Agent Based Diagnostic System for the Defect Analysis during Chemical Mechanical Polishing (CMP)

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Geleitwort der Herausgeber

Über den Erfolg und das Bestehen von Unternehmen in einer marktwirtschaftlichen Ordnung entscheidet letztendlich der Absatzmarkt. Das bedeutet, möglichst frühzeitig absatzmarktorientierte Anforderungen sowie deren Veränderungen zu erkennen und darauf zu reagieren.

Neue Technologien und Werkstoffe ermöglichen neue Produkte und eröffnen neue Märkte. Die neuen Produktions- und Informationstechnologien verwandeln signifikant und nachhaltig unsere industrielle Arbeitswelt. Politische und gesellschaftliche Veränderungen signalisieren und begleiten dabei einen Wertewandel, der auch in unseren Industriebetrieben deutlichen Niederschlag findet.

Die Aufgaben des Produktionsmanagements sind vielfältiger und anspruchsvoller geworden. Die Integration des europäischen Marktes, die Globalisierung vieler Industrien, die zunehmende Innovationsgeschwindigkeit, die Entwicklung zur Freizeitgesellschaft und die übergreifenden ökologischen und sozialen Probleme, zu deren Lösung die Wirtschaft ihren Beitrag leisten muss, erfordern von den Führungskräften erweiterte Perspektiven und Antworten, die über den Fokus traditionellen Produktionsmanagements deutlich hinausgehen.

Neue Formen der Arbeitsorganisation im indirekten und direkten Bereich sind heute schon feste Bestandteile innovativer Unternehmen. Die Entkopplung der Arbeitszeit von der Betriebszeit, integrierte Planungsansätze sowie der Aufbau dezentraler Strukturen sind nur einige der Konzepte, welche die aktuellen Entwicklungsrichtungen kennzeichnen. Erfreulich ist der Trend, immer mehr den Menschen in den Mittelpunkt der Arbeitsgestaltung zu stellen - die traditionell eher technokratisch akzentuierten Ansätze weichen einer stärkeren Human- und Organisationsorientierung. Qualifizierungsprogramme, Training und andere Formen der Mitarbeiterentwicklung gewinnen als Differenzierungsmerkmal und als Zukunftsinvestition in *Human Resources* an strategischer Bedeutung.

Von wissenschaftlicher Seite muss dieses Bemühen durch die Entwicklung von Methoden und Vorgehensweisen zur systematischen Analyse und Verbesserung des Systems Produktionsbetrieb einschließlich der erforderlichen Dienstleistungsfunktionen unterstützt werden. Die Ingenieure sind hier gefordert, in enger Zusammenarbeit mit anderen Disziplinen, z. B. der Informatik, der Wirtschaftswissenschaften und der Arbeitswissenschaft, Lösungen zu erarbeiten, die den veränderten Randbedingungen Rechnung tragen.

Die von den Herausgebern langjährig geleiteten Institute, das

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arbeiten in grundlegender und angewandter Forschung intensiv an den oben aufgezeigten Entwicklungen mit. Die Ausstattung der Labors und die Qualifikation der Mitarbeiter haben bereits in der Vergangenheit zu Forschungsergebnissen geführt, die für die Praxis von großem Wert waren. Zur Umsetzung gewonnener Erkenntnisse wird die Schriftenreihe „IPA-IAO - Forschung und Praxis“ herausgegeben. Der vorliegende Band setzt diese Reihe fort. Eine Übersicht über bisher erschienene Titel wird am Schluss dieses Buches gegeben.

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Stuttgart, Juni 2005 Akhauri Prakash Kumar

Contents

0 Acronyms and Variables

General

ANSI		American National Standards Institute
ASIC		Application Specific Integrated Circuit
BPSG		Boron-Phosphorous-Silicate Glass
CORBA		Common Object Request Broker Architecture
CMP		Chemical Mechanical Polishing
CVD		Chemical Vapor Deposition
DCOM		Distributed Component Object Model
DE		Defect Evaluation
DIN		Deutsches Institut für Normung
DRAM		Dynamic Random Access Memory
E	[N/m^2]	Young's Modulus
E-2, E-3		Roll-off at the wafer edge in directions 2, 3
E-4, E-5		Roll-off at the wafer edge in directions 4 and 5
FDC		Fault Detection and Classification
FPD	[µm]	Focal Plane Deviation
FQA	[µm^2]	Flatness Quality Area
G	[N/m^2]	Shear Modulus
GBIR	[µm]	Global Back surface Ideal Range
GEM		Generic Equipment Model
GFLD	[µm]	Global Front surface Least squares Deviation
GFLR	[µm]	Global Front surface Least squares Range
IC		Integrated Circuit
IEP		Isoelectric Point
JNI		Java^{TM} Native Interface
LLS		Localized Light Scattering
LPD		Light Point Defect
LT2-4	[µm]	Linear Taper in directions 2-4
LT3-5	[µm]	Linear Taper in directions 3-5
MPU		Microprocessor Unit
MTTR		Mean Time to Repair
MVA		Multivariate Statistical Analysis
NLT 2-4	[µm]	Non Linear Taper in directions 2-4
NLT 3-5	[µm]	Non Linear Taper in directions 3-5
OEE		Overall Equipment Effectiveness
PDL		Parameter Definition Language
pH		the negative base 10 logarithm of the hydrogen ion concentration $pH = -\log_{10} a_{H+}$
PLC		Programmable Logic Control

POU		Point of Use
RMI		Java™ Remote Method Invocation
r, θ, z		Polar coordinate system
SBID	[µm]	Site Back surface Ideal Deviation
SBIR	[µm]	Site Back surface Ideal Range
SECS		Semiconductor Equipment Communication Standard
SEM		Scanning Electron Microscope
SEMI		Semiconductor Equipment and Materials Institute
SFLD	[µm]	Site Front surface Least squares Deviation
SFLR	[µm]	Site Front surface Least squares Range
SFPD	[µm]	Site Focal Plane Deviation
SFQD	[µm]	Site Front surface Least squares Site Deviation
SOG		Spin on Glass
SPC		Statistical Process Control
SRAM		Static Random Access Memory
STIR	[µm]	Site Total Indicator Reading
TCP / IP		Transmission Control Protocol / Internet Protocol
TIR	[µm]	Total Indicator Reading
TTV	[µm]	Total Thickness Variation
WSDL		Web Service Description Language
x, y, z		Cartesian coordinate system
XML		Extensible Markup Language
Chapter 2		
A_k		parameter drift constant k^{th} process run
b_k		offset drift constant for k^{th} process run
e_k		noise factor for k^{th} process run
k		k^{th} process run number
PR_k		k^{th} process run
RbR		Run by Run process control
r_k		k^{th} process recipe
$\boldsymbol{S}^{-1}$		inverse of the sample covariance matrix (n x n) for the n machine variables
T^2		Hotelling's T^2 control chart
$\boldsymbol{x}_i$		(1xn) row vector of tool-state variables
$\bar{\mathbf{x}}$		(1xn) row vector of means for the tool-state variables
y_k		actual value of the recipe for k^{th} process run
Chapter 3		
a	[µm]	distances from the upper help planes to the front wafer surface
A	[µm^2]	contact area between the polishing pad and the wafer

a_c	[μm^2]	contact area
A_c	[μm^2]	total contact area
A_p	[μm^2]	total pad contact area
A_s	[μm^2]	total surface area
b	[μm]	distances from the lower help planes to the back surface of wafer
β	[μm]	radius of pad asperity
c		particle fill factor at the surface
c_l	[N]	contact load
C_L	[N]	total contact load
d	[μm]	diameter of the abrasive particle
d_1, d_2	[μm]	distances from upper and lower curvatures of wafer from the help planes
d_{max}	[μm]	maximum wafer thickness
d_{min}	[μm]	minimum wafer thickness
d_{zi}	[μm]	central thickness of Site$_i$
δ	[μm]	indentation/penetration depth of the abrasive particle
δ_{th}	[μm]	layer thickness
E'	[N/m^2]	effective Young’s Modulus of pad surface
η	[$N.s / m^2$]	fluid viscosity
F	[N]	applied mechanical force
FPD_{fi}	[μm]	Focal Plane Deviation on the edge of the reference position
FPD_{bi}	[μm]	Focal Plane Deviation away from the center of Site$_i$
FPD_{zi}	[μm]	Focal Plane Deviation in the center of Site$_i$
$FPD_{max\ i}$	[μm]	maximum Focal Plane Deviation in Site$_i$
$FPD_{min\ i}$	[μm]	minimum Focal Plane Deviation in Site$_i$
γ	[N/m^2]	shear strain
ΔH	[μm]	height of the surface
h	[μm]	film thickness between wafer and pad surface
κ	[kg/m^3]	asperity density
K_p		Preston's coefficient
L	[μm]	substrate length
λ	[kg/m^3]	fluid density
NF		Norm Factor
ν		Poisson's ratio
ω	[radians/min]	angular velocity of polishing plate with pad
ω_2	[radians/min]	angular velocity of the wafer on the carrier plate
ω_s	[radians/min]	relative angular velocity radians per minute
P	[N/m^2]	applied pressure
φ	[°]	angle

Φ_β		normal distribution of pad asperity's radius β
Φ_z		normal distribution of pad asperity's height z
q	[N]	applied force
r	[mm]	radius
r, r_1	[mm]	radii
r_b ,r_{fi}	[mm]	radial distances from the center of the wafer where the measured points lie
r_c	[µm]	contact radius
r_p	[µm]	abrasive particle radius
ρ	[mm]	distance of any point on the circle from the pole of the circle (polar coordinates)
ρ_0	[mm]	distance between the pole and the centre of the circle (polar coordinates)
Δs	[µm]	distance
SF		Scaling Factor
$SFLD_i$	[µm]	SFLD value in Site_i
Δt	[s]	time elapsed
τ	[N/m^2]	shear stress
thk_{fi}	[µm]	measured thickness at the position "i" on the wafer surface
thk_{center}	[µm]	thickness of the wafer at its center
θ	[°]	angle
U	[m/s]	fluid velocity
v	[m/s]	relative velocity between polishing pad and a point on the wafer
v_s	[m/s]	relative velocity between any wafer position and the polishing pad for $\omega = \omega_2$
$v_e(r)$	[m/s]	radial relative velocity at distance r
$w(r)$	[µm]	pad deformation
x		variable
$\|x\|$	[µm]	maximum positive deviation from the reference plane
$\|y\|$	[µm]	maximum negative deviation from the reference plane
z	[µm]	pad asperity height

Chapter 5

$\boldsymbol{B}$		parameter behavior vector
$\boldsymbol{BP}$		behavioral pattern characteristics vector
C_a		threshold conditional probability
$C_l(\boldsymbol{BP})$		conditional error probability
$\boldsymbol{D}$		defect class vector space

$D_1, \ldots, Dd$		defect class vectors
$\boldsymbol{E}$		expected characteristics vector
e^*		optimal error probability
$e_1, \ldots, e_n$		unit vectors
$\boldsymbol{I}$		information characteristics vector
$I_1(t), \ldots, I_n(t)$		linearly independent vectors in vector space $\boldsymbol{I}$
$\boldsymbol{M}$		CMP machine parameter vector
$m_i(t)$		linearly independent vectors $\boldsymbol{M}(t)$
ω_0, ω_l		defect classes for Bayes theorem
Ω_A		set of all classified defect class regions with known behavioral pattern characteristics
Ω_R		set of all unknown defect class regions with unknown behavioral pattern characteristics
Ω_0		defect class region containing set of all unclassified defect classes
Ω_m		defect class region containing set of all unknown behavioral pattern characteristics
$p(\omega_l)$		a priori probability
$f(\boldsymbol{BP}\|\omega_j)$		conditional probabilities of Behavior Pattern characteristics
$\boldsymbol{PT}$		CMP process parameter vector
$pt_i(t)$		linearly independent vectors $\boldsymbol{PT}(t)$
$\boldsymbol{P}(S_{ps})$		CMP process vector
$\boldsymbol{P}^n$		CMP process space
Φ		empty set
$\boldsymbol{R}^d$		d-dimensional defect class Space
S_{ps}		processing State
S_{pt}		processing State transition
$\boldsymbol{T}$		transformation vector
t_0	[s]	start time
t_n	[s]	end time
Δt	[s]	duration
$\boldsymbol{T_P}$		CMP process transformation vector
$t_{process\ state\ start}$	[s]	process state start time
$t_{process\ state\ end}$	[s]	process state end time
$t_{state\ transition\ start}$	[s]	process state transition start time
$t_{state\ transition\ end}$	[s]	process state transition end time

1 Introduction

1.1 Problem definition

The manufacturing facilities in semiconductor industries are getting very complex in their construction and functionalities because of the rapidly changing trends towards small, dense and compact structures of logic products such as Microprocessor Units (MPUs) and Application Specific Integrated Circuits (ASICs) [ITRS 2002]. Figure 1.1 shows the future trends [ITRS 2002] of these products. The IC manufacturers are demanding very high surface planarity and uniform surface topography of the starting substrate material (wafer [SEMI M1 2002]). The Site flatness [DIN 50441/4 1991] control for these devices requires the measuring of topographical deviations and the allowed defect size on the wafer backside in nanometers. However, the redetection size of these defects should not exceed approximately 40% of the size of the Site flatness. The wafer manufacturers have therefore, very short delivery times to provide wafers with continuously decreasing defect densities and very tight tolerances to the IC manufacturers after the final planarization step, which is Chemical Mechanical Polishing (CMP) [Steigerwald 1997, WSAG 1997-2003, ITRS 2002, TIN 2003]. To accomplish the specified wafer geometry with very tight tolerances and constantly changing wafer specifications, a very high degree of automation grade and flexibility of the CMP process machine is required [WSAG 1997-2003].

Characteristics	**2003**	**2005**	**2007**	**2010**	**2013**	**2016**
Transistor density SRAM products (transistors/cm^2)	305M	504 M	827 M	1718 M	3532 M	7208 M
Transistor density for logic products (transistors/cm^2)	61.2 M	97.2 M	154.3 M	309 M	617 M	1235 M
DRAM ½ Pitch (nm)	100	80	65	45	32	22
MPU/ASIC ½ Pitch (nm)	107	80	65	45	32	22
Site flatness (nm)	≤ 100	≤ 80	≤ 65	≤ 45	≤ 32	≤ 22
Wafer backside 200mm (defect size nm)	200	100	100	100	60	50
Redetection: minimum defect size (nm)	44	30	26	18	13	9
DRAM (defects/m^2) for Generic Tool Type scaled to 75nm critical defect size or greater						
CMP Clean	610	318	171	78	30	14
CMP Insulator	472	246	132	60	23	11
CMP Metal	723	378	203	92	36	17
MPU (defects/m^2) for Generic Tool Type scaled to 75nm critical defect size or greater						
CMP Clean	228	127	78	37	18	8
CMP Insulator	552	308	189	90	43	20
CMP Metal	623	348	213	102	48	23

Figure 1.1: IC manufacturing characteristics and future trends [ITRS 2002]

For product quality, yield and throughput improvement, the in-situ defect detection, the real-time analysis of non-visual defects, the simultaneous differentiation of multiple defect types and the high capture rates of the detected defects [Shaw 1993, Chillarege 1997, Devriendt 2000] are turning out to be the major challenges for wafer suppliers [WSAG 1997-2003]. The CMP process depends upon many parameters that influence the process independently or in conjunction with each other or in different constellations [Steigerwald 1997, Boning 1999, WSAG 1997-2003, TIN 2003]. During CMP process the wafer is pressed faced down on a polishing pad, therefore it is extremely difficult to access the information about chemical and mechanical mechanisms taking place during processing. The time dependency [Gamper 1996] of the properties of these parameters during CMP process and the non-trivial causal [Jordan 1991] coherence among the different CMP process steps and the related parameters further complicates the understanding of the CMP process [Steigerwald 1997]. The drift or shift of these parameters leads to the origination of defects i.e. undesired topographical irregularities on wafer surface [WSAG 1997-2003]. On the other hand, the high complexity of the CMP process [TIN 2003, WSAG 1997-2003] makes the localization (i.e. to find out the defected area, the type and the cause) and control of the process and machine parameters responsible for defect origination during a process run very difficult. This leads to intolerable machine downtimes caused by the time-consuming defect localization procedures [KLA-Tencor 1999]. The cause detection and localization of the detected defects is mostly done by the CMP process expertise offline [Devriendt 2000, Luo 2003]. The deductions of corrective actions and the establishment of correlations between the detected defects and the process parameters is mostly based on the long year CMP process experience of the process engineers [WSAG 1997-2003].

The currently deployed process control approaches for CMP process machines are Statistical Process Control (SPC) and Run-to-Run process control [Leang 1991, Boning 1996, Castillo 1998, Musacchio 1999, Smith 1999A]. These approaches have a drawback, as they are unable to provide mechanisms to detect defects during their origination [Straatum 2000]. In addition to this, these approaches do not support the time dependent changes of the properties [Gamper 1996] of CMP process and machine parameters and their causal coherence to the different CMP process steps during the CMP process run.

To comply with the continuously changing demands of the IC manufacturers, the wafer manufacturers require a system, which integrates the expert knowledge of the CMP process expertise directly to enhance the functionalities of CMP process controller [TIN 2003]. The system should provide in-situ diagnosis (recognition, localization, representation and required corrective actions) [Puppe 1996, Puppe 1997] of the defects at a very early stage to improve the CMP process capability during the CMP process run [KLA-Tencor 1999, Wang 2001, TIN 2003]. This system should work autonomously without intervening in the activities of the existing CMP process controller [WSAG 1997-2003].

An agent [Wooldridge 1995, Wagner 1996, Schroeder 1998], which works autonomously and collects continuously the CMP process runtime information without intervening the regular CMP process activities provides this information to the diagnostic system [Puppe 1996, Puppe 1997]. The diagnostic system encompasses of knowledge base [Oberholthaus 1995, Puppe 1998, Schmitte 1999] and an inference engine [Schroeder 1998, Schilstra 2001] components.

1.2 Objectives and approach

The objective of this work is to develop and implement an in-situ agent based diagnostic system for defect analysis during CMP process. This system examines, evaluates, analyzes and predicts the origination of defects at a very early stage during CMP process in the production environment. This system, thus, provides the prerequisites for the wafer manufacturers to supply the products with demanded precision and short delivery time to the IC manufacturers.

The approach for the development of the in-situ agent based diagnostic system is to investigate at first the state of the art describing the analysis of currently deployed approaches to control this process. In the next step, the theoretical analysis of the CMP process and the CMP process machine is carried out by investigating the individual CMP process steps and the influencing process and machine parameters during these steps.

The theoretical analysis is used as basis to develop the design of agent based diagnostic system for defect analysis, which includes the development of the problem domain model of the CMP process machine. The design of defect evaluation system consists of development of a model to evaluate defect classes and the responsible process and machine parameters using stochastic methods. The design of diagnostic system comprises of the knowledge base design and inference engine design, based on the problem domain model and the defect evaluation system. The agent designed finally is to control and coordinate the defect evaluation system and the diagnostic system.

The implementation of the agent based diagnostic system is done based on its design. The implemented system during run time, thus, takes into account all the process steps and the related process and machine parameters, along with the time dependencies of their properties to recognize and establish the non-trivial coherence among them. It diagnoses the exact contributor responsible for the origination of a defect using the knowledge base.

The agent based diagnostic system for defect analysis is then tested in-situ in the production environment and the results are evaluated regarding its applicability and practicability in the production environment.

2 State of the art

2.1 Chemical Mechanical Polishing terms and definitions

2.1.1 Integrated Circuit manufacturing

In the *Integrated Circuit* (IC) manufacturing [ITRS 2002, Luo 2003], depending upon the *wiring levels* (the interconnect levels in an IC) required, the *surface planarization* (flatness [DIN 50441/4 1991]) is a necessary process step per level [TIN 2003]. The methods used traditionally for planarization were for example high temperature annealing (Boron-Phosphorous-Silicate Glass BPSG) and *Spin on Glass* (SOG) [Ouma 1998B]. The main problem with even the best techniques was that they achieved local planarization only. *Chemical Mechanical Polishing* (CMP) is the only technique that performs a global planarization of the wafers. The basic process is to deposit the silicon oxide thicker than the final thickness required and polish the material back until the step heights are removed [Steigerwald 1997]. This provides a good flat surface for the next level. In addition, the process can be repeated for every wiring level that is added [TIN 2003].

2.1.2 Wafer manufacturing

In the *wafer* [SEMI M1 2002] manufacturing process, after creation of *polycrystalline silicon* (substrate material), the *silicon crystal ingot* is pulled, which can have 150 mm, 200 mm and 300 mm as diameters. This silicon ingot characterized by the orientation of its silicon crystals and sliced into individual wafers with a precision saw [WSAG 1997-2003, TIN 2003]. The sliced wafers are lapped mechanically. The sliced wafers are etched in a solution of nitric/acetic acid or sodium hydroxide to remove microscopic cracks or surface damages created by the lapping process. Finally, the CMP process [WSAG 1997-2003] then polishes the etched wafers. These wafers are cleaned, packed and then shipped for the IC manufacturing.

2.1.3 CMP process

This section gives an overview of the CMP process and the CMP *process machine* (figure 2.1) [WSAG 1997-2003] studied in the industrial context for this work. The lapped and etched wafers are mounted on the *carrier plates* (ceramic plates), using wax as adhesive to fix them firmly before the CMP process. These carrier plates are at first cleaned thoroughly and then a thin film of wax is *spin coated* (SOG method [Ouma 1998B]) to obtain a homogeneous wax layer on the carrier plates. The carrier plate is heated in the *heating stations* after homogeneous temperature is reached throughout the plate; six 200 mm wafers are then automatically mounted on the carrier plate by pressing the wafers on the plate and cooling the carrier plate along with the wafers. The wafers are mounted under clean room conditions [Schließer 1999] to avoid any particle contamination [Philipossian 2001] between the wafers and the carrier plates and on the surfaces of wafers and the carrier plate. These carrier plates are mounted on the *rotating cylinder head* in the CMP process machine. Figure 2.1 shows the general set-up of studied CMP process machine.

In a typical CMP process, a rotating cylinder head holds a carrier plate with wafers having the active wafer surface facing the rotating *polishing plate* (platen) [Steigerwald 1997, TIN

2003]. On top of the polishing plate is porous polyurethane *polishing pad* on which *slurry* with *abrasive* material of colloid dispersed silica (silica particles of size 50-100 nm) suspended in aqueous solution is poured. The *pH* value of slurry and the *temperature* of the polishing plate influence the optimization of the *chemical removal rate*, which is the loosening of material from the wafer surface due to *chemical reactions*. The control of accurate pH value of the slurry is very important during the polishing process as higher alkali value results in a steep decline of *removal rates* (rate at which the material is removed from the wafer surface), caused by chemical oxide formed at the wafer surface. The concentration of ions regulated by pH value of the slurry is actually responsible for microscopic ("atom for atom“) removal.

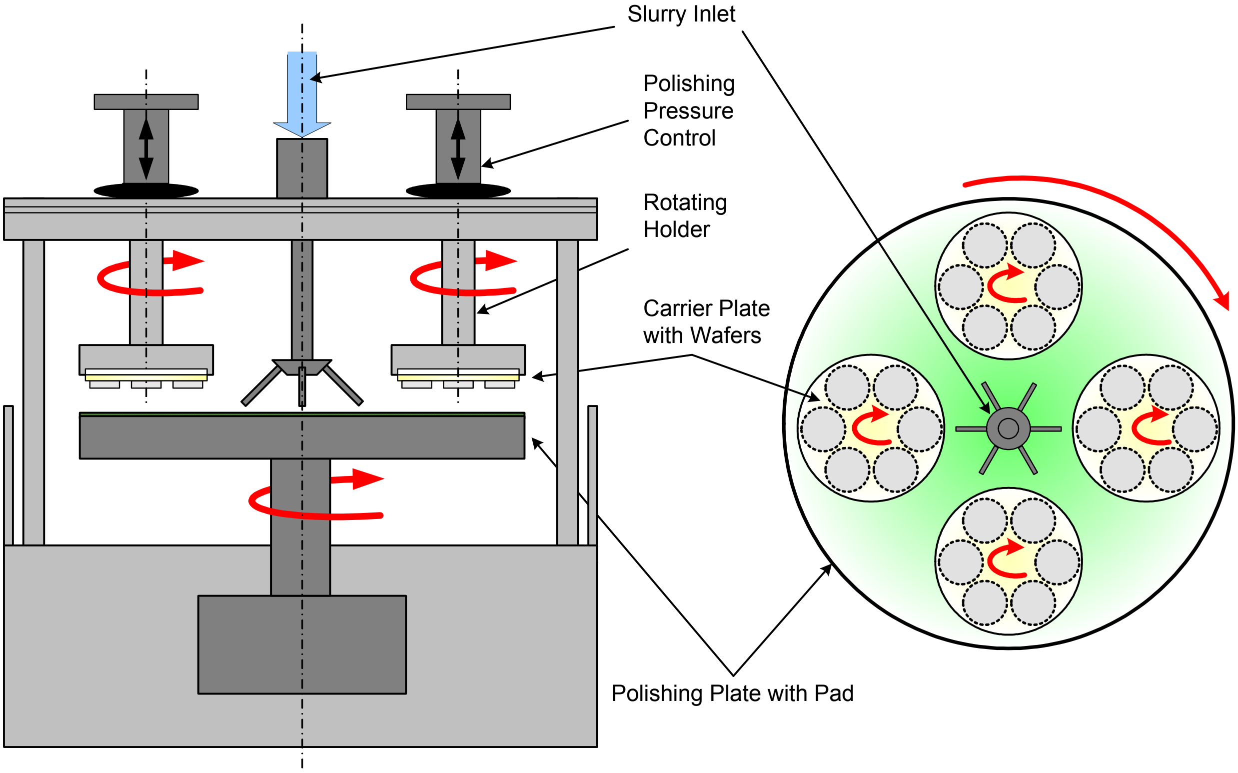


Figure 2.1: CMP process machine for wafer polishing [WSAG 1997-2003]

Slurries with different chemical compositions are used to polish metal and other films. The polishing plate temperature also influences the removal rate as increasing the temperature increases the chemical reaction rate. The carrier plates and the polishing plate rotate in the same direction on their own *rotating axes*. The rotating axes of rotating cylinders holding carrier plates are not concentric and possess a certain offset to the rotating axis of the polishing plate. The carrier plates therefore exhibit an orbital motion. Thus, this arrangement results in a relative linear motion between any position on the wafers on four carriers and the polishing pad at any time during polishing. The slurry reacts with the wafer surface chemically and together with the *polishing pressure* exerted by the rotating cylinders holding carrier plate, the pad and the colloidal silica particles, the surface of all the wafers is abraded [Ouma 1998B]. The *material removal* not only depends on the *relative motion* between the wafer and pad surface but also on the *chemical reaction*. The polishing pad surface becomes glazed after number of process runs, resulting in a lower removal rate. Therefore, for maintaining the *polishing integrity* [Steigerwald 1997] of the pad after certain process runs the *pad conditioning* is done with a diamond tipped conditioner to minimize the glazing effect by scratching the surface of the pad.

Every wafer thus produced undergoes a quality control where the *geometrical* parameters (wafer thickness, wafer flatness and wafer surface topography) and *electrical* parameters (resistivity) are tested against the wafer specification. The wafers having *geometrical defects* (scratches, edge) are then sorted out [WSAG 1997-2003].

In the wafer manufacturing process the *oxide CMP* [Philipossian 2001], as described above is the final step to achieve global planarization. On the other hand, during the IC manufacturing process *metal CMP* [Steigerwald 1997] is often used. The blanket metal film is deposited thick enough to fill interconnects and then the metal is removed by CMP process. The metals, which are deposited, are tungsten, copper and aluminium. The CMP process to remove these metals is therefore called *tungsten CMP* [Philipossian 2001], *copper CMP* [Steckenrider 2001] and *aluminium CMP* [Steigerwald 1997].

The study showed that the CMP process depends upon many process parameters such as slurry composition, slurry pH value, chemical reaction, abrasive size, abrasive properties, cylinder head rotation speed, polishing plate rotation speed, polishing pressure and polishing plate temperature. All these parameters together can cause process shifts individually or in combinations, resulting in undesired wafer surface topographies i.e. deviation of geometrical parameters. The in-situ analysis and correlations of these parameters during CMP process run is currently missing.

2.2 Typical defects generated during CMP processing

The quality of CMP process [KLA-Tencor 1999, Devriendt 2000] depends upon the process parameters as discussed above. The removal rate control by influencing these parameters, at any time actually is the greatest challenge in the CMP process [TIN 2003]. Although this process has matured now, still research work [Runnels 1994, Vasilopoulos 2000A, Lee 2000] is being done to gain more information about the chemistry of the process and the mechanical and material properties of the CMP process machine.

The reason is still to:

1. Achieve very good product quality [TIN 2003]
2. Achieve a very high automation grade [ITRS 2002]
3. Produce multiple products on the same machine (high flexibility) [WSAG 1997-2003]
4. Have a continuous production [TIN 2003]
5. Reduce Mean Time to Repair (MTTR) [ITRS 2002]
6. Improve the Over all Equipment Effectiveness (OEE) [WSAG 1997-2003]

During continuous processing due to wear, tear and mechanical fatigue certain process parameters start drifting, which when not immediately corrected can lead to some *typical defects* (topological irregularities) as described here.

2.2.1 Defects in oxide CMP

During the wafer production process, depending upon the pressure and relative rotational speed between the carrier and polishing plate these defects can be originated. Figure 2.2 shows a typical *edge defect* (a, b), a *pit* (c) (depression of wafer surface with steeper slopes) [SEMATECH 1995, SEMI M52 2002] caused by the water drop in the wax, a *dimple* (d) (shallow depression on wafer surface) [SEMATECH 1995, SEMI M1 2000] and a *Roll Off* (e).

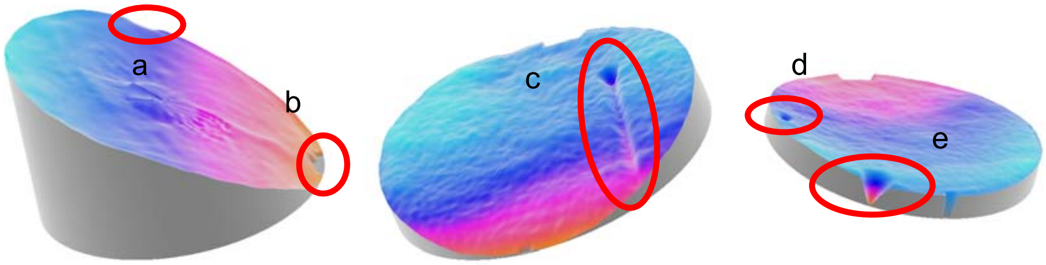


Figure 2.2: Oxide CMP defects: edge defect (a, b), pit (c), dimple (d) and Roll Off (e) Defects in oxide CMP [WSAG 1997-2003]

The microscopic planarization requires a very precise removal process. The influence of mechanical and chemical parameters on each other during this process is so sensitive that minute parameter value shift leads to nanoscopic defects. Figure 2.3 shows further the oxide CMP defects: *rip out* of CMP oxide (a), *large particle* (b), *micro scratch* (c), and residual slurry (d).

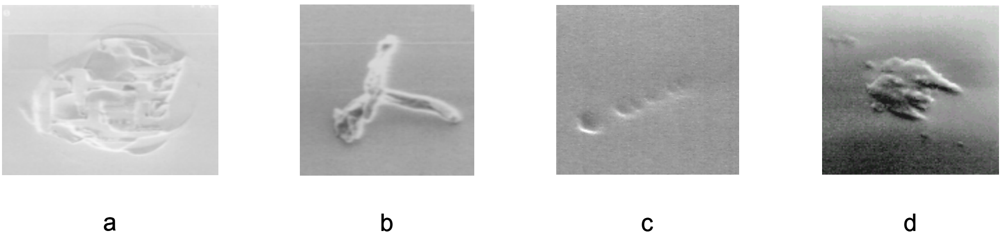


Figure 2.3: Oxide CMP defects: rip out (a), large particle (b), micro scratch (c) and residual slurry (d) [Philipossian 2001]

2.2.2 Defects in tungsten CMP

No matter whether it is oxide CMP or tungsten CMP, both these processes are very sensitive. Minute environmental changes lead to origination of nanoscopic defects. It can be due to the tungsten puddle or due to slurry residue remains on the surface observed only under Scanning Electron Microscope (SEM). Figure 2.4 shows the tungsten CMP defects: *residual slurry* (a), *recessed tungsten* (b), empty *micro scratch* (c), and *tungsten puddle* (d).

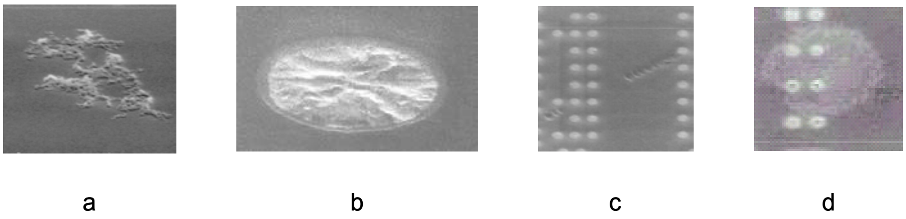
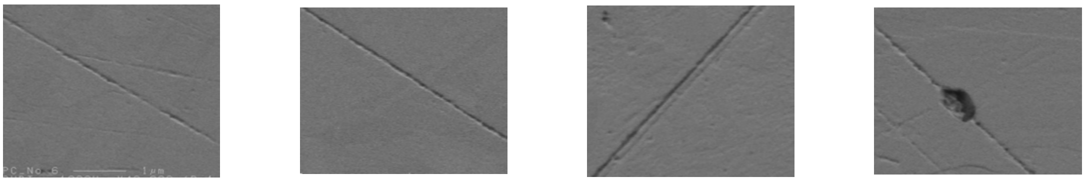


Figure 2.4: Critical tungsten CMP defects: residual slurry (a), recessed tungsten (b), empty micro scratch (c) and tungsten puddle (d) [Philipossian 2001]

2.2.3 Defects in copper CMP

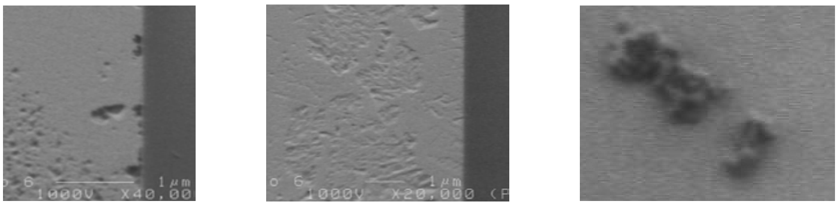
Typical copper defects [Vasilopoulos 2000B, Steckenrider 2001] originated due to particles in the slurry. Figure 2.5 (a, b and c) shows *scratches*: *shallow, middle* and *deep* caused by the particles in the slurry depending upon the sizes. Figure 2.5 (d) shows a *blister* with a middle scratch. The cause of the scratches is usually a residual slurry particle or the abraded particle, which could not be transported by the slurry during polishing process.



a b c d

Figure 2.5: Copper defects: Scratches (a, b and c) and a scratch with blister (d) [Vasilopoulos 2000B]

Figure 2.6 (a, b) shows typical examples of *surface pitting* and figure 2.6 (c) shows a large particle on the surface. All these defects can be reduced by using Point of Use (POU) filtration of the slurry. The defects observed during aluminium CMP are mostly scratches due to its high malleability and softness [Steigerwald 1997].



a b c

Figure 2.6: Copper defects: Surface pitting (a, b), large particle (c) [Vasilopoulos 2000B]

All CMP processes, whether it is oxide CMP, tungsten CMP, copper CMP or aluminium CMP, require slurries with different chemical compositions. The slurry thus selected should have following properties:

- It should transport the abrasives
- It should not build conglomerates
- It should be free from big particles
- It should be able to transmit mechanical forces between the wafer and the pad

These properties should be analyzed and controlled in-situ during a particular process run to achieve the product quality (defects reduction) as demanded by the IC manufacturers.

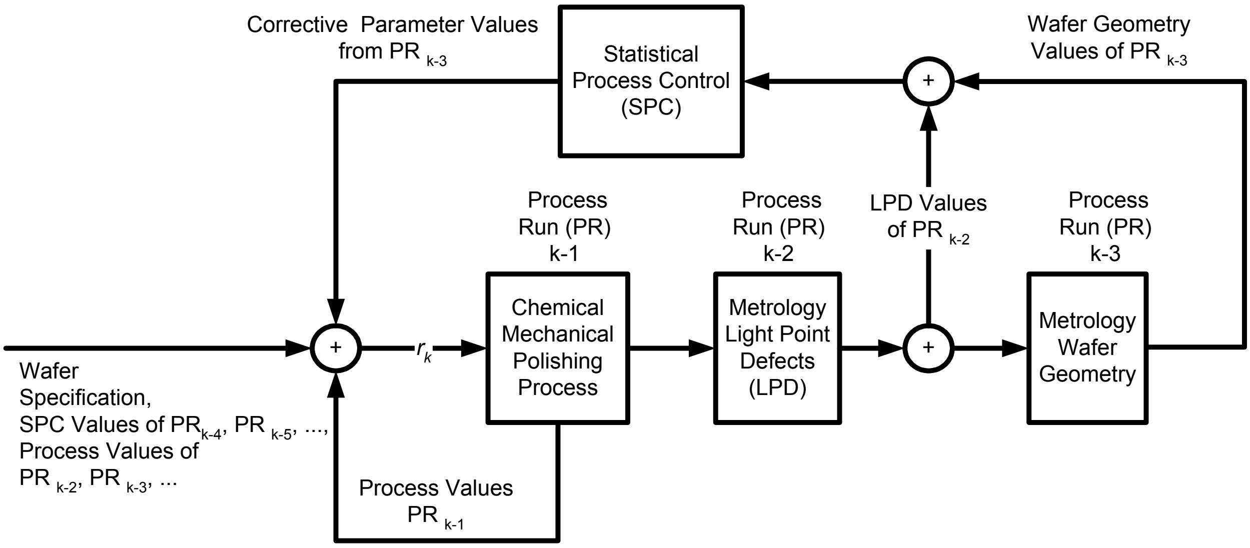
The defect analysis at present is the correlation of geometrical irregularities to the drifts and shifts of process parameters and machine parameters. This correlation is done offline after the geometrical measurement of wafer is made and when the irregularities are observed. The defect analysis is done after the defects are there. For the avoidance of above defects many process control methods are deployed, the state of the art of the process control methods is discussed in the next paragraphs.

2.3 Process control during CMP process

In the manufacturing process of wafers or integrated circuits, a very high availability and high quality of this process is required. Therefore, it is becoming very important to observe and control the process, to avoid the defect originations and unscheduled shutdown of the CMP process machine. To avoid the process parameter drifts, shifts and inconsistent CMP process machine operation resulting in the above-discussed defects, CMP process control is gaining industrial recognition. The advanced process models represent the real world behavior of the CMP process, therefore the CMP processing quality improves, as many multi-step process optimizations and control mechanisms are possible. The most important process control approaches are discussed here.

2.3.1 Statistical Process Control

In the CMP process, as the wafer is pressed faced down on a polishing pad, it is extremely difficult to access the information about chemical and physical mechanisms taking place during processing. The ex-situ geometry measurements provide exact information about the process. The geometrical measurement data is fed into a Statistical Process Control (SPC) system [Leang 1991, Smith 1999A], where the deviations between process outputs and process target is evaluated and the feedback is used to compensate the process parameters to control the CMP process and thus, to avoid further defects. Figure 2.7 shows the SPC feedback control loop for CMP process. The calculation of the current recipe r_k depends upon the wafer specification, SPC values tuple not before k-3rd process run (PR) and the process values tuple of previous process runs for the CMP process machine under investigation. The SPC is done for wafer geometry values of k-3rd process run, Light Point Defect (LPD i.e. increased light scattering intensity on the wafer surface due to a particle or a pit on the wafer surface) [SEMI M1 2002] values of k-2nd process run and the previous trend charts.



$r_k = f(\text{Prod Spec, SPC values of } (PR_{k-3}, PR_{k-4}, \ldots), \text{Process values of } (PR_{k-1}, PR_{k-2}, PR_{k-3}, \ldots))$

Figure 2.7: Statistical Process Control feedback control loop for CMP process

The SPC feedback control loop is an established system as long as the CMP process machine is producing products. The ex-situ measurements are only possible if the wafer is available and therefore the defects can be avoided only for the next wafer fabrication cycle. The CMP process machine with time experiences regular shifting in its output although SPC catches these errors, but the random drifting, to and from the target output of the processes requires significant engineering effort.

2.3.2 Multivariate Statistical Analysis process control

Multivariate Statistical Analysis (MVA) includes reduction of SPC charts and inclusion of covariance measurements as compared to variance measurements used by SPC [White 2001, Goodlin 2002]. These techniques are also used for fault classifications of the process and the process machine. The statistical methods are used to create a model, which is then used to identify probable fault contributors to a particular fault classification by repeating process runs. This method combines all tool-state variables together when possible into one multivariate control chart. The most popular way to do this is with a multivariate Hotelling's T^2 control chart. The calculation of single sample T^2 statistic [White 2001, Goodlin 2002] is described by the equation 2.1:

$$T_i^2 = \left(\boldsymbol{x}_i - \overline{\boldsymbol{x}}\right)\boldsymbol{S}^{-1}\left(\boldsymbol{x}_i - \overline{\boldsymbol{x}}\right)^T \tag{2.1}$$

Where "i" is the wafer number, $\boldsymbol{x}_i$ is the (1xn) row vector of tool-state variables, $\overline{\boldsymbol{x}}$ is the (1xn) row vector of means for the tool-state variables and $\boldsymbol{S}^{-1}$ is the inverse of the sample covariance matrix (n x n) for the n machine variables. The means and covariance are calculated on the normal process wafers only. The typical process excursions are flagged out immediately as multivariate Hotelling's T^2 control chart and have the highest sensitivity to identify faults that occur as a mean shift from the normal data population [White 2001, Goodlin 2002]. MVA process control indicates the fault classification and the fault contributors. It means that the wafer being processed currently has a defect. It provides the fault contributors for correction of the next process run.

2.3.3 Run by Run process control

Run by Run (RbR) control [Smith 1999A, Smith 1999C] is often referred also as run-to-run control or model-based control [Musacchio 1999]. It monitors process parameters similar to SPC; however, unlike SPC and MVA techniques, RbR makes continuous changes to the process in order to compensate drifts and shifts in the process outputs after every run based upon some objective functions such as distance from target. Adjusting the process machine setting controls the process outputs, as the weighted average of the process offset is used to update the dynamic model of the process. In order to control the process adequately, it is necessary to obtain the critical parameters. To achieve this, large amount of metrology and in-situ sensor development is necessary [Smith 1999A, Smith 1999C].

RbR very often uses models to describe key relationships in a process; these models are developed through process characterization and are often a mixture of first principles [Musacchio 1999] and experimental results. Models are used to describe the relationship between measurement and process variables, and can be used to facilitate control strategies. Advanced RbR control strategies [Smith 1999C] extend the use of models to include upstream tool information and incoming product variation in determining control adaptation as shown in the figure 2.8. The recipe parameters r_{k+1} are generated after evaluating the current process and machine parameter drifts, current offset drifts and the measurement noise based upon the control strategies as developed in the model. The earlier process and machine parameters trends are also taken into consideration by the model to evaluate the new process recipe parameters.

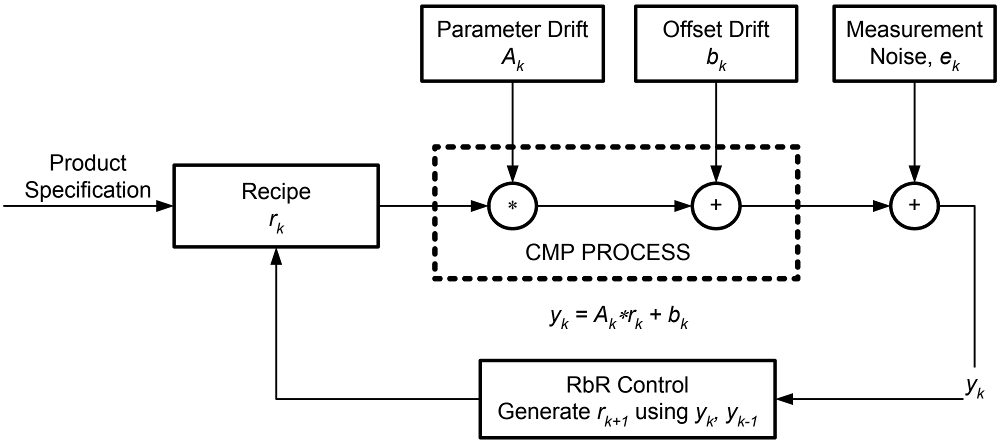


Figure 2.8: RbR Process Control for CMP process [Musacchio 1999]

Figure 2.9 shows the advanced RbR process control with in-situ metrology, feed forward and feed backward control strategies [Straatum 2002].If the process or machine parameter drift is detected, the fault detection algorithm evaluates this drift and classifies it accordingly to the corresponding faults in the model. The fault contributors are then evaluated and new process parameters values are provided for the feedback as well as for the feed forward process control.

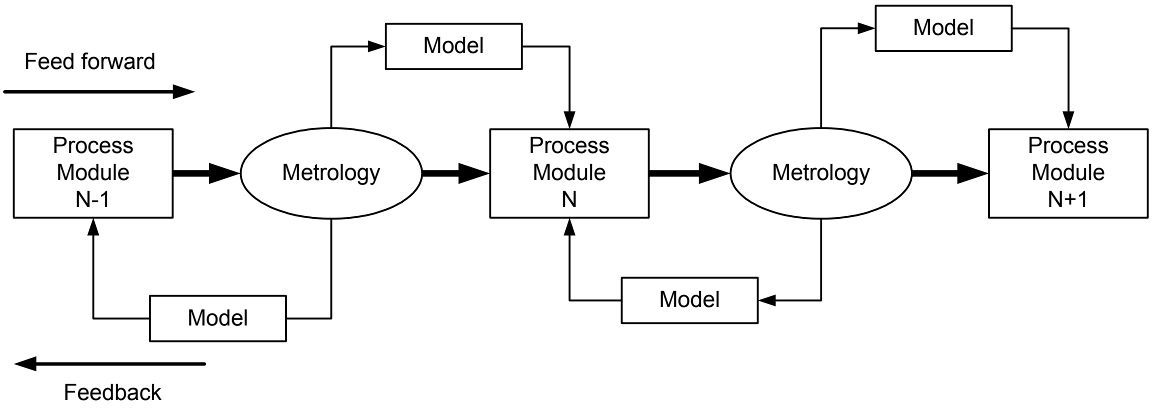


Figure 2.9: Advanced Process Control with RbR Process Control [Straatum 2002]

Advanced RbR process controller found a very large acceptance in the semiconductor industry as in mid 1990s many algorithms (e.g. neural network controllers [Sniderman 1997], adaptive controllers [Castillo 1998]) and a lot of in-situ sensors [Smith 1999A] and on-line metrology techniques were developed. The benefits of this method brought with it as compared to SPC and MVA [Smith 1999A, Smith 1999C] are:

- Increased throughput
- Operating errors reduction
- Wafer to wafer and lot to lot variability improvement
- Within-wafer and within-die variability reduction

The RbR process control reduces random tool process variability and increases long-term processing variability using in-situ sensors (e.g. acoustic emission sensor [Hwang 2001-02]) and inline metrology.

The inline metrology increases production time, as after every process run measurements are to be made, which has an influence on the throughput and in addition to this judgment about the process can be made only after the wafer is measured. The in-situ sensors give information only about certain critical process parameters that reflect a particular behavior of the process model and not the complete behavior of the process machine model.

2.3.4 Knowledge based process control

The knowledge based process control systems used for inline process control have to fulfill strict real-time requirements of the process and machine model [Knight 1997, Straatum 2002]. These systems have specific goals, different decision strategy, input and output information but require the same basic technical model of process and machine. The knowledge based process control systems discussed here are not yet deployed for CMP process machines. State of the art of these systems is discussed here:

2.3.4.1 Knowledge based process control for Plasma Etch and Chemical Vapor Deposition process

This approach [Straatum 2002] embeds an impedance sensor, which is tool and process sensitive, applicable currently only for Plasma Etch process and Chemical Vapor Deposition (CVD) process. This sensor has electrical signals (power, voltage and amperage) as input such as for pressure and temperature i.e. it observes the tool hardware, which builds the bases of contributors for the Fault Detection and Classification (FDC) using MVA techniques. The Fourier component of the impedance sensor is used to classify the faults. Fourier spectrum of the forced input changes, is then correlated to the corresponding tool process hardware parameters (e.g. power drop). The fault classification is done in the production environment with the expert knowledge of process engineer using MVA techniques. The collection of fault classes builds the basis for knowledge based process control and it is used for hardware fault detection.

Figure 2.10 shows a knowledge based process control for Plasma Etch process [Straatum 2002]. The advanced integrated sensors on the tool provide the inline tool state and process state information. This information is evaluated and a plasma index is calculated. The plasma index along with the process drift, offset drift and wafer specification is fed to the fault detection and classification engine by the knowledge based process control, which evaluates and generates decisions for the knowledge based process control to calculate the new process parameters, machine parameters and corresponding corrective actions.

The chemistry of the process is not controlled by this approach. The knowledge based process control is currently being deployed only for the Plasma Etch process and CVD but can be extended to any other semiconductor-processing machine.

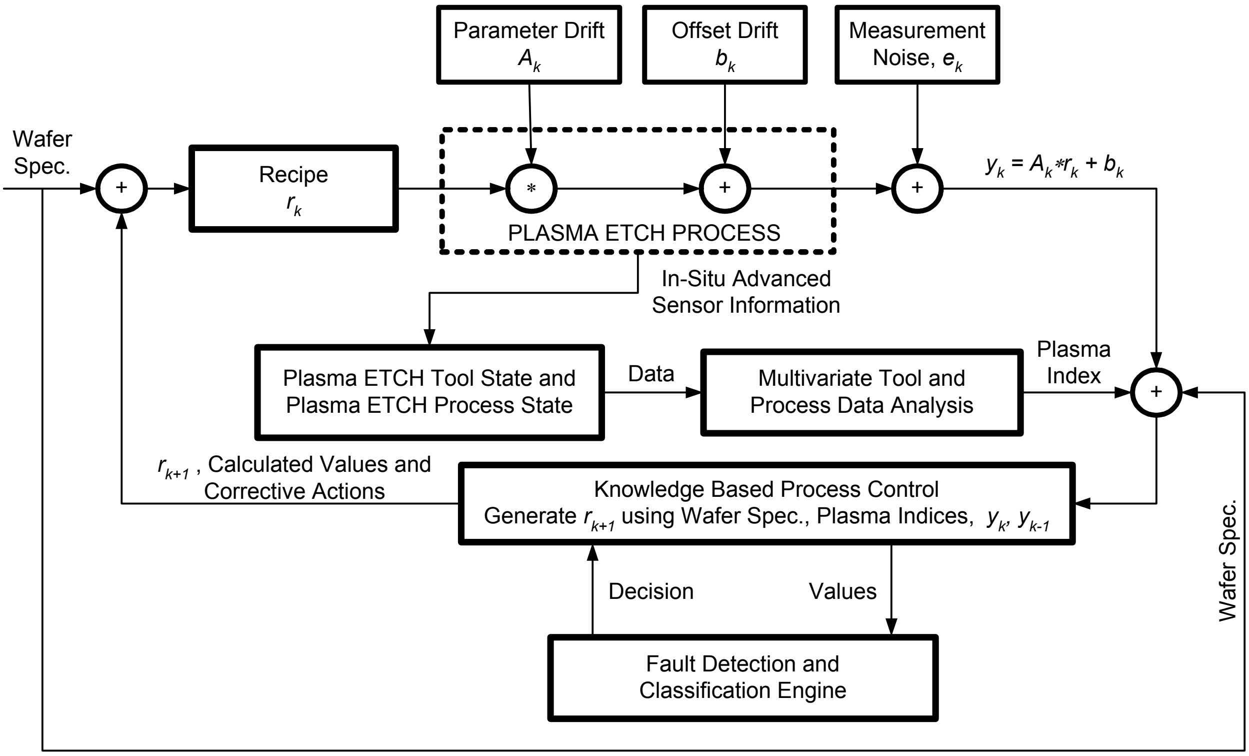


Figure 2.10: Knowledge based process control for Plasma Etch process

2.3.4.2 Diagnostic system an enhancement of supervisory control system for Photolithography process machine

The diagnostic system based on conventional probability theory compliments [Leang 1997] the existing supervisory control system consisting of feedback control loop and a feed-forward control loop for the Photolithographic process machine. It enhances the existing control system by detecting and correcting the process drifts and generating customized recipes for the next process steps or generating new recipes to counteract a particular process trend.

For every process run the supervisory control system [Leang 1997] with its feedback control loop tracks the performance of the Photolithographic process machine using adaptive process machine models. With its feed-forward loop, it tracks the standard process machine settings on subsequent process steps for correct wafer processing, thus improving significantly the process capability of photolithographic sequence. During the tracking of process machine performance and process machine settings, process machine malfunctioning or control alarm can be generated. To find the exact cause and the source of this malfunctioning or control alarm the diagnostic system is then activated. The diagnostic system calculates the probability of faults and determines which customized recipe is to be used next or generates a new recipe to counter the process trend. The diagnostic system is activated only for the suspicious wafers, which have generated a control alarm or malfunction alarm. The diagnosis is not performed on every wafer because the sensitivity of the diagnostic system here is limited. The supervisory control system tracks the process machine performance, process machine settings after every process run and therefore cannot detect the origination of a defect during a process run. If there is a control alarm or malfunction alarm the diagnostic system estimates the probability of faults and the corresponding contributors after an alarm has occurred and not during its occurrence.

Figure 2.11 shows schematically how the diagnostic system enhances the supervisory control system for particular Photolithographic process machine.

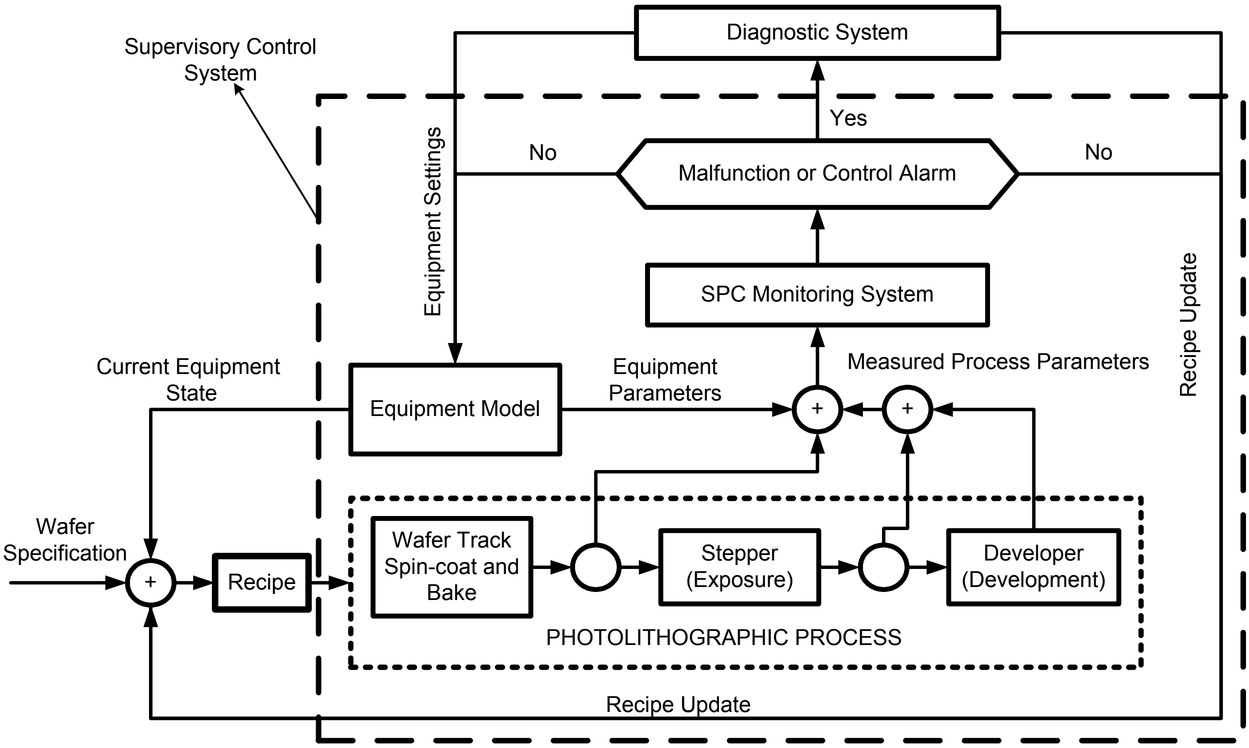


Figure 2.11: A diagnostic system: an enhancement of supervisory control system for Photolithography process machine

All The process controllers discussed here, generate a new process recipe before a process run is started. The process recipe is then downloaded by the CMP process automation controller [Kumar 1998] on the CMP process machine and the process run is started (point of no return) by the operator, it means that the calculated process recipe parameters cannot be changed by the operator after starting the process run. If some process alarm is registered by the process controller, it provides the operator a corrective action or list of corrective actions to clear the process alarm during a particular process run. A corrective action can be for example, an abort, which means an immediate stop of the process machine, or the recovery of wafers present in the process machine, or the complete initialization of the process machine and it is necessary to calculate a new process recipe.

2.4 Summary

To reduce the origination of defects during processing it is necessary to improve the existing control strategies. The defects are mostly detected after ex-situ measurements and the responsible process and machine parameters are correlated by the CMP process expertise offline. The correlations can lead to the generation of a new process recipe, or corrective actions for operator, or an immediate stop of the CMP process machine. If the CMP process expertise had the possibility to collect the process and machine parameter deviations inline, a time intensive correlation for defect analysis can be saved.

The studied CMP process machine uses SPC method to control the highly automated CMP process machine. The CMP process automation controller here generates a new recipe based on the feed back of geometrical deviations provided after k-3rd process run (section 2.3.1) for the current (kth) process run. The calculation of the new process recipe is based on the correlation between the deviations of measured geometrical values and the process and machine parameter values in the past. Another drawback here is that during unscheduled downtime of CMP process machine, there are no feedback geometrical values from the polished wafers, because the current state of the CMP process machine has changed. This leads to a problem i.e. to control the process and machine parameters the CMP process automation controller requires the SPC trends of geometrical values of wafers processed under the changed process conditions and process environment and these SPC trends are not available. For example in case of polishing pad renewal the CMP process machine has to be stopped. The CMP process machine is started again as there are no new wafers available for measurement at the metrology station polished by the renewed polishing pad. The SPC provides the first trends of geometrical values at least after third process run. To regulate and control the CMP process machine after a stop it requires at least ten process runs.

The MVA process control discussed in section 2.3.2 is an enhancement of SPC process control, as it will reduce the number of control parameters but will also provide the trends as the SPC process controller discussed above after the ex-situ measurements. RbR process control discussed in section 2.3.3 controls the parameter deviation after a process run, not during a process run. The drawback here is that the potential cause of a parameter drift cannot be analyzed as it controls only the process parameters involved during CMP process and not the machine parameters.

The knowledge based process control for Plasma Etch and CVD process as discussed in section 2.3.4.1 has been developed for Plasma Etch process. The integrated impedance sensors observe in-situ the process machine, the process states and provide the deviations to the knowledge based process controller, which further forwards these deviations to the fault detection and classification engine. The main drawbacks here are the adaptability of the knowledge based process controller to the changing stable process characteristics of studied CMP process machine, and controlling the chemistry of the process. This method requires a hardware change i.e. integration of advanced sensors, which is not desired at present in the studied CMP process machine. The supervisory control of Photolithography Process machine with diagnostic system (section 2.3.4.2) provides a very profound design and implementation of diagnostic system. However, the process controller has a drawback for the current CMP process machine as the diagnostic system is activated only by the SPC for the suspicious wafers and the sensitivity of the diagnostic system limits to carry out the diagnosis of every wafer. The detection of defect origination is not possible as it can only be activated after a process run is completed and only then when a suspicious wafer is detected.

None of the above process controller takes into consideration the in-situ time dependencies of the properties of process and machine parameters, therefore, an advanced process model describing completely the real time regular and irregular behavior of CMP process machine as well as of the CMP process is required. The expert knowledge about the CMP process and the CMP process machine builds the basis for the advanced process model and the in-situ sensors and ex-situ metrology results provide information to improve and optimize this model.

3 Theoretical and problem domain analysis of CMP process

3.1 Mechanical and chemical aspects of the CMP process during wafer manufacturing

Figure 3.1 shows in general the process flow and material flow during CMP process of the studied CMP process machine [WSAG 1997-2003]. In this section, the mechanical and chemical aspects of the CMP process during the final step of wafer manufacturing process are analyzed.

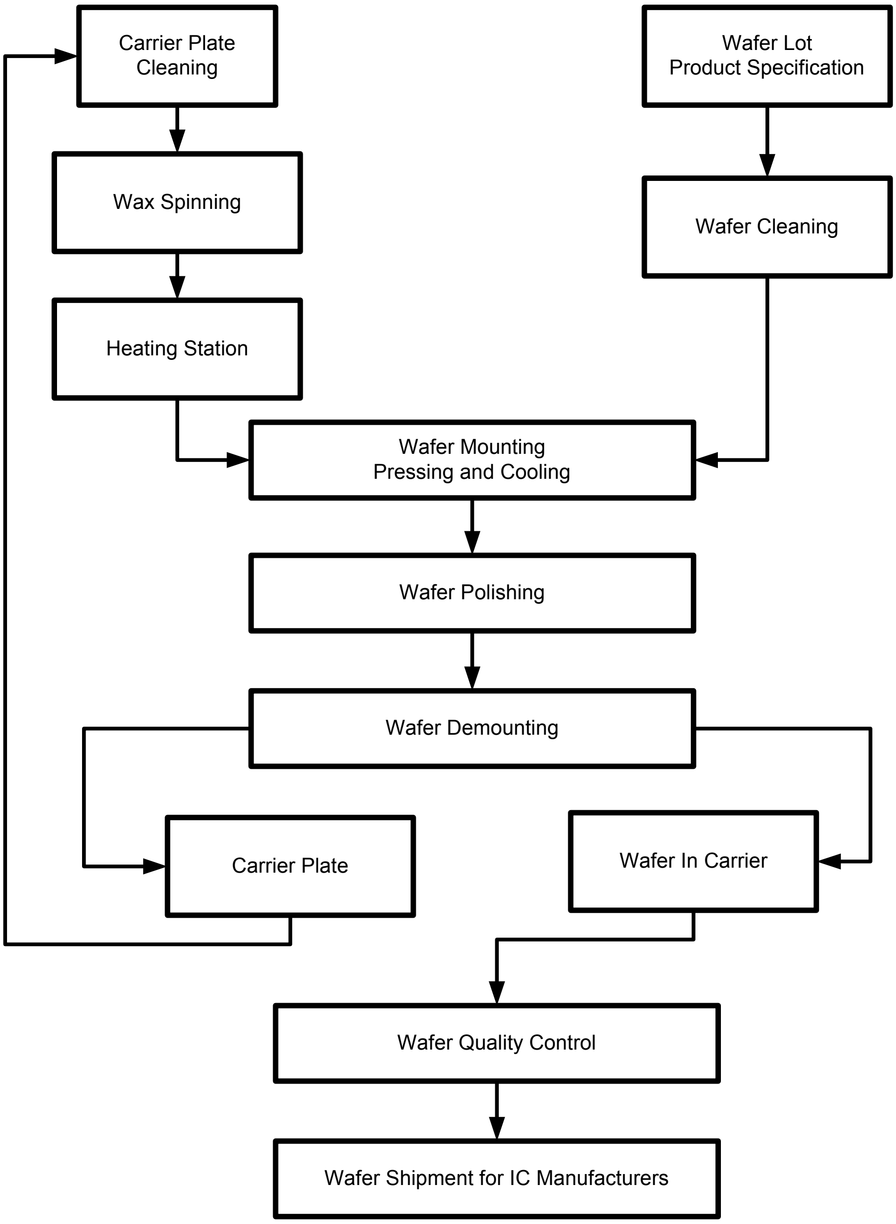


Figure 3.1: Process flow and material flow in general during the CMP process

3.1.1 The material flow logistics of the studied CMP process machine

Figure 3.2 shows the schematic diagram of the material flow during CMP process [Schweiker 1998]. The wafers (nominal diameter 150 mm, 200 mm or 300 mm) are brought to the wafer-cleaning unit. They are cleaned there and mounted on a carrier plate. As next step the carrier plates with mounted wafers are brought to the loading station on a conveyer belt for polishing. The loading station has a capacity to hold four carrier plates. The carrier plates are then picked up by portals having four independent rotating cylinders and are brought to the polishing plate, the portals move on rails.

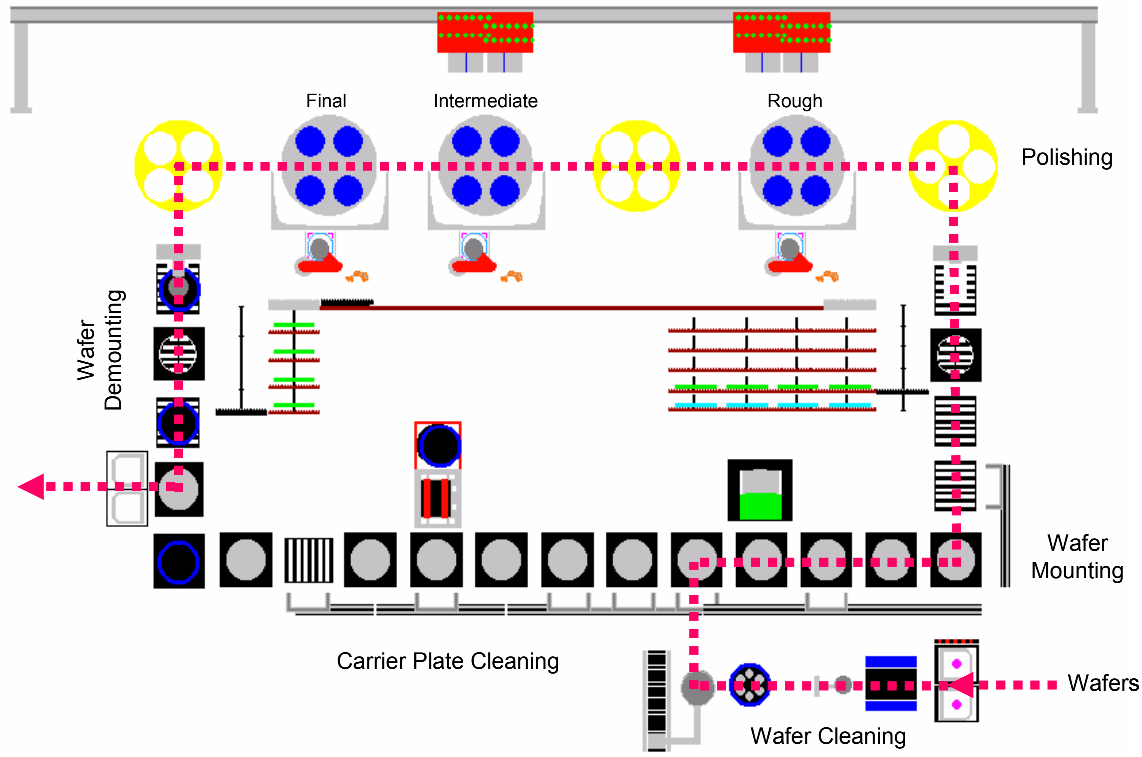


Figure 3.2: Material flow in the large volume wafer manufacturing CMP process machine [Schweiker 1998]

The mounted wafers are polished single sided in three steps, first step is rough polishing here 12 µm material from wafer surface is removed. The second polishing step is intermediate polishing, which reduces the localized light scattering defects (LLS) [SEMI M1 2002] (also known as LPD), i.e. the material removed here is between 0.8 µm to 1 µm. The third and the final polishing step is to reduce the haze defect [SEMI M1 2002], i.e. the material removed here is approximately 0.1µm.

The CMP process is described in chapter 2, section 2.1.3. Between the polishing step one and polishing step two there is an intermediate station where the four carrier plates wait to be picked up by second portal, which brings the mounting plates from intermediate polishing station to final polishing station. Before starting the polishing step, a polishing recipe calculated by the CMP process automation controller [Kumar 1998] is downloaded to the CMP process machine. The recipe contains the process and machine parameter values, which are regulated and controlled by the hardware components of the CMP process machine. The differences between the three polishing steps are the polishing pad, the slurry used and the control parameters, which are not required during polishing step 2 and polishing step 3.

After the polishing step 3 is finished the carrier plates are brought to the unload station, where the wafers are demounted from the carrier plate. The demounted wafers are put in a wafer carrier in a well-defined order. The carrier plates are finally cleaned and are mounted again with new wafers. The demounted wafers in a carrier are brought to a special metrology tool to measure the wafer geometry. After the quality control, the wafers are cleaned, packed and shipped to the semiconductor manufacturer [WSAG 1997-2003].

3.1.2 Wafer mounting and demounting process

The defects (see also section 2.2) origination in CMP process can start very early as all the surfaces, which are exposed for polishing should be free from contamination (metals, adhesive rests, medium residues and slurry rest). Certain defects are also caused if there is some contamination between the wafer, adhesive and the carrier plate; therefore, contamination free wafer mounting during wafer fabrication is a challenge in itself. The CMP process machine studied here has its own wafer mounting process and demounting process. The wafers are mounted under clean room conditions [Schließer 1999], where the particle concentration in clean air, DI water and other mediums are monitored continuously. The cleanliness of the surfaces during mounting process plays an important role during wafer fabrication, as it has direct impact on the quality of the product, i.e. the wafer geometry. The wafer mounting process includes following steps:

- **Carrier plate cleaning**

The carrier plate is cleaned thoroughly before it is spin-coated with wax. Any contamination on the surface of the plate will increase the risk of origination of a defect. The plate is cleaned with brushes after wafer demounting then it is put in ultrasonic warm water bath and finally scrubbed with soft brushes using DI water having 60°C inflowing temperature. After cleaning the plate it is either stacked at 35°C environment temperature in a buffer or it is moved further for wax coating under clean room conditions.

- **Wax spin coating**

The wax is spin-coated on the plate using SOG principle to hold the wafers during polishing, as any movement of wafers relative to rotating carrier or to polishing plate can lead to breakage of the wafer, that means a complete production stop. The wax must therefore posses certain characteristics, which is required during polishing process. The wax should:

1. Build a homogenous thin (3-7 µm) film on the carrier plate surface
2. Have low sticking zone temperature (65-75°C)
3. Not allow any wafer movement under polishing conditions (50-55°C)
4. Provide easy wafer demounting characteristics at (20-30°C)
5. Have high aqueous solubility
6. Contain resins with low molecular weight
7. Be contamination free
8. Not build any agglomerates

The thickness of the wax film formed on the carrier plate depends upon the wax amount; spinning speed, spin duration and the above wax characteristics. The homogeneity of wax film influences the wafer geometry directly.

- **Carrier plate heating**

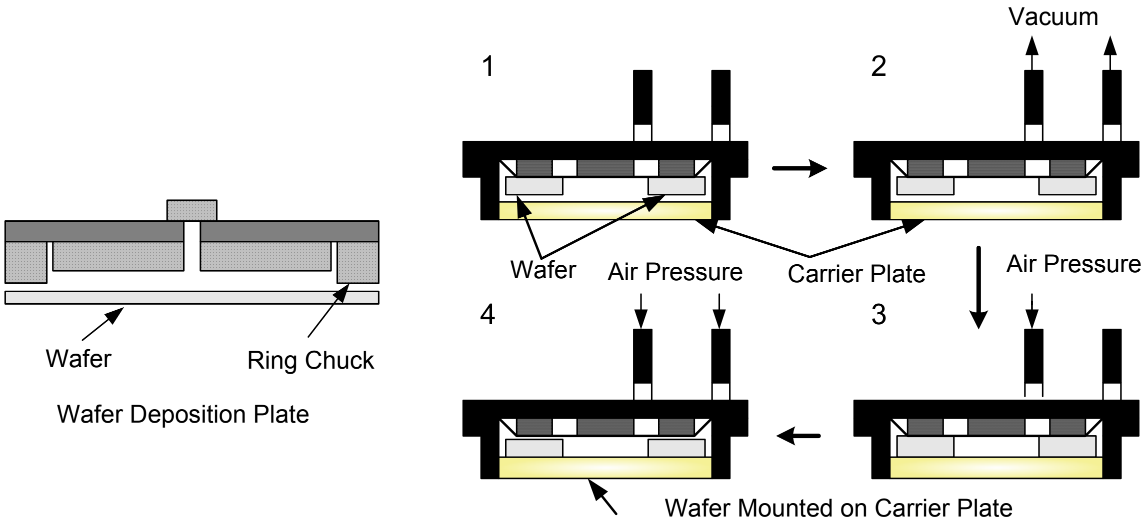
The carrier plate coated with wax is heated to a sticking zone temperature of 65 to 75°C. Heating is done gradually to avoid any thermal shock, i.e. the breakage of the carrier plate and the achievement of homogenous temperature profile all over the carrier plate. At any time, the sensors control the carrier plate temperature and the wax temperature. The temperature is regulated either by adjusting the duration of heating or by changing the temperature. The wafers are then placed on the carrier plate when the target (mounting) temperature ≥ 65 to 75°C has been reached.

- **Wafer cleaning**

Wafers are cleaned and dried in a wafer-cleaning machine parallel to the carrier plate cleaning and heating. The wafers are cleaned individually and are placed on a pick up pallet having a capacity for six 200 mm wafers. The six selected wafers, which are to be mounted on a carrier plate, have a maximum allowed thickness deviation of ± 1 μm.

- **Wafer pressing**

The wafers are transported from the pick up pallet to the carrier plate coated with wax at mounting temperature by means of a mechanical arm. The mounting mechanism provides the possibility of regulating the wafer curvature or its thickness variations (figure 3.3). This is accomplished by air pressure, when wafers are being pressed down on the carrier plate. Figure 3.3 shows the wafer mounting process and a wafer deposition plate, where a ring chuck uses vacuum for holding the wafers.



Wafer Deposition Plate

Wafer Mounting

Figure 3.3: Wafer deposition plate having six ring chucks and wafer mounting process [WSAG 1997-2003]

The six wafers are then lowered down to the carrier plate (figure 3.3) with regulated lowering speed. The defect origination here can be due to contamination, as there are moving parts, which due to friction can contaminate the wax or the carrier plate. Pressing is therefore done under controlled clean room conditions. To avoid any wafer breakages an accurate and uniform pressure under control is applied over the complete surface area of the wafer. The wafers are pressed on the wax slowly and during lowering of wafers the concavity or convexity of its curvature is individually regulated as the wafer mounting recipe parameters provide these values. The mounted wafers are then brought to the cooling station.

- **Carrier plate cooling along with mounted wafers**

The wafers mounted on the carrier plate are cooled down gradually 2-3°C by blowing air, which dries and lowers the carrier plate and wax temperature from 65 to 75°C down until the final temperature 30 to 40°C is reached. After the carrier plate, along with wafers is cooled down to the desired temperature the remaining wax is washed away with water jets. Figure 3.4 shows the mounted wafers on a carrier plate. Important information to localize and control defects is the wafer location on the carrier plate, as the SPC evaluates the LPD values [SEMI M1 2002] and wafer geometry values per wafer (see chapter 2, section 2.3.1) to calculate exactly the new recipe parameters for the next wafer lot.

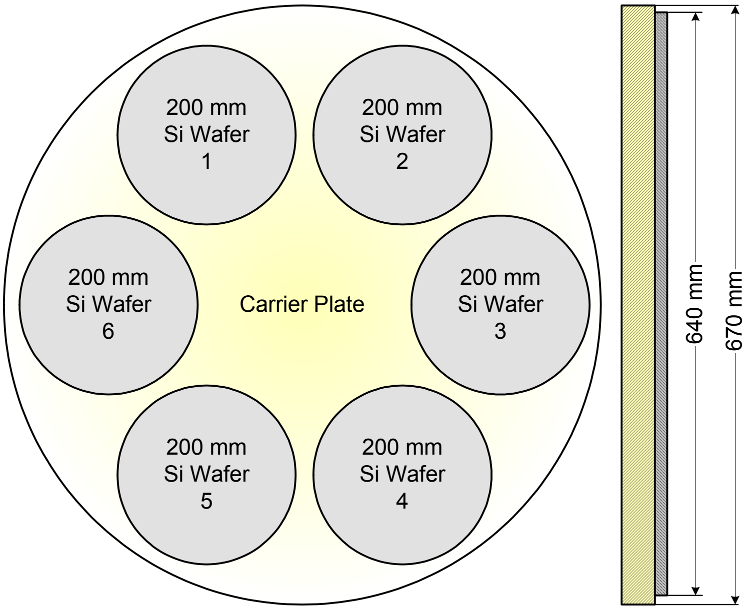


Figure 3.4: Mounted wafers on a carrier plate [WSAG 1997-2003]

- **Wafer demounting process**

After the CMP process, the wafers are demounted automatically from the carrier plate. The demounted wafers are placed in a carrier, building a group of six wafers and are put in the carrier in the same order as they were mounted on the carrier plate. The reason here is to correlate the measured geometrical parameters after CMP process with the corresponding process and machine parameters, which influence the CMP process such as pressure and velocity control of the rotating head holding the carrier plates.

3.1.3 Wafer polishing process

During wafer polishing process (see chapter 2, section 2.1.3) the material removal depends on the exerted mechanical forces and the chemical reaction taking place between the wafer and suspended colloid dispersed silica particles (size 50 - 100 nm) in an aqueous solution having a pH value around 12.5. Thus, the wafer polishing process depends upon many process parameters and machine parameters, which directly or indirectly influence the quality of polishing and thus build, alone or in combination, a basis for defect origination. A thorough investigation of the influence of these parameters is therefore necessary. In the next sections, the basic fundamental concepts of the CMP process are analyzed.

- **Polishing Rate**

The polishing rate is determined empirically by the Preston's equation [Preston 1927]. It states that the polish rate is directly proportional to the pressure exerted and the relative velocity:

$$\frac{\Delta H}{\Delta t} = -K_p \, P\left(\frac{\Delta s}{\Delta t}\right) \qquad 3.1$$

Where ΔH is the change in height of the surface, Δt is the time elapsed, K_p is the Preston's coefficient, P is the applied pressure and Δs / Δt is the relative velocity between pad and the wafer. The applied pressure $P = F/A$, where F is the applied mechanical force and A is the contact area between the polishing pad and the wafer. The Preston's coefficient K_p depends on process variables such as slurry composition, pad properties, mechanical abrasion and chemical effects during polishing process. Many models [Cook 1990, Runnels 1994, Runnels 1998, Tseng 1997 and Ouma 1998A] have been developed to understand the polishing rate with Preston's empirical equation 3.1 as basis, considering the mechanical and chemical properties of wafer, polishing pad and slurry. These models have discussed the mechanical aspect of polishing. The exact role of chemistry rate during this process is still hidden in the Preston's coefficient, which can be observed by the behavioral pattern characteristics during polishing.

- **Calculation of relative velocity during CMP**

The polishing plate and the carrier plates as described in chapter 2, section 2.1.3 rotate in the same direction as shown in figure 3.5. The Preston's equation 3.1 provides a dependency of removal rate based on the relative velocity and pressure within some region of the wafer [Ouma 1998B, Boning 1999]. For a particular studied machine configuration, figure 3.5, the relative velocity can be straightforward calculated by applying Preston's model. In figure 3.5 A is the center of the polishing plate and C is the axis of rotation of carrier plate, B is a particular point on the wafer, which lies on the circle of radius *r* centered at C, where the relative velocity between pad and wafer is calculated. The aim is to determine the effective relative velocity at any point on the ring. The carrier plate is assumed to oscillate along AC to ensure uniform and even pad degradation [Steigerwald 1997, Ouma 1998B] and ρ_0 is the average offset along AC. Let the angular velocity of the wafer on the carrier plate be ω_2 (in radians per minute) and that of the polishing plate be ω (in radians per minute). The relative velocity between the polishing pad and the point B on the wafer is given as [Preston 1927]:

$$v = v_s\left(1 + r_1^2\omega_s^2 + 2r_1\omega_s\cos\theta\right)^{1/2} \qquad 3.2$$

Where $v_s = \rho_0\omega$ is the relative velocity between the polishing pad and any wafer position, when the angular velocity of wafer and pad is equal (i.e. $\omega = \omega_2$), $r_1 = r/\rho_0$ and $\omega_s = 1 - \omega_2/\omega$. For $x = r_1\omega_s$ equation 3.2 can be written as [Boning 1999]:

$$v = v_s\left(1 + x^2 + 2x\cos\theta\right)^{1/2} \qquad 3.3$$

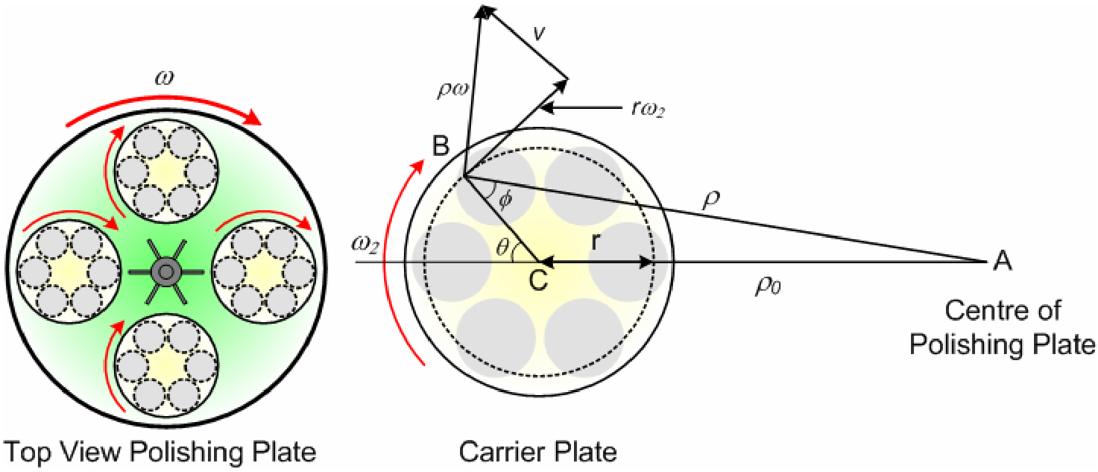


Figure 3.5: Velocity vectors of interest during CMP process

The equation 3.3 gives relative velocity *v* at any point on the circle with center at C and radius *r*, the effective relative velocity at distance *r* from the center can be given by [Steigerwald 1997, Ouma 1998B]:

$$v_e(r) = \frac{v_s}{\pi}\int_0^{\pi}\left(1 + x^2 + 2x\cos\theta\right)^{1/2} d\theta \qquad 3.4$$

Assuming the radial symmetry, substituting $\theta = 2\varphi$ and $\cos\theta = 1 - 2\sin^2\varphi$ the effective radial relative velocity $v_e(r)$ during CMP process is given by [Ouma 1998B, Boning 1999]:

$$v_e(r) = \frac{v_s(1+x)}{\pi}\int_0^{\frac{\pi}{2}}\left(1 - \frac{4x}{(1+x)^2}\sin^2\varphi\right)^{1/2} d\varphi \qquad 3.5$$

The equation 3.5 is an elliptical integral of second kind and is evaluated numerically. During CMP process, any drift or shift in the angular velocity of carrier plate or of polishing plate has a direct impact on the removal rate as given by Preston's equation 3.1, therefore these velocities play a very significant role for searching the cause of origination of defects during the CMP process.

- **Penetration depth**

The penetration depth or indentation depth δ of the abrasive particle (figure 3.6) is given by the equation 3.6 [Steigerwald 1997]:

$$\delta = \frac{3}{4}d\left(\frac{P}{2cE}\right)^{2/3} \qquad 3.6$$

Where *d* is the diameter of the abrasive particle, *P* is the exerted pressure and *c* is particle fill factor at the surface. The contact area A_c is given by the equation 3.7 [Steigerwald 1997]:

$$A_c = \pi r_c^2 = \pi\left(d\delta - \delta^2\right) \qquad 3.7$$

In the figure 3.6 the indentation depth is δ, abrasive particle radius r_p and contact radius r_c. The polishing pad as well as the wafer surface is abraded during polishing, after certain process runs the polishing pad shows a glazing affect, which again is the cause of defect origination and has to be observed during polishing process.

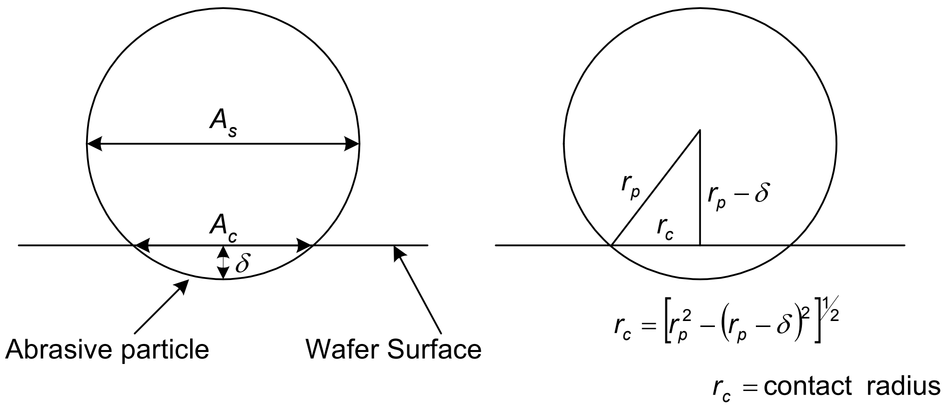
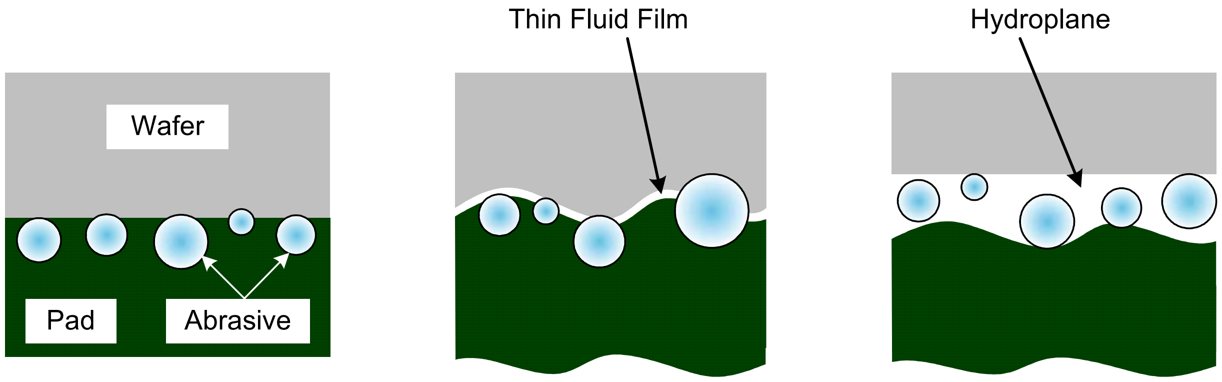


Figure 3.6: Abrasive particle with contact area A_c, surface area A_s and indentation depth δ [Steigerwald 1997]

- **Slurry characteristics and its role in CMP**

The colloid dispersed silica particles suspended in aqueous solution (slurry) builds an interacting lubricating fluid layer between wafer surface and pad. The relative sliding motion between the wafer and pad [Zhang 1999 and Philipossian 2001] supports the load (figure 3.7):

1. Directly via wafer-pad contact
2. Partially by wafer-pad contact and partially by hydrodynamic pressure provided by the lubricating fluid layer between them
3. By the fluid layer between wafer and pad by building an hydroplane between the two (no wafer-pad contact)



1. Wafer - Pad full Contact Mode

2. Wafer - Pad partial Contact Mode

3. Wafer - Pad no Contact Mode

Figure 3.7: Wafer-Pad contact modes for supporting the load

In the first case, the maximum frictional wear is there because of reduced chemical activity due to poor slurry flow, high mechanical abrasion, high temperature, reduced transport of abraded particles, and therefore severe damages on the polished surface.

In the second and third cases where slurry plays a very important role, as it builds the basis for chemical activity between wafer surface and pad (i.e. metal solubility and metal dissolution), has lubricating characteristics, builds boundary layers, provides hydrodynamic pressure, transmits heat, provides the abrasive particles and transports the abraded particles during polishing. In fact, the polishing process takes place under partial-contact mode. Pad asperities and fluid forces against the wafer surface carry abrasive particles in slurry during polishing, the pad is in partial contact with the wafer and there is a very thin discontinuous fluid film between the wafer and the pad. The load is, therefore supported by both the pad and the fluid layer [Steigerwald 1997, Zhang 1999].

In CMP process, the slurry builds a thin fluid film between the wafer and the pad therefore, from the aspect of defect origination, boundary layer consideration between the surface being polished and the slurry, which transports new reactants to the wafer surface and takes away the abraded particles from wafer surface continuously, is very important. In CMP process boundary layers limit the rate of the chemical activity-taking place between the slurry and the surface being polished [Steigerwald 1997], because they act as diffusion barriers to the reactants and the products of the chemical reactions. The formation of these layers can be categorized as follows:

1. *Stagnant boundary layer:* Develops at the fluid solid interface where the flow velocity is zero due to frictional forces of the wafer on the moving fluid. The influencing parameters for this layer are fluid viscosity η, fluid density λ and fluid velocity U as boundary layer thickness δ_{th} is given by [Steigerwald 1997]:

$$\delta_{th} = \frac{2}{3}L\left(\frac{\eta}{\lambda UL}\right)^{1/2} \quad 3.8$$

2. *Boundary layer*: Develops due to accumulation of electric charges at the contact surface [Steigerwald 1997]. The attraction and repulsion of reactants and products is caused by the charges built on the surface layer. For insulators and metal, charges accumulate at the surface because of adsorbed charge species. For Example at the SiO_2 surface either positively charged $Si\text{-}OH_2^+$ or neutral Si-OH or negatively charged $Si\text{-}O^-$ bonds are formed. The pH value of the slurry can shift this equilibrium in either direction, if the pH value is low then a positive charge is developed on the surface and vice versa, which directly affects the polishing rate, and thus pH value of the slurry plays an important role supporting the material removal during the polishing process.
3. *Metal surface film*: Develops because of chemical modification of the metal. This film is produced due to chemical reaction between metal surfaces and the slurry chemicals and thus affecting the diffusion of reactants and abraded particles. The chemical reaction is corrosive and thus builds a barrier for reactants and products.

The slurry, thus supporting the chemical as well as mechanical component of CMP, provides the breaking up of the boundary layers by abrasive particles and supporting the transportation of reactants to the surface being polished and products away from it [Steigerwald 1997]. Any drift or shift in slurry characteristics influences the CMP process and thus the product quality directly. Therefore, to avoid the defect origination, the observation of slurry characteristics is inevitable.

- **Polishing pad and its characteristics**

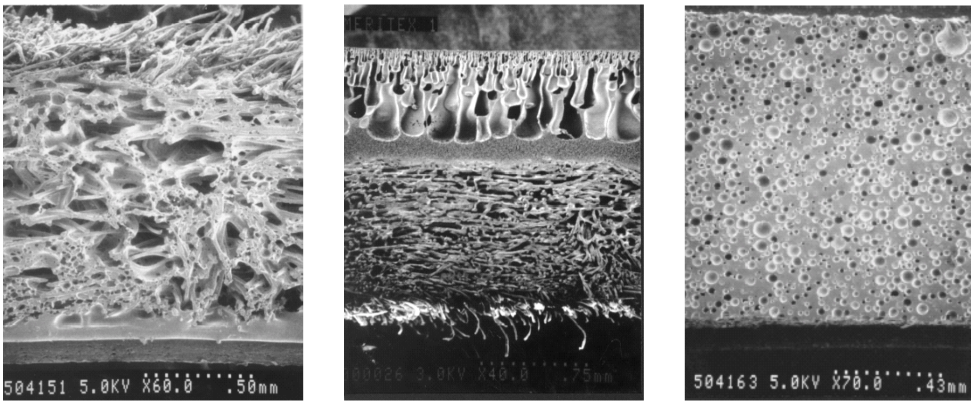
In CMP process the polishing pad during its polishing life cycle influences the product quality [Ouma 1998B, Philipossian 2001, James 2001], as it:

1. Delivers slurry, water and chemicals to the wafer
2. Transports water, chemical, abraded particles, pad fragments and unused slurry away from the wafer

3. Influences the polishing rate and polishing ability of CMP process
4. Should be resistant to harsh chemical and mechanical environments

Therefore, it requires a very thorough investigation as it plays a very significant role for the origination of defects. The resulting chemical and mechanical properties characterizing a polishing pad [Philipossian 2001 and James 2001] to fulfill the above requirements are:

1. Material of construction (e.g. polyurethane, etc.) see figure 3.8.



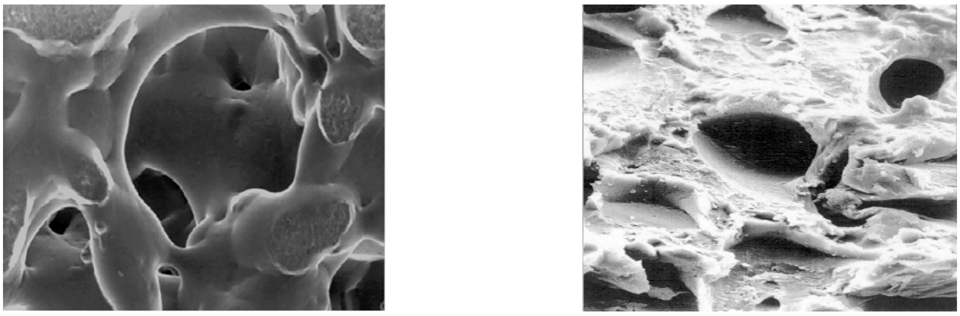
SUBA IV^{TM}
source Rodel

Politex
source Rodel

IC 1000
source Rodel

Figure 3.8: Microstructure of base polishing pads (Rodel [Philipossian 2001, James 2001])

2. Specific gravity (influences pad porosity i.e. slurry transport to and away from the wafer) see figure 3.9.



EPIC Pore Shape
source Cabot

Polyurethane Pore Shape
source Rodel

Figure 3.9: Polishing pad pore shapes (Rodel, Cabot [Philipossian 2001, James 2001])

3. Pad elasticity and viscoelasticity (influences polishing rate). The elastic behavior of the pad is given by equation 3.9 [Timoshenko 1970], where τ is shear stress, γ is shear strain and G is shear modulus related to Young's modulus as shown in equation 3.10 [Timoshenko 1970] where ν is the Poisson's ratio.

$$\tau = G\gamma \qquad 3.9$$

$$G = \frac{E}{2(1+\nu)} \qquad 3.10$$

The viscous behavior of pad is given by the equation 3.11 [Steigerwald 1997], where η is the viscosity. The strain in a viscous material remains after the stress removal and it is a linear function of time.

$$\tau = \eta\gamma \qquad 3.11$$

The viscoelastic behavior of the pad is given by the equation 3.12 [Steigerwald 1997]. The viscoelastic material relaxes with exponential time dependence as given by the equation 3.13, where t is the elapsed time and $\tau_r = \eta/G$:

$$\tau = G\gamma + \eta\gamma \qquad 3.12$$

$$\gamma = \frac{\tau}{G}\left[1 - e^{-t/\tau_r}\right] \qquad 3.13$$

4. Surface roughness (influences polishing rate) is based on the distribution of pad asperities (high points on the pad surface, figure 3.10). These asperities actually have been exposed to the wafer during polishing and are assumed to be spherical at their summit [Yu 1993] and their height z, radius β are normally distributed (Gaussian distribution). As the polishing takes place in wafer-pad partial contact mode [Zhang 1999], see figure 3.7 and 3.10, the pad asperities are in direct contact with the wafer surface. The contact area a_c and the contact load c_l is given by the following equations [Yu 1993, Steigerwald 1997]:

$$a_c = \pi\beta\,(z - h) \qquad 3.14$$

$$c_l = \frac{4}{3}E'\beta^{0.5}(z - h)^{3/2} \qquad 3.15$$

Where h is the film thickness between wafer and pad surface, z is pad asperity height, and E' is an effective modulus of pad surface.

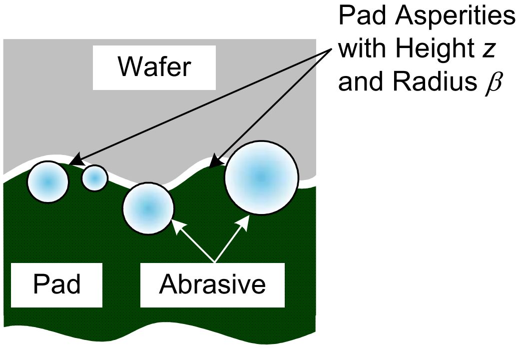


Figure 3.10: Pad asperities in wafer-pad partial contact mode

The total pad contact area A_p and total contact load C_L over a given pad area A is given by equation 3.16 and 3.17 [Yu 1993, Steigerwald 1997]:

$$A_p = \kappa A \int_h^\infty \int_0^\infty a_c \; \Phi_\beta \, \Phi_z d\beta \; dz \qquad 3.16$$

$$C_L = \kappa a_c \int_h^\infty \int_0^\infty c_l \Phi_\beta \, \Phi_z d\beta \; dz \qquad 3.17$$

Where κ is the asperity density, Φ_β and Φ_z are normal distribution of β and z.

5. Average cell size, size distribution and cell density (influences slurry transport to and away from the wafer).

6. Hardness, tensile strength, compressibility and thickness (influence polishing rate): The polishing pad deformation characteristics [Boning 1999] depends on the applied loads, relative speeds and the polishing pad thickness. The analytic solution for the deformation of a polishing pad can be given by a set of two equations 3.18 and 3.19 [Timoshenko 1970]. Assuming that pad is an elastic material, which has a thickness relative to the vertical deformation and has a deformation force q applied over a circular region of radius r_1 (figure 3.11). The equation 3.18 and 3.19 represent deformations within and outside the circular radius over which the force is applied. The deformation at any radius $r < r_1$ is given by equation 3.18:

$$w(r) = \frac{4\left(1-\nu^2\right) q\, r_1}{\pi E} \int_0^{\frac{\pi}{2}} \sqrt{1 - \frac{r^2}{r_1^2} \sin^2\theta}\; d\theta \qquad 3.18$$

Where ν is Poisson's ratio, q is applied force and E is Young's modulus of the polishing pad.

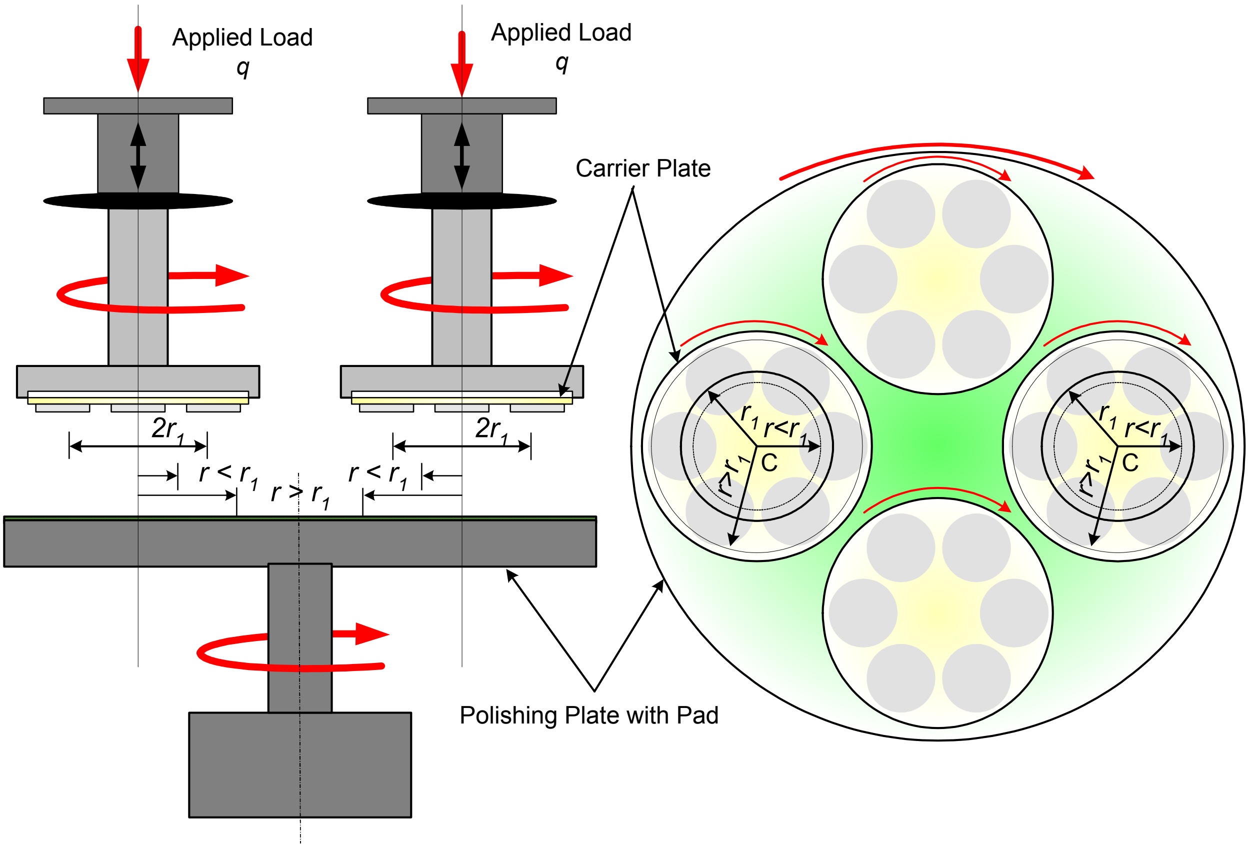


Figure 3.11: Pad deformation

For $r > r_1$ is given by the following equation:

$$w(r) = \frac{4\left(1-\nu^2\right) q\, r}{\pi E} \left[\int_0^{\frac{\pi}{2}} \sqrt{1 - \frac{r_1^2}{r^2} \sin^2\theta}\, d\theta - \left(1 - \frac{r_1^2}{r^2}\right) \int_0^{\frac{\pi}{2}} \frac{d\theta}{\sqrt{1 - \frac{r_1^2}{r^2} \sin^2\theta}} \right] \qquad 3.19$$

According to equations 3.18 and 3.19 the pad deformation is directly proportional to the applied force q and is inversely proportional to the pad material stiffness [Boning

1999]. The maximum deformation occurs when $r = 0$, is given by the equation 3.20 [Boning 1999]:

$$w_{\max} = \frac{2\left(1-\nu^2\right) q\, r_1}{\mathrm{E}} \qquad 3.20$$

In addition, the deformation at the edge of force area for $r = r_1$ is given by equation 3.21 [Boning 1999]:

$$w_{r=r_1} = \frac{4\left(1-\nu^2\right) q\, \mathrm{r}_1}{\pi \mathrm{E}} \qquad 3.21$$

The hardness, compressibility and thickness of polishing pad influence its life cycle and material removal characteristics. The pad undergoes plastic deformation after a certain number of polishing runs in production environment and starts glazing thus resulting in the reduction of the removal rate.

7. Water absorption at room temperature (influences chemical activity of CMP process).
8. Perforation patterns and density (influences slurry transport to and away from the wafer).
9. Groove pattern (i.e. concentric or tiled), profile (i.e. V-shaped, U-shaped or Wedge-shaped) and dimensions (i.e. depth, width and pitch).

The CMP process is a very dynamic process. After certain process runs, the polishing pad surface starts glazing due to plastic deformation resulting in low polish rates. The refreshing of the polishing pad is done by the pad conditioning, which maintains the porosity and roughness of the pad. The conditioning involves removal of deformed pad material, removal of used slurry and polish by-products. The in-situ control of polishing pad characteristics is therefore very important.

Shift in any of the above characteristics of polishing pad becomes a possible cause of defect generation. The polishing pad is therefore under continuous surveillance during the CMP process.

➢ Abrasives

The abrasives responsible [Westkämper 1991, Steigerwald 1997] for mechanical abrasion and pad glazing, play a key role during CMP process. Abrasives commonly used are made up of materials [Philipossian 2001] like silicon oxide, aluminium oxide or ceria oxide having a size [Westkämper 1996] between 50 -100 nm. To avoid the sedimentation and building of agglomerates the abrasive particles are kept in a colloidal silica suspension, which is done by using the zeta potential of these particles. The zeta potential is a surface charge developed on small particles in an ionic solution and depends upon the particle composition and the solution pH. The abrasive particles develop a positive surface charge in an alkaline pH solution. Due to these positive charges, they repel each other; therefore, they build no agglomerates, which further avoid the sedimentation of abrasive particles in the suspension. The mechanical properties, size, concentration, physical shape, zeta potential, chemical reactivity with surrounding materials and the relationship to materials to be polished, pad and slurry chemistry are typical characteristics of abrasives, which are to be considered for optimizing a CMP process. During the CMP process, the typical defects caused by abrasives are micro scratches, pitting and rip-offs [Vasilopoulos 2000B].

- **Chemistry of polishing**

The chemical composition of wafer being polished, polishing pad and slurry play a very crucial role during the CMP process. The chemical interactions induced by the chemicals (organic and inorganic acids or bases, anti-coagulating agents, corrosion inhibitors, oxidizers) in slurry, wafer surfaces and polishing pad surfaces during CMP process determine [Steigerwald 1997]:

1. The formation of a passivating layer at the wafer surface caused by oxidizers
2. Dissolution of:
    a. Wafer, pad surface
    b. The mechanically abraded wafer, pad fragments
    c. Atoms or molecules of the wafer or of the passivated layer formed on the wafer surface
3. The Isoelectric point IEP, which is the solution pH where the zeta potential of a given submerged surface is zero, related to abrasive and wafer surface charged layers
4. Polished material effectively removed and its redeposition
5. Contamination of polished wafer surface
6. Post-CMP neutralization and hydrophilization
7. Pad life cycle and pad properties

The chemistry of polishing is very complicated; it influences the quality of the CMP process directly. Change in any of the chemical properties of slurry, wafer and pad results in the origination of defects or combination of defects. These defects can be correlated with the present knowledge in certain known cases and require a very thorough study to understand the correlations completely [Cook 1990, Runnels 1994].

3.2 The geometrical aspects of wafer surface to assure the quality of CMP process

In the wafer manufacturing process, for a specified nominal wafer diameter (150 mm, 200 mm, 300 mm) the wafer surface should conform to the geometrical dimension [DIN 50441/1 1991, DIN 50441/4 1991] and its tolerances as specified in the standard [SEMI M1 2002]. The CMP process is the final step during the wafer manufacturing process and the objective here, is therefore to accomplish the specified geometrical dimensions of wafer surface within the specified tolerances. The geometrical dimensions of wafer surface after CMP process exactly qualifies the quality of the CMP process. The geometrical deviations are used as one of the inputs by the process controller to adjust the process and machine parameters for the compensation of the deviation between the process output parameters and the target parameters. The specified geometrical dimensions according to the SEMI standards [SEMI M1 2002] are wafer surface flatness, bow and warp [DIN 50441/1 1991, DIN 50441/4 1991], which are explained here.

3.2.1 Wafer surface flatness

Table 3.1 shows the letter codes used according to SEMI Norm [SEMI M1 2002] and Table 3.2 shows the SEMI Norms and the corresponding geometrical indices to characterize wafer flatness. The wafer flatness, can be either global or local (flatness measured on Sites), is the deviation of the front surface relative to reference plane when the back surface of wafer is ideally flat [DIN 50441/4 1991, SEMI M1 2002].

Position	Letter	Description
1	S / G	Site / Global
2	F / B	Front / Back i.e. reference surface of the wafer
3	L / Q / I	Least Square Global / Least Square Site / Ideal
4	R / D	Range / Deviation

Table 3.1: Letter code according to SEMI Norms [SEMI M1 2002]

Geometrical Indices	SEMI Norm
TTV: Total Thickness Variation	GBIR
TIR best fit: Total Indicator Reading	GFLR
FPD best fit: Focal Plane Deviation	GFLD
STIR max. back ref. Site Total Indicator Reading	SBIR max.
STIR max. front ref. focal range	SFLR max.
STIR max. best fit	SFQR max.
SFPD max. back ref. Site Focal Plane Deviation	SBID max.
SFPD max. front ref. focal range	SFLD max.
SFPD max. best fit	SFQD max.

Table 3.2: Geometrical indices and corresponding SEMI Norms

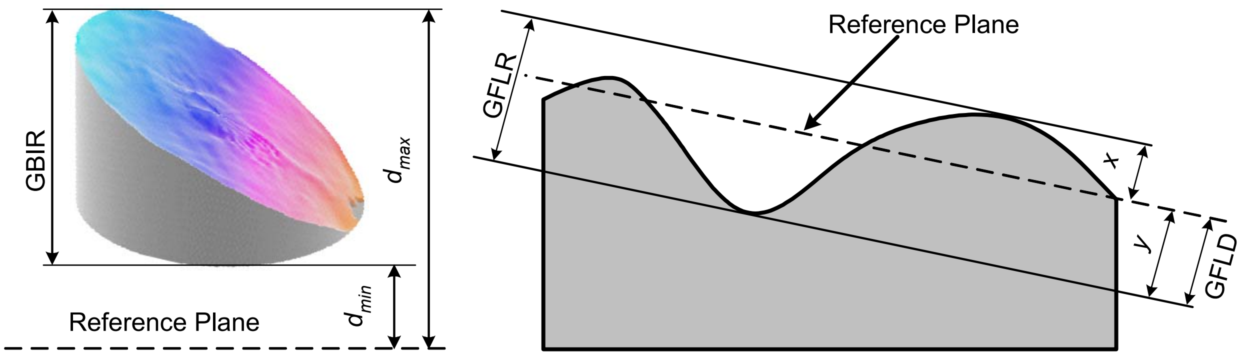
3.2.1.1 Global geometrical indices

All the global geometrical indices begin with the letter "G" (Table 3.2) and define the global geometrical dimensions of the wafer.

- **Total Thickness Variation (TTV) or Global Back surface Ideal Range**

TTV [DIN 50441/1 1991] or GBIR is defined as the linear thickness variation and is the difference between the maximum wafer thickness and minimum wafer thickness (see figure 3.12 a) from a reference plane [SEMI M1 2002]. GBIR is given by the equation 3.22:

$$\mathrm{GBIR} = d_{\max} - d_{\min} \tag{3.22}$$



a) TTV / GBIR

b) TIR / GFLR, FPD / GFLD

Figure 3.12: Global Parameters a) Total Thickness Variation (TTV) or GBIR, b) Total Indicator Reading or GFLR, Focal Plane Deviation (FPD) or GFLD [WSAG 1997-2003]

- **Focal Plane Deviation (FPD) or Global Front surface Least squares Deviation (GFLD)**

FPD [DIN 50441/1 1991] or GFLD is defined as maximum value among the maximum positive deviation (i.e. modulus |x|) and the maximum negative deviation (i.e. modulus |y|) from the reference plane (figure 3.12 b) and is given by the equation:

$$\begin{aligned} \text{GFLD} &= \pm \max.\left(|x|,|y|\right) \\ &+ \text{if}\left(|x| \geq |y|\right) \\ &- \text{if}\left(|x| < |y|\right) \end{aligned} \qquad 3.23$$

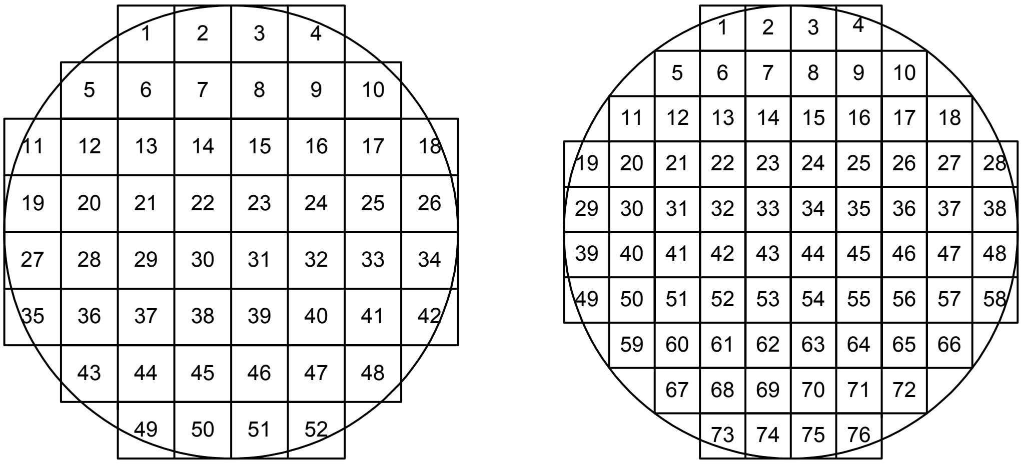
- **Total Indicator Reading (TIR) or Global Front surface Least squares Range GFLR**

TIR [DIN 50441/1 1991] or GFLR is a nonlinear thickness variation and is defined as the sum of the maximum positive deviation modulus $|x|$ and the maximum negative deviation modulus $|y|$ (equation 3.24) on the front surface of the wafer from the reference plane (figure 3.12 b):

$$\text{GFLR} = |x| + |y| \qquad 3.24$$

3.2.1.2 Local geometrical indices

All the local geometrical indices begin with the letter "S", which stands for “Site” (Table 3.1). It is defined according to SEMI standards as a rectangular area on the front surface of the wafer, whose sides are parallel and perpendicular to the notch bisector and whose center falls with in the Flatness Quality Area (FQA) [DIN 50441/1 1991, DIN 50441/4 1991, SEMI M1 2002]. Figure 3.13 shows two examples of Site-partitions on 200 mm wafer with 25*25 mm squares dividing it into 52 Sites and 20 partials and 20*20 mm squares dividing it into 76 Sites and 24 partials, having an edge exclusion of 3 mm (194 mm as diameter for FQA). These geometrical indices reveal the wafer topologies locally, precisely and are helpful to specify the wafer topographical anomalies exactly.



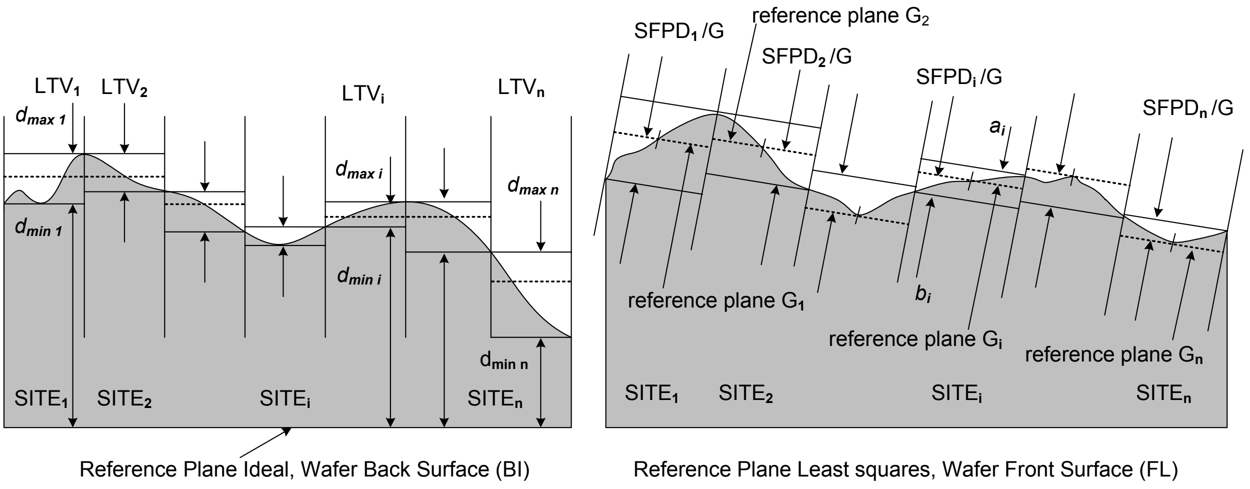
a) 52 Sites and 20 Partials

b) 76 Sites and 24 Partials

Figure 3.13: Example of Sites on the front surface of the wafer [WSAG 1997-2003]

- **Site Focal Plane Deviation (SFPD) or Site Back surface Ideal Deviation SBID**

SFPD or SBID as shown in figure 3.14 a, is given by the equation 3.25:



a) SFPD / SBID and LTV / SBIR

b) SFPD / SFLD and STIR /SFLR

Figure 3.14: Local geometrical indices: a) reference plane as wafer back surface and b) reference plane as wafer front surface [WSAG 1997-2003]

$$
\begin{aligned}
SBID_i &= \pm \max\left(\left|d_{\max i} - d_{zi}\right| \wedge \left|d_{\min i} - d_{zi}\right|\right) \qquad 3.25\\
&\quad + \text{if } \left(\left|d_{\max i} - d_{zi}\right| \geq \left|d_{\min i} - d_{zi}\right|\right)\\
&\quad - \text{if } \left(\left|d_{\max i} - d_{zi}\right| < \left|d_{\min i} - d_{zi}\right|\right)
\end{aligned}
$$

$$
\mathrm{SBID}_{\max} = \pm\, Maximum\left\{\left|SBID_1\right|, \left|SBID_2\right|, \ldots, \left|SBID_i\right|, \ldots \left|SBID_n\right|\right\} \qquad 3.26
$$

Where $SBID_i$ is the SBID value in Site$_i$, $d_{max\ i}$, $d_{min\ i}$ are the maximum, minimum wafer thickness in Site$_i$ measured from wafer back surface as reference plane (Ideal), d_{zi} is the central thickness of Site$_i$ and n is the number of Sites.

- **Site Local Thickness Variation (LTV) or Site Back surface Ideal Range SBIR**

In figure 3.14 a SBIR is the difference between maximum wafer thickness and the minimum wafer thickness in Site$_i$. This is measured from the wafer back surface as reference plane (Ideal), and is given by the equation 3.27.

$$\mathrm{SBIR}_i = d_{\max i} - d_{\min i} \qquad 3.27$$

$$\mathrm{SBIR}_{\max} = \pm\, Maximum\{SBIR_1, SBIR_2, \ldots, SBIR_i, \ldots, SBIR_n\} \qquad 3.28$$

- **Site Focal Plane Deviation (SFPD) or Site Front surface Least squares Deviation (SFLD)**

SFPD / SFLD as shown in figure 3.14 b, is given by the equation 3.29:

$$\begin{aligned} SFLD_i &= \pm \max\left(\left|FPD_{\max i} - FPD_{zi}\right| \wedge \left|FPD_{\min i} - FPD_{zi}\right|\right) \qquad 3.29\\ &\quad + \text{if } \left(\left|FPD_{\max i} - FPD_{zi}\right| \geq \left|FPD_{\min i} - FPD_{zi}\right|\right)\\ &\quad - \text{if } \left(\left|FPD_{\max i} - FPD_{zi}\right| < \left|FPD_{\min i} - FPD_{zi}\right|\right) \end{aligned}$$

$$\mathrm{SFLD}_{\max} = \pm\, Maximum\{\left|SFLD_1\right|, \left|SFLD_2\right|, \ldots, \left|SFLD_i\right|, \ldots \left|SFLD_n\right|\} \qquad 3.30$$

Where $SFLD_i$ is the SFLD value in Site$_i$, $FPD_{max\ i}$, $FPD_{min\ i}$ are the maximum, minimum focal plane deviation in Site$_i$ measured from wafer front surface as reference plane (using Least square), FPD_{zi} is the focal plane deviation in the center of Site$_i$ and n is the number of Sites.

The calculation for SFQD is similar to that of GFLD as given by equation 3.23 and is limited only to a particular Site

- **Site Total Indicator Reading (STIR) or Site Front surface Least squares Range (SFLR)**

In figure 3.14 b SFLR is the difference between maximum focal plane deviation and minimum focal plane deviation Site$_i$ measured from the wafer front surface as reference plane (using Least squares), and is given by the equation 3.31.

$$\mathrm{SFLR}_i = FPD_{\max i} - FPD_{\min i} \qquad 3.31$$

$$\mathrm{SFLR}_{\max} = \pm\, Maximum\{SFLR_1, SFLR_2, \ldots, SFLR_i, \ldots, SFLR_n\} \qquad 3.32$$

The calculation for SFQR is similar to that of GFLR as given by equation 3.24 and is limited only to a particular Site.

3.2.2 Geometrical deformation of wafer due to residual stress

After wafer manufacturing process due to residual stress there can be a deformation of wafer surface known as warp and bow [DIN 50441/1 1991, SEMI M1 2002] as discussed later. These deformations are measured on a freely lying wafer on three specified points. These three specified points build the reference plane and all the distance measurements are made relative to this plane.

- **Warp**

Warp is defined as modulus of the difference between maximum deviation d_{max} and the minimum deviation d_{min} of the median area from the reference plane (figure 3.15). The median area is locus of set of all points, which are equidistant from wafer front and back surface. The accessibility of median area is difficult for measurements, thus two help planes parallel to reference plane for front and back surface of wafer are used to evaluate Warp [Lehnicke 1999] and is given by:

$$\mathrm{Warp} = \left| d_{\max} - d_{\min} \right| \qquad 3.33$$

$$\mathrm{Warp} = \frac{1}{2}\left[(b-a)_{\max} - (b-a)_{\min} \right] \qquad 3.34$$

Where *a* and *b* are the distances from the upper and lower help planes to the front and back surface of wafer respectively.

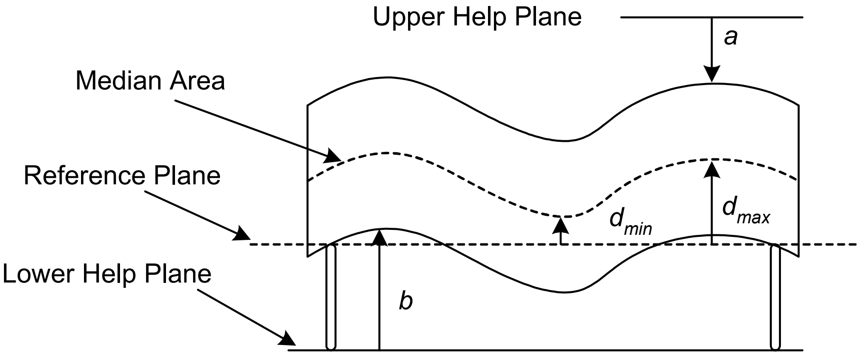


Figure 3.15: Definition of Warp [DIN 50441/2 1991]

- **Bow**

The Bow (figure 3.16) is a measure of wafer surface curvature. It is defined as the distance to the center point of the median area of an unclamped wafer from the reference plane. The Bow has either a plus (convex) or a minus (concave) sign depending upon the convexity or concavity of the wafer surface curvature [Lehnicke 1999]. The influence of the gravitational force can be compensated through calculation. Bow is given by the equation 3.35:

$$\mathrm{Bow} = \frac{1}{2}\left(d_2 - d_1 \right) \qquad 3.35$$

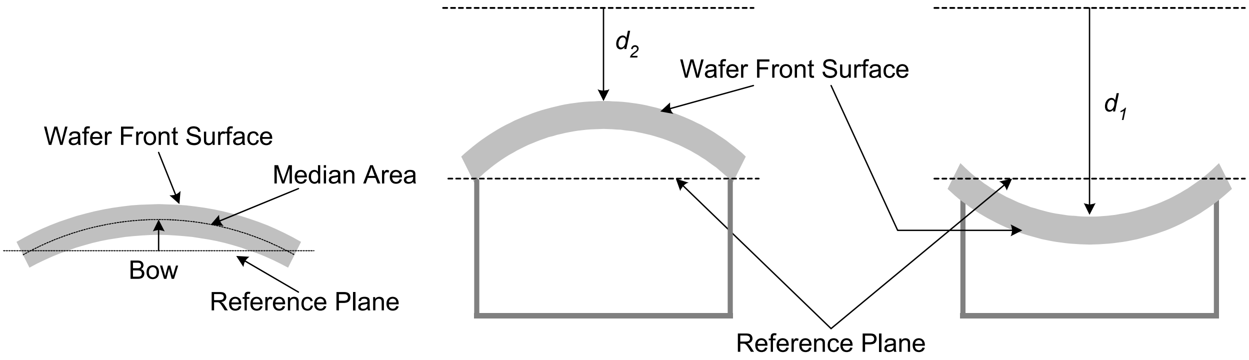
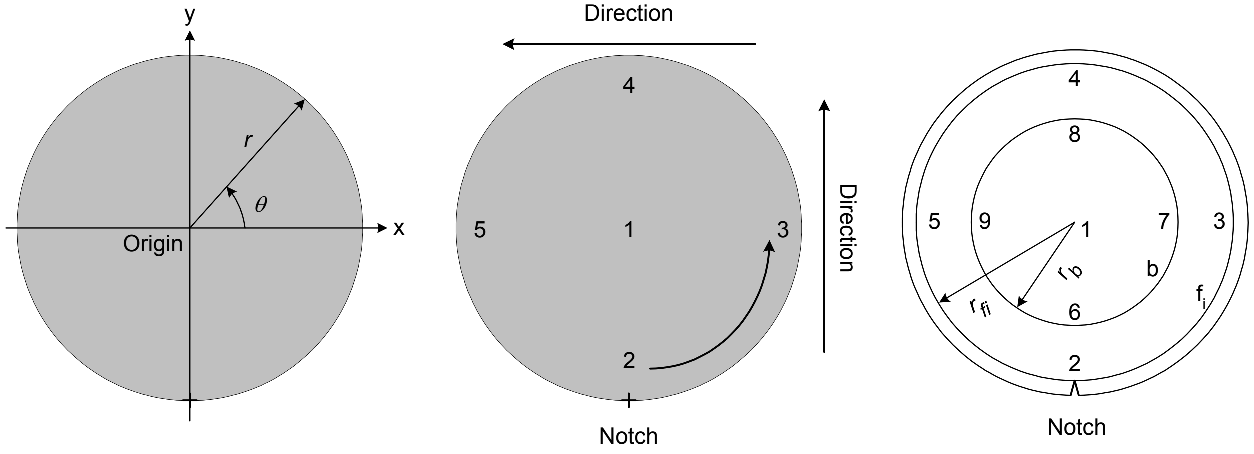


Figure 3.16: Definition of Bow [DIN 50441/2 1991]

3.2.3 Mapping of the geometrical indices to process control indices

In the studied CMP process machine setup, to suffice the customer specification, different process and machine parameters are controlled and adjusted during processing by means of either generating a new recipe or correcting the current one. In this section, the analysis of process control indices in correlation to the discussed geometrical indices is done (see section 3.2.1 and section 3.2.2). The process control indices are the machine and process parameters, which influence the wafer geometry by adjusting them directly. Figure 3.17 shows the geometrical dimensions and wafer orientation as used by the studied CMP machine. The notch on the wafer as defined in SEMI standards [SEMI M1 2002] is used for referencing and orientation of wafer during processing and metrology.



Wafer Coordinates

Reference Points on Wafer for Orientation

Points on Wafer Surface to Calculate Process Control Indices

Figure 3.17: Wafer coordinates orientation and points on wafer surface to calculate process control indices [WSAG 1997-2003]

Polar coordinate system (r, θ, z) or Cartesian coordinate system (x, y, z) [SEMI M20 1998] depending upon the customer specification is the basis to specify data points on the wafer surface. The positions 1, 2, 3, 4 and 5 are the reference points on the wafer surface (figure 3.17). Where the reference position 1 is always at the center (origin figure 3.17) of the wafer, reference positions 2 and 4 are on y-axis whereby reference position 2 is at the notch and reference positions 3 and 5 are counter clockwise on the x-axis of the wafer respectively. The reference positions 2-4 on the wafer are traversed along the y-axis and reference 3-5 along the x-axis. The reference positions 2-4 and 3-5 are defined as traversing directions to define linear and nonlinear polishing indices. r_b and r_{fi} (figure 3.17) are the radii of the measuring data points on the measuring circles b and f_i, which builds the basis to calculate the process control indices.

- **Linear Taper: LT2-4 / LT3-5**

The commonly used process control indices for the linear taper on the y-axis are LT2-4 and on the x-axis LT3-5. Figure 3.18 shows the linear taper (GBIR), which is the difference of the thickness at reference position 2 and 4 in vertical direction or between reference positions 3 and 5 in horizontal direction on the wafer surface. For orientation, calculation and corrective actions the exact position of notch plays a very significant role. In the studied CMP machine, the notches of the wafers during wafer mounting process is directed away from the center of the carrier plate and is placed on the radial axis of the carrier plate.

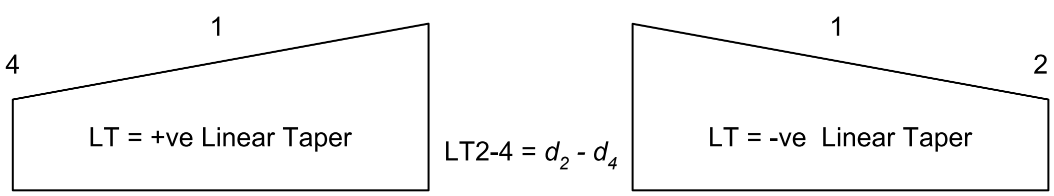


Figure 3.18: Process control indices linear taper LT2-4 [WSAG 1997-2003]

The calculation of linear taper is given by the equations:

$$\text{LT}2-4=\frac{thk_{f2}-thk_{f4}}{r_{f2}-r_{f4}}SF \qquad 3.36$$

$$\text{LT}3-5=\frac{thk_{f3}-thk_{f5}}{r_{f3}-r_{f5}}SF \qquad 3.37$$

Where thk_{fi} and r_{fi} are the measured thickness and radius at the position i (approximately 64000 data points on 200 mm wafer surface are measured), *SF* is the scaling factor in mm. These indices are directly correlated to Global flatness and Site flatness as described in sections 3.2.1.1, 3.2.1.2, as the corresponding measured points on the wafer surface build the basis of calculations of Global and Site flatness. Changing the process parameters as shown in the figures 3.19, 3.20, 3.21 and 3.22 influences the positive linear taper and the negative linear taper.

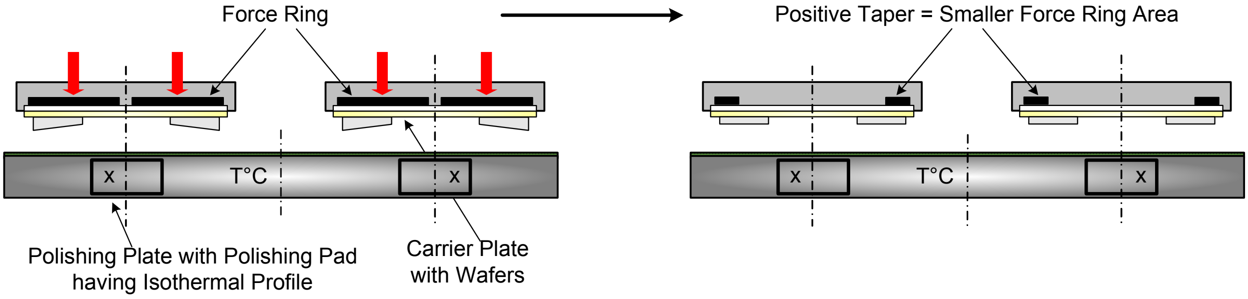


Figure 3.19: Force ring influence on positive taper [WSAG 1997-2003]

The applied force distribution through force rings on the carrier plate is used to bend the carrier plate to influence the linear taper accordingly. The smaller force ring area influences the positive linear taper (figure 3.19) during the material removal and the broader force ring area influences the negative taper (figure 3.20).

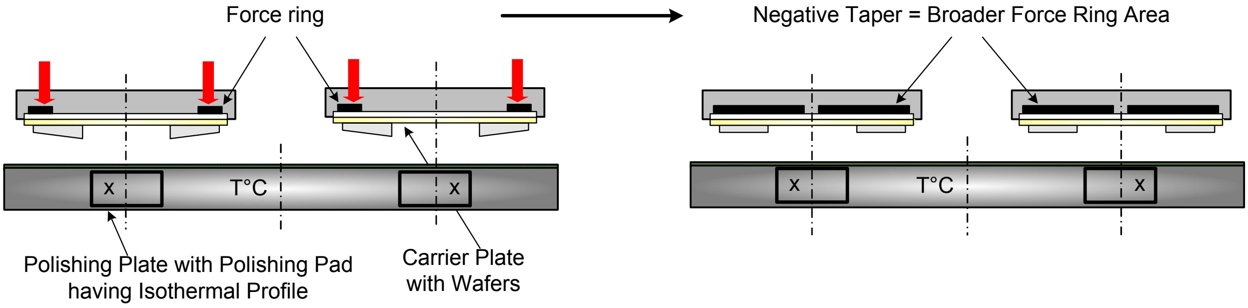


Figure 3.20: Force ring influence on negative taper [WSAG 1997-2003]

If the force distribution is kept constant increasing or decreasing the polishing plate temperature, which enhances the chemical reaction rate accordingly, also influences these tapers. By decreasing, the temperature of isothermal lines passing through "x" on the polishing plate the positive taper is influenced (figure 3.21).

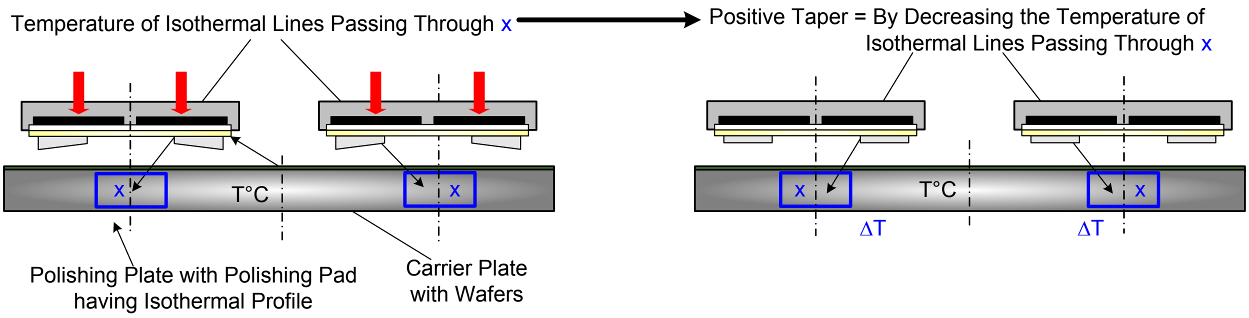


Figure 3.21: Influence of polishing plate temperature on positive taper [WSAG 1997-2003]

If the temperature of isothermal lines passing through "x" on the polishing plate is increased, (i.e. there is an increase in chemical reaction rate) the negative taper (figure 3.22) is influenced, because the material removal rate at reference position 4 increases.

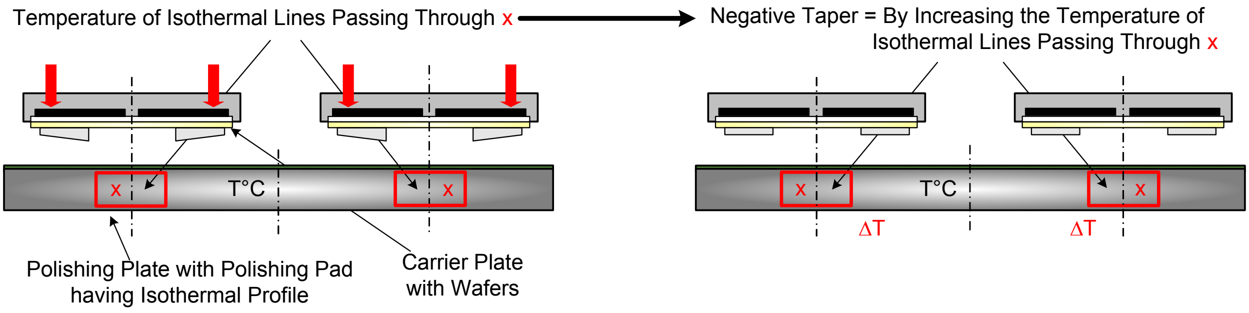


Figure 3.22: Influence of polishing plate temperature on negative taper [WSAG 1997-2003]

The process control index linear taper LT2-4 provides the information about the influencing process and machine parameters like polishing pad characteristics, carrier plate characteristics and polishing plate characteristics. The process control index LT3-5 provides the information about slurry characteristics and the relative velocity between the polishing plate and the carrier plates.

- **Nonlinear Taper NLT2-4 / NLT3-5 and Roll-off (E2, E3, E4 and E5)**

The non-linearity (GFLR) on the wafer surface is the peak to valley variations [SEMI M40 2000] between different points. To calculate the non-linearity, at least three points on the wafer surface are required. One of them is the height deviation from the mean at the center of the wafer. The non-linearity is either positive (convex) or negative (concave) depending upon the height variation with respect to the height measured at the center. Non-linearity is caused due to CMP process machine kinematics or due to lack of slurry between wafer and pad.

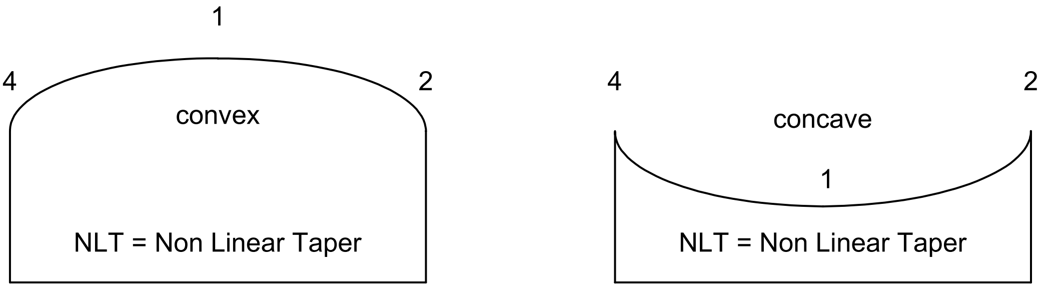


Figure 3.23: Process control indices for nonlinear taper NLT2-4 [WSAG 1997-2003]

The wafer non-linearity (figure 3.23) is given by:

$$\mathrm{NLT2-4} = \frac{thk_{f2} + thk_{f4}}{2} - thk_{center} \quad 3.38$$

$$\mathrm{NLT3-5} = \frac{thk_{f3} + thk_{f5}}{2} - thk_{center} \quad 3.39$$

Where thk_{fi} is the measured thickness at the position *i,* and thk_{center} is the thickness of the wafer at its center (origin figure 3.17).

The Roll-off is the non-linear height variation of the wafer surface (i.e. the convex profile near wafer periphery, figure 3.24) and is given by the equation 3.40. Figure 3.23 shows a wafer Roll-off at the wafer edge. This defect can propagate from the edge towards the center of the wafer. The process control indices at the reference positions 2, 3, 4 and 5 are E-2, E-3, E-4 and E-5, which can be regulated by the process parameters respectively.

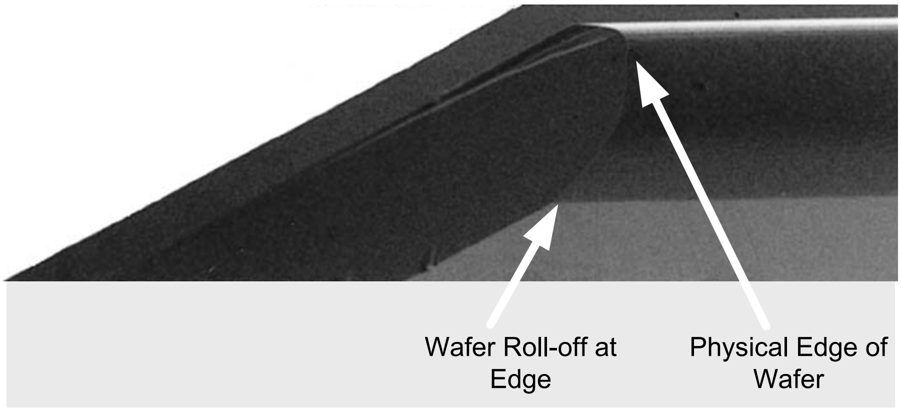


Figure 3.24: Wafer Roll Off at the edge [Kimura 1999]

$$\mathrm{E_i} = \frac{\left(FPD_{fi} - FPD_{bi}\right)}{r_{fi} - r_b} NF \text{ ; for } i = 2 \ldots 5 \quad 3.40$$

Where FPD_{fi} is the measured focal plane deviation on the edge of either of the reference positions 2, 3, 4, 5 and FPD_{bi} is the corresponding focal plane deviation away from the center of FPD_{fi}. The r_{fi} and r_b are the corresponding radial distances from the center of the wafer where the measured points lie. The distance between the two points depends upon the minimum ring spacing distance (here 7.5 mm) of the metrology tool, the norm factor (*NF*) for this tool is 15. When the material removal rate at the edge region of reference position 2 (i.e. E-2) and in region NLT2-4 is high, then the wafer gets a typical nonlinear defect in the 2-4 direction. This defect can be regulated by abrading the polishing pad (figure 3.25) with a special grinding mechanism. The grinding mechanism can also be used to grind inside or outside of the polishing plate by varying the pressure and the process time.

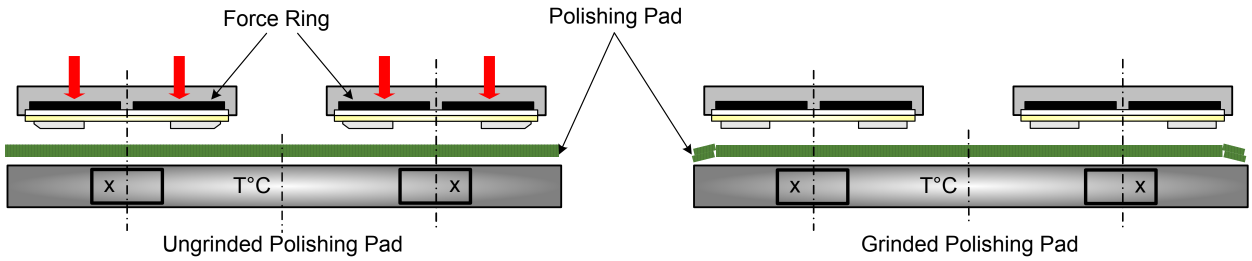


Figure 3.25: Polishing pad correction for E-2 in the reference position 2 region and NLT2-4 defects [WSAG 1997-2003]

The process control indices LT2-4, NLT2-4, E-2 and E-4 provide the information about:

1. Pad characteristics (LT2-4)
2. Pad correction (E-2, NLT2-4)
3. Polishing plate characteristics (LT2-4, NLT2-4, E-2, E-4)
4. Pressure cylinder characteristics (LT2-4, NLT2-4, E-2, E-4)
5. Carrier plate characteristics (LT2-4, NLT2-4)
6. Slurry characteristics (LT3-5, NLT2-4, NLT3-5, E-2, E-3, E-4, E-5)
7. Angular velocities of the polishing plate and carrier plates (LT3-5, NLT3-5, E-3, E-5)

The linear and non-linear process control indices are influenced by the same process characteristics and machine characteristics. These indices provide the information about GBIR (Total Thickness Variation TTV) and GFLR (Total Indicator Reading TIR) geometrical indices respectively. The geometrical indices are calculated by evaluating all the 64000 measured data points and from the generated height maps showing isolines. The height maps are further analyzed by examining the peak to valley variations, height variations and focal plane deviations globally and locally (per Site). The process control indices give then the feed back information to process controller to regulate and adjust the process and machine parameters for the next process run.

3.2.4 Defect classes

The geometrical indices and process control indices build the basis to regulate and control the CMP process, but still during the CMP process, the process and machine parameter drifts and cause the undesired defects. In this section, the typical defects generated during CMP process for wafer fabrication are classified and depicted. The defects here are geometrical deviations from the required specification and caused due to the irregularities of process and machine parameters. The most probable correlation to the process and machine parameters of these defects are discussed in section 3.3. Every wafer after CMP process is measured in the production environment and its quality is checked against the specified geometrical indices. Following figures are the height maps showing the isolines, i.e. the elevations and crater or peaks and the valleys on the wafer surface as measured by the special metrology machine for this purpose. Table 3.3 contains the measured values (i.e. GBIR, GFLR, GFLD, center thickness, maximum wafer thickness, minimum wafer thickness and the distance of all isoline values measured in µm) and the corresponding figure number.

Figure Nr.	GBIR [µm]	GFLR [µm]	GFLD [µm]	Center Thickness [µm]	Max. Wafer Thickness [µm]	Min. Wafer Thickness [µm]	Line Distance [µm]
3.26	1.35	1.46	-0.98	728.41	728.89	727.55	0.05
3.27	3.08	2.22	-1.53	727.30	728.51	725.43	0.05
3.28	3.85	3.66	-2.96	726.92	727.67	723.81	0.05
3.29	1.74	1.67	-1.04	726.58	727.08	725.34	0.05
3.30	3.69	1.03	0.62	695.67	697.20	694.51	0.05
3.31	4.49	0.91	0.66	723.73	726.19	721.70	0.05
3.32	1.67	1.32	-0.79	725.64	726.36	724.69	0.05

Table 3.3: Measured values of corresponding figures [WSAG 1997-2003]

- **Water drop and particle in wax layer**

In figure 3.26 the typical defects, "a" water drop in the wax layer and "b" a particle in the wax layer, observed during CMP processing are due to the presence of water drops or due to a contaminated wax layer (figure 3.26 "a" and "b") causing small depressions on the wafer surface. Examining the isolines in the height map shows these defects can be classified to the global flatness (global geometry) defect class and to the site flatness defect classes, (local geometry) see also table 3.3 row "Figure Nr. 3.26". These defects are specified by the deviations of the geometrical indices from the required customer specifications. The defect "c" in the figure 3.26 is a typical Roll-off at notch (E-2) near the edge of the reference position 2, assigned to E-x defect class, where x = 2,3,4 or 5.

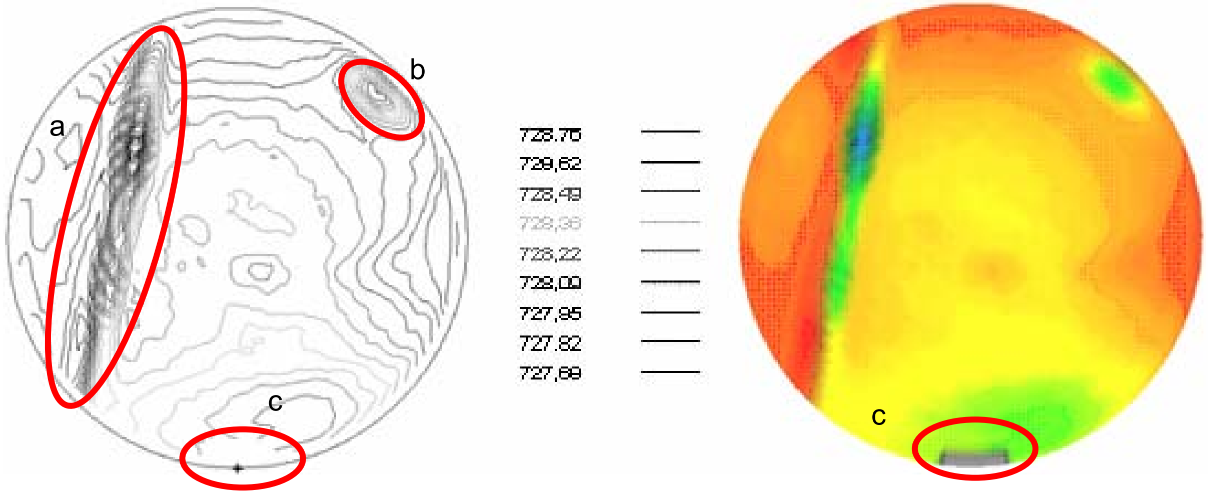


Figure 3.26: Defect "a" is a water drop in the wax layer, defect "b" is due to a particle in the wax layer and defect "c" is a typical Roll Off at notch [WSAG 1997-2003]

In figure 3.27, "d" shows a particle in the wax layer causing a small depression of wafer surface in the region of reference position 4 and the global and local geometry defects, see Table 3.3 row "Figure Nr. 3.27". These defects are classified according to SEMI standards, as dimples (shallow depression on wafer surface) or as pits (depression of wafer surface with steeper slopes) [SEMATECH 1995, SEMI M52 2002]. The dimples and pits are deviations of local geometrical indices.

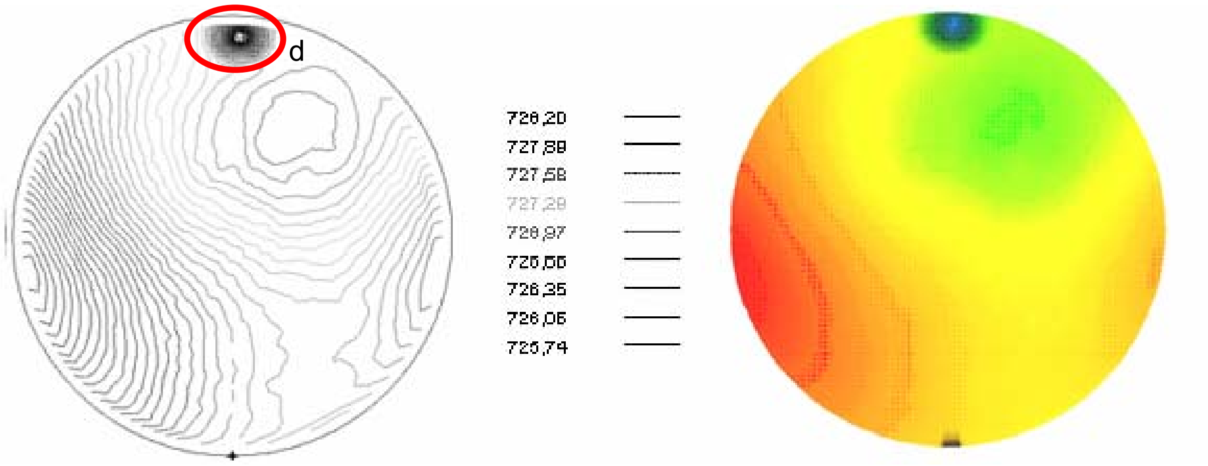


Figure 3.27: Particle in wax layer and geometry defects [WSAG 1997-2003]

- **Air trapped between mounted wafer and the wax layer**

In figure 3.28, "e" shows depression in wafer surface caused by air trapped between the mounted wafer and the wax layer on the carrier plate during pressing. The air gets trapped as during the pressing process an air cushion builds between the wafer and the carrier plate, due to the applied pressure. The pressing is required to accomplish the corresponding adhesive forces to hold the wafer firmly during polishing. This defect occurs, when the wafer sticks firmly at the edge first and then due to the pressure distribution the air gets trapped between the two surfaces. This defect class according to [SEMI M52 2002] can be a dimple or a pit depending upon the measured local geometrical indices.

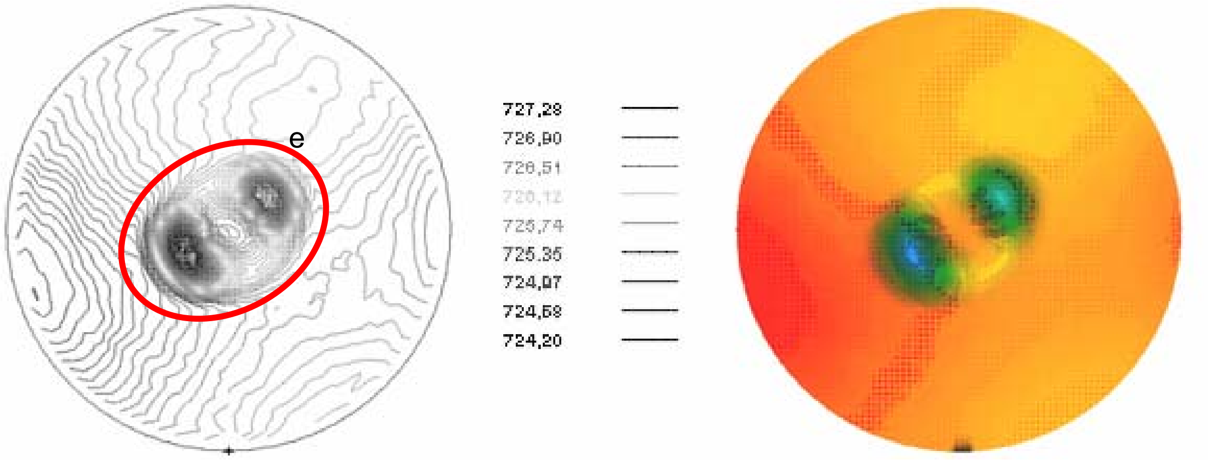


Figure 3.28: Air trapped in between the mounted wafer and the wax layer on the carrier plate [WSAG 1997-2003]

- **Electro Static Charge defect**

In figure 3.29, "f" shows the defect caused by electrostatic charging of wafer surface. The suspended abrasives and the immersed wafer in the slurry get charged by adsorbing ions from the slurry. The equal and opposite diffused charge density in the slurry balances the compact charge density on the wafer surface. Total charge density on wafer surface and in the slurry must be equal and opposite in sign. The compact charges move along with the wafer and diffused charges along with the slurry resulting in electro kinetic potential or zeta potential, which is regulated by the pH value of slurry and should be zero during CMP process (see also section 3.1.3). If the zeta potential value is not zero it means that, the slurry pH value has changed resulting in electrostatic charging of the wafer and causing the non-linear defect in the 2-4 direction NLT2-4 and is classified as Non Linear Taper defect class.

In figure 3.29 "g" shows defect caused by trapped air during pressing and in figure 3.29 "h" shows Roll-off at notch. Table 3.3 row "Figure Nr 3.29" shows the global and local geometrical indices deviations indicating non-linear defects.

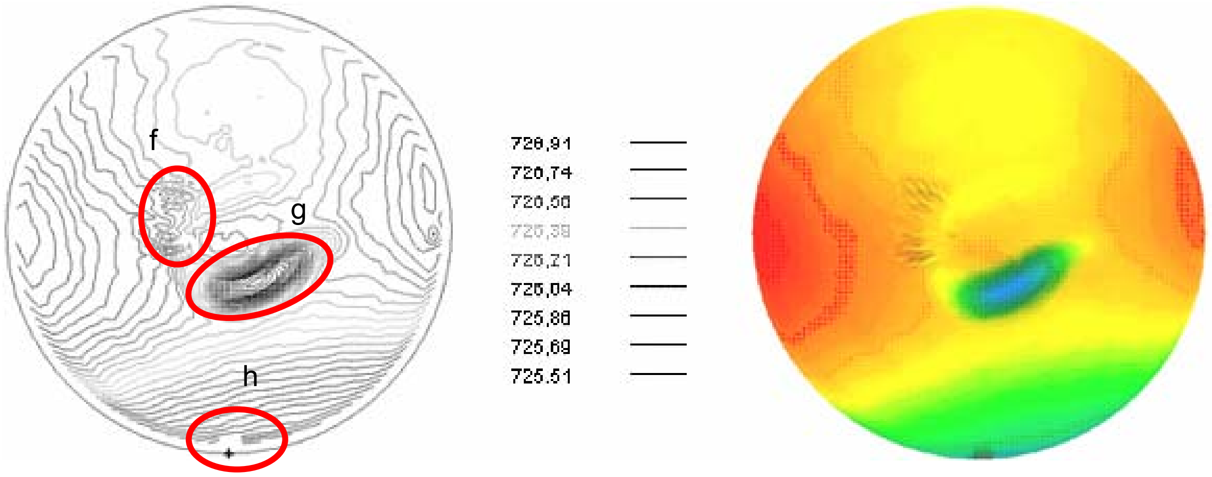


Figure 3.29: Electrostatic charging of wafer "f"; "g" is the air trapped between the mounted wafer and the wax layer on the carrier plate and "h" is a typical Roll-off at notch [WSAG 1997-2003]

- **Linear taper LT2-4 and Dimple**

Figure 3.30, 3.31 and the Table 3.3 rows “Figure Nr 3.30, Figure Nr 3.31” show the typical positive linear taper LT2-4 (GBIR) in the reference direction 2-4, and are classified as Linear Taper defect class. In figure 3.30 "i" is classified as dimple defect [SEMI M52 2002]. The process control index LT2-4 depends upon the polishing pad state (pad life cycle), CMP process machine down time (duration), the geometrical characteristics of carrier plate (carrier plate profile) and the temperature profile of polishing plate. Any change in these characteristics can cause this defect class.

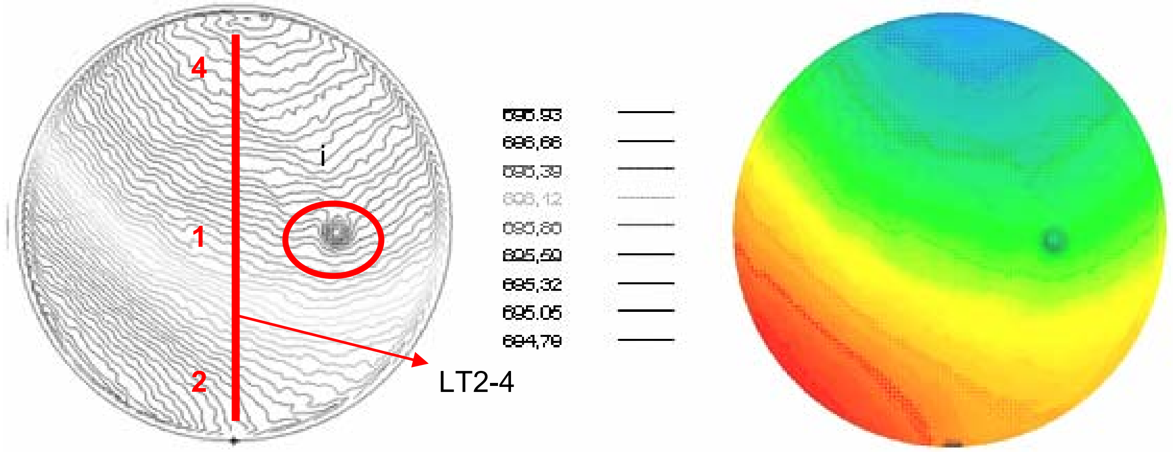


Figure 3.30: Linear taper LT2-4 and "i" is a small dimple [WSAG 1997-2003]

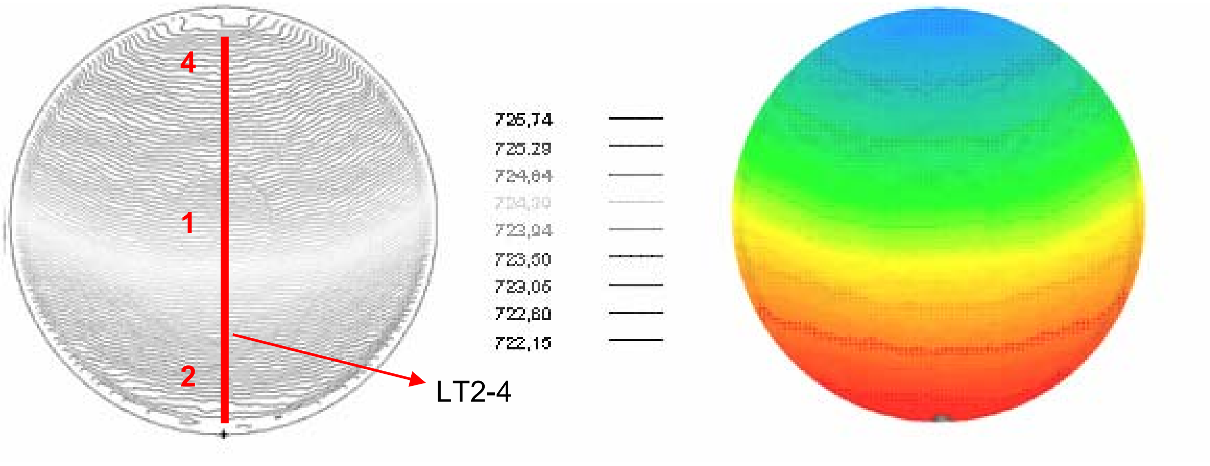


Figure 3.31: Linear Taper LT2-4 [WSAG 1997-2003]

- **Non Linear taper NLT3-5 and Edge defect**

Figure 3.32 and Table 3.3 row "Figure Nr 3.32" shows the typical non linear taper NLT3-5 (GFLR) in the reference direction 3-5. This index depends upon the relative angular velocities of carrier plates and polishing plate or on the slurry characteristics (amount, flow rate).

In figure 3.32, "j" is a typical edge defect, see chapter 2, section 2.2.1. It belongs to non-linear defect class and is caused by high material removal rate at the edges. The responsible parameters for this defect are polishing pressure, high relative velocity between polishing plate and carrier plate, and high temperature. In the next section the process and machine parameters, which influence the wafer surface geometry, are analyzed.

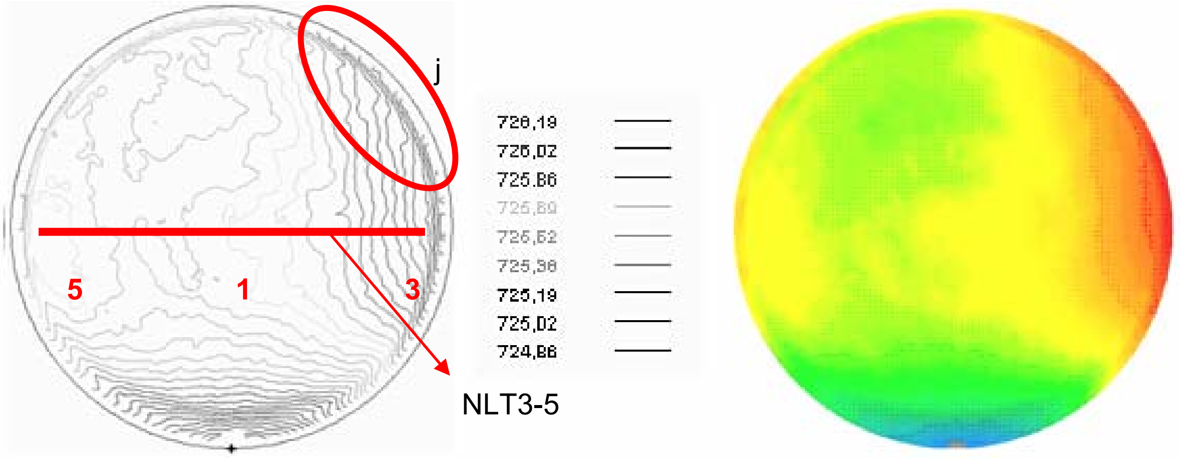


Figure 3.32: Nonlinear taper NLT3-5 and edge defect [WSAG 1997-2003]

3.3 Process and machine parameters analysis and their correlation to wafer geometry defects

The quality of the CMP process as discussed in section 3.1 depends upon the dynamic characteristics, behavior and control of the parameters (figure 3.33) involved. During the CMP process, all involved parameters are in dynamical equilibrium and any shift or drift of these parameters influence the process characteristics and thus its control.

The chemical or mechanical interaction of the process parameters during processing is difficult to determine. As discussed in section 3.1, it appears that certain parameters have only mechanical interaction and others only chemical interaction during polishing. However, in reality it is very difficult to differentiate their influence on the CMP process. For example, the removal rate according to Preston's equation 3.1 is directly proportional to the pressure and velocity. Both parameters at first sight can be treated as interacting mechanically during the CMP process. By changing these affects the slurry flow across the wafer thus influencing the film thickness between the wafer and the pad. Slurry transport and film thickness further influence the diffusion of chemical reactants and products to and away from wafer, which further affects the chemical reaction rates and finally the removal rate. It shows that pressure and velocity influence both mechanical and chemical interactions.

The process and machine parameter interdependencies and their dynamical interaction among themselves makes it very difficult to correlate the geometrical deviations, experienced during CMP process on the wafer surface to the corresponding process and machine parameters. Figure 3.33 shows in general different process and machine parameters, which influence the quality of the CMP process. A particular parameter, e.g. slurry flow rate influences the CMP process. The flow rate depends upon the slurry properties such as viscosity, which further depends upon the concentration of the suspension. The suspension concentration depends upon the concentration of abrasives, reactants, oxidizers. On the other hand, slurry flow rate in combination with polishing pressure and relative velocity influences the removal rate. The removal rate characteristics over the whole wafer surface area are determined by the geometrical distinctiveness of the wafer surface. However, after the geometrical measurement surface depression on the wafer was found. This can have many causes e.g. slurry flow rate, polishing pressure, relative velocity or due to the slurry properties in combination with pressure and relative velocity or due to an abrasive particle in the slurry, which slipped through point of use filtration of slurry or the surface depression can have another cause. The fact is that there are so many interdependencies of parameters among themselves and dynamical interactions between them, so it becomes very difficult to find the exact cause of a particular geometrical deviation.

The quality of the CMP process is judged by the geometrical measurements made after process, therefore this section deals with the process and machine parameters (figure 3.33), which influence directly or indirectly the wafer geometry in the production environment and their correlation to the most probable wafer geometry defect classes. The correlation to the corresponding defect classes is based on the expert knowledge and experience of process engineers in the production environment of the studied CMP process machine. At first the parameters during the Wafer mounting process and then during Wafer polishing process are discussed.

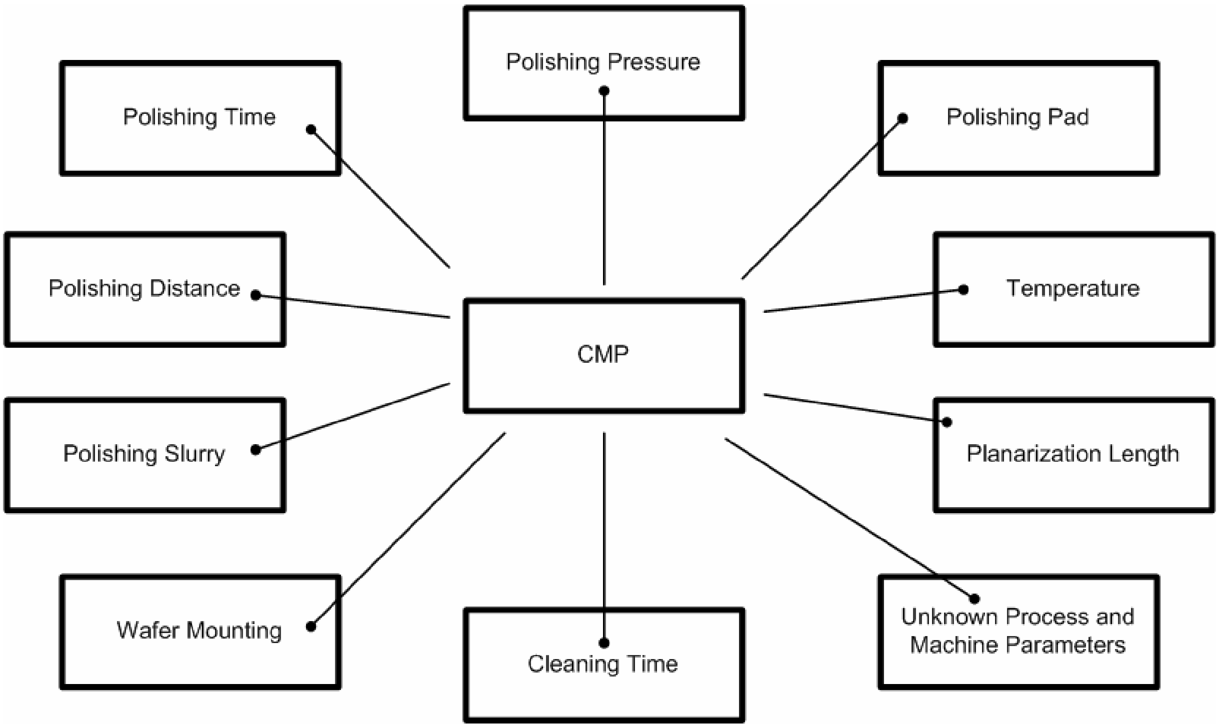


Figure 3.33: Process and Machine parameters in general

3.3.1 Correlation and influence of process and machine parameters during wafer mounting process

The theoretical aspects of wafer mounting process section 3.1.2 and the defect classes section 3.2.4 build here the basis of correlating process and machine parameters to the process index deviations or geometrical index deviations. The wafer mounting process requires a very clean process environment, which is strictly monitored regarding particle concentration. The wax coating mechanism and wafer pressing mechanism play a significant role in the defect origination. The main aim at the end of wafer mounting process is that all the mounted wafers should sit firmly on the carrier plate.

Table 3.4 shows the steps required during the mounting process. The expected results of the process step, i.e. the output parameters and the most probable parameters that influence the output parameters of this process step. It further shows the most probable correlation between the process step and the process control index or geometrical index deviations or the process deviations during this particular process step.

Mounting Process Steps	Output Parameters	Most Probable Influencing Parameters	Most Probable Correlations*
Carrier Plate Cleaning	Clean, tempered carrier plates	Buffer air temperature 35°C	Carrier plate too cold
	Carrier plate cleanliness	Brush cleaning characteristics, mechanical failure	Carrier plate stops moving in cleaning station
		Particle count	Pits, SFLR (STIR)
		DI water temperature 60°C	Carrier plate too cold
	Tenside supply	Tenside concentration too low or too high	Carrier plate sides are not clean or too many bubbles on carrier plate
		Tenside exchange after 900 cleaning cycles	
Wax Spin Coating	Thin wax film on the carrier plate	Wax properties	Wax nose, flow marks, imprints
	Homogenous wax coating	Wax amount	Wax backflow during cleaning
		Spinning speeds	Dimple, pit, SFLR (STIR)
		Spin duration	E-2, E-3, E-4, E-5
		Process environment	Blurred wafer
Carrier Plate Heating	Wax sticking zone temperature (65 to 75°C)	Temperature of heating stations	Breaking of carrier plate due to thermal shock
	Homogenous carrier plate and the wax film temperature	Mounting temperature 75 °C	Non uniform carrier plate temperature profile
		Carrier plate temperature profile	Wafer "swim"
	Heating time	Heating duration	Blurred wafer
		Gradual heating of carrier plate	Pits, SFLR (STIR)
		Particle count	Waviness, plane parallelism
		Air circulation rate underneath the carrier plates 2m/s	Wafer "swim", wafer breakage
Wafer Cleaning	Wafer cleanliness	Washing medium, washing mechanism	Wafer breakage
		Particle count, rolling shaft speed	Pits, SFLR (STIR)
		Wafer pre alignment functionality	
	Wafer placement on pick up pallet	Position, location	
		Orientation	
Wafer Pressing	Wafer placement on carrier plate	Pressure and temperature	Damaged wafer
		Exhaust pressure	Wafer "swim", dimple, edge defect
		Pressure distribution	Wafer breakage, center mark
		Pressing duration, time	Imprints
		Wafer location, orientation	
	Firm wafer fixing on the wax	Wafer deformity on the wax (convex or concave)	GBIR (TTV), LT2-4
		Placing unit adjustment, wafer lowering speed	Roll off, E-2, E-3, E-4, E-5, SFLR (STIR)
		Taper and roll off parameters	Plane parallelism
		Membrane temperature 80°C	
		Membrane cleanliness	
Carrier Plate Cooling along with Mounted Wafers	Solid wax film	Gradual temperature drop of carrier plates aprox. 30-40 °C	Carrier plate breakage
		Cooling duration	
		Air circulation temperature and air flow	
Carrier Plate Front Side Cleaning along with Mounted Wafers	No wax remains on the carrier plates	Air pressure for wax removal	Wax remains
	Drying of carrier plate	Water flow for wax removal (two water jets)	SFLR (STIR)
	Roughness	Measured: 5 µm-polishing lot, 1.2 µm - carrier plate	
	Convexity	Carrier plate profile geometry	

* = The most probable correlations between the process step and the process control index deviations, geometrical index deviations, or individual process step deviations

Table 3.4: Process and machine parameters, which influence the wafer geometry during wafer mounting process

3.3.2 Correlation and influence of process and machine parameters during wafer polishing process

The theoretical aspects of wafer polishing process section 3.1.3 provides the process and machine parameters affecting the wafer surface quality during CMP process and the sections 3.2.1, 3.2.3 and 3.2.4 provide the geometrical indices, process control indices and the corresponding defect classes respectively.

Table 3.5 shows the different parts of studied CMP process machine (e.g. polishing plate, polishing pad, etc.), which are actively involved during polishing. The target or output parameters of these parts are to be regulated during polishing. The table 3.5 further shows the parameters that most probably influence the output parameters and the most probable correlations between the parameters of the CMP process machine parts and the process control index or the geometrical index deviations.

In the production environment, the parameter values are calculated before every process run. These parameter values, grouped together in a recipe structure, are downloaded to the CMP process machine. The evaluation of parameter values in the recipe is done based upon the deviation of the process control indices calculated after the wafer surface geometry measurements. The values of certain interdependent parameters in the recipe structure are calculated using special control algorithms, which are developed by the process engineers based on the experimental results and their process experience.

Some of the parameters depend upon the earlier process runs, such as polishing pad characteristics depends upon its life cycle (i.e. number of polishing cycles this particular pad has undergone). This parameter affects CMP process quality directly, as with the time the polishing pad starts loosing its material removal characteristics due to plastic deformation, resulting in its replacement. The parameters responsible for plastic deformation are for example applied polishing pressure, relative velocities, polishing pad thickness, therefore, for the calculation of polishing pressure and relative velocities the current pad state plays a very important role. The main aim here is to optimize the calculation so that the polishing pad can be used for a longer time, as polishing pad replacement reduces the wafer production time and thus the yield.

It is very difficult to predict and to correlate exactly the process control index deviation to a particular parameter, as a particular parameter affects the CMP process not individually but in combination with other process and machine parameters. The process engineers having long-term high volume wafer manufacturing experience can only make the correlations and predictions of CMP process dynamics, chemical and mechanical behavior of the parameters. The correlation between parameters and defects in table 3.5 is a combination of expert knowledge of process engineers, their CMP process experience and experimental results.

Polishing Machine	Output Parameters	Most Probable Influencing Parameters	Most Probable Correlations*
Polishing Plate	Polishing rate uniformity	Temperature	+LT2-4, -LT2-4, GBIR (TTV)
	12 µm material removal	Isotherms	+LT2-4, -LT2-4, GBIR (TTV)
	Geometrical shape	Pressure (force rings)	Micro scratches
	Chemical reaction rate	Pressure (cylinder)	Central thickness, removal rate
	Atom to atom removal rate	Polishing time and steps	Removal rate
		Rotation speed (platen)	LT 2-4, GFLR (TIR), SFLR
		Rotation speed (cylinder)	LT 3-5+, LT 3-5 -
		Wafer shape	NLT 2-4, NLT3-5, SFLR
		Slurry flow rate	LT2-4, GFLR (TIR)
		Isoelectric point (slurry pH) zeta potential	LT2-4, GFLR (TIR)
		Abrasive (size, cocentration, shape)	Micro scratches
		OH-ions concentration	Chemical removal rate, LT2-4, GFLR (TIR)
		DI water	E-2
		Carrier plate geometry	NLT 2-4, NLT3-5, SFLR
		Pad exchange	Pad damage
		Pad correction	E-2, NLT2-4
		Downtime	LT2-4, GBIR (TTV)
Polishing Pad	Stock removal rate	Porosity (pore diameter)	Removal rate
		Fibre structure	Pad damage
		Chemical durability	Grooves
		Chemical resistivity	Pad damage
		Slurry transportation	SFLR, NLT3-5,NLT2-4
		Surface roughness	GBIR (TTV)
		Thickness and texture	Pad deformation, GBIR (TTV)
		Specific gravity	Downtime
		Compressibility	LLS (LPD), edge defect
		Hardness (elasticity, viscoelasticity)	E-2, NLT2-4, edge defect
		Life cycle	
		Perforation and groove patterns	
		Conditioning	
Pad Cleaning Unit	Pad correction	Grinding medium	Pad damage
	Pad cleaning	Grinding angles	E-2, scratches
		Outer edge deformation	E-2
		Duration	Pit, SFLR(STIR)
		Controlling the brushes	
Cylinder Head	Stock removal	Pressure (force rings)	LT2-4
	Ellipsoidal path	Pressure (cylinder)	Central thickness
	Security of carrier plates	Oscillation	LT2-4, GFLR (TIR)
		Distance	Standard thickness
		Vacuum	
Loading Station	To keep wafer wet	DI water bath	LPD
Hydrophilization	To keep wafer wet	Hydrophilisation suspension, water coating	Hydrophobie
	Hydrophilation	DI-failure	

* = The most probable correlations between the polishing components and the process control index deviations, geometrical index deviations, or the deviations of individual polishing components

Table 3.5: Influence of the process and machine parameters on the wafer geometry during wafer polishing process

3.4 Problem domain analysis

The quickly changing trends towards smaller structures, as in the case of microprocessors, demand very high wafer surface planarity and uniform wafer surface topography [ITRS 2002, TIN 2002, TIN 2003]. The flatness control for these devices requires the measuring of topographical deviations in nanometers. To accomplish the specified wafer geometry with very tight tolerances and very high throughput, a very high degree of automation grade and flexibility of CMP process machine is required. The CMP process automation controller of the studied CMP process machine [WSAG 1997-2003] satisfies these requirements. Therefore, the in-situ diagnostic system for defect analysis should not intervene in the activities of CMP process automation controller. On the other hand, it should also have a very high availability to support the CMP process automation controller and CMP process expertise during defect analysis.

The mechanical and chemical aspects of CMP process discussed in section 3.1 show the complexity of the CMP process (number of process and machine parameters influencing the CMP process) and the qualitative claim (i.e. minimization of wafer surface geometry deviations) on the CMP process from the IC manufacturing industry. The analysis in section 3.1 showed that the CMP process is in a continuous state of dynamical equilibrium. Where the mechanical actions at polishing pad and wafer surface, chemical actions of slurry weakening the atomic or molecular layer of the wafer surface and the slurry particles along with the pad asperities responsible for the final removal of material from the wafer surface, are in dynamical balance. It is a great challenge to control CMP process, to achieve continuous state of dynamical equilibrium in the production environment (i.e. wafer fabrication 24 hours a day, seven days a week and 365 days a year). Any drift or shift in any of these activities during CMP process, away from the equilibrium point results in defect origination (section 3.2.4), which requires to be correlated with the geometry measurement results determined by ex-situ metrology. The surface quality of the wafer is an indication of the expected yield and the reliability of the CMP process. Every wafer, thus produced by the CMP process is measured and checked against the geometrical specifications (section 3.2.1). Any deviation of the geometrical indices, causing the deviation of process control indices (section 3.2.3) during the CMP process, leads to the origination of defects (section 3.2.4). These indices therefore, provide a basis for the CMP process automation controller to observe and influence the process and machine parameters, which can be correlated (section 3.3.1 table 3.4 and section 3.3.2 table 3.5) directly or indirectly to these indices. The most probable correlations between the geometrical deviations and the influencing process and machine parameters during CMP process require a long term and a thorough knowledge of this process.

The process and machine parameters involved during individual process steps and their correlation to the process control indices or geometrical indices show, that a particular deviation can have many probable process and machine parameters as originator of the deviation and thus complicating the determination of the exact source of its originator. The above-consolidated analysis builds the fundament of this work to optimize the process controller.

The studied CMP process machine has a yield of 96% and it produces 200000 wafers per month [WSAG 1997-2003]. Today the CMP process and CMP automation engineers are looking forward for potential optimizations to increase the yield from 96% to 100% and a target of manufacturing 250000 wafers per month. The CMP process engineers are experimenting in the laboratories to improve the polishing behavior of the CMP process machine in the production environment. The CMP process engineers are developing technologies to gather more and more information from the CMP process machine during polishing to understand and correlate the CMP behavior to the process and machine parameters.

The in-situ diagnostic system should be able to embed the knowledge of CMP process engineers and CMP automation engineers in the knowledge base and should save them effort required for defect correlation and localization. It should provide them the possibility to detect new causes and defect contributors and it should provide them the different correlation permutations and combinations for defect analysis.

Currently the process automation engineers are looking forward for new hardware (sensors and actuators) and software technologies to optimize the current configurations and to fulfill the requirements of the CMP process engineers and IC manufacturers [TIN 2003]. The time in which the improvements can be made, is very narrow as the overall effectiveness of the improvement should be cost-effective. The current software advances and results as discussed in chapter 2, section 2.3 show that efforts are being made to reduce the defect densities by observing, understanding and correlating the drifts of process and machine parameters. At the same time the wafer geometry tolerances are becoming tighter and the geometrical deviations, which were tolerated earlier are now treated as defects resulting in even more tighter surveillance of the process and machine parameters to catch the drifts as early as possible to control the defect origination and take corrective actions to avoid them. The machine and parameter values, which characterize the particular process step and the process environment, have to be investigated in the production environment. For this, it is necessary to examine not only the CMP process and CMP process machine information, but also the source of information generators. This is required to correlate the defect originators with the originating defects.

- **The information flow analysis during the CMP process**

The information flow (figure 3.34) generated by the studied CMP process machine [WSAG 1997-2003] for large volume wafer fabrication can be divided into following five functional groups:

1. CMP process as discussed in chapter 2, section 2.1.3, sections 3.1.2 and 3.1.3, and the mechanical construction
2. CMP process machine hardware parts such as sensors, actuators and PLC
3. Software for the automation and control of the hardware components
4. Ex-situ metrology and statistical process control software
5. CMP process automation controller software

The wafers after CMP process (functional group 1) are measured externally (functional group 4) immediately after the post CMP cleaning and the measured values per wafer are fed to the SPC software (functional group 4, quality control), which determines the trend of geometrical indices (sections 3.2.1, 3.2.2) and process control indices (section 3.2.3). These trends are one of the input information to the CMP process automation controller (functional group 5). The next set of input information, i.e. wafer mounting trace data and wafer polishing trace data (both the functional groups 2 and 3), see figure 3.34, are provided directly by the wafer mounting process and wafer polishing process respectively to the CMP process automation controller (functional group 5). The CMP process automation controller analyzes the input information based on the table 3.4 and table 3.5, as discussed in sections 3.3.1 and 3.3.2 respectively, along with the wafer specification. It generates a new mounting recipe and a new polishing recipe for the next process run (see chapter 2, section 2.3.1 and figure 2.7). The CMP process automation controller calculates a new process recipe before the start of every process run. It downloads the mounting recipe and the polishing recipe to the CMP process machine, which then starts the CMP process.

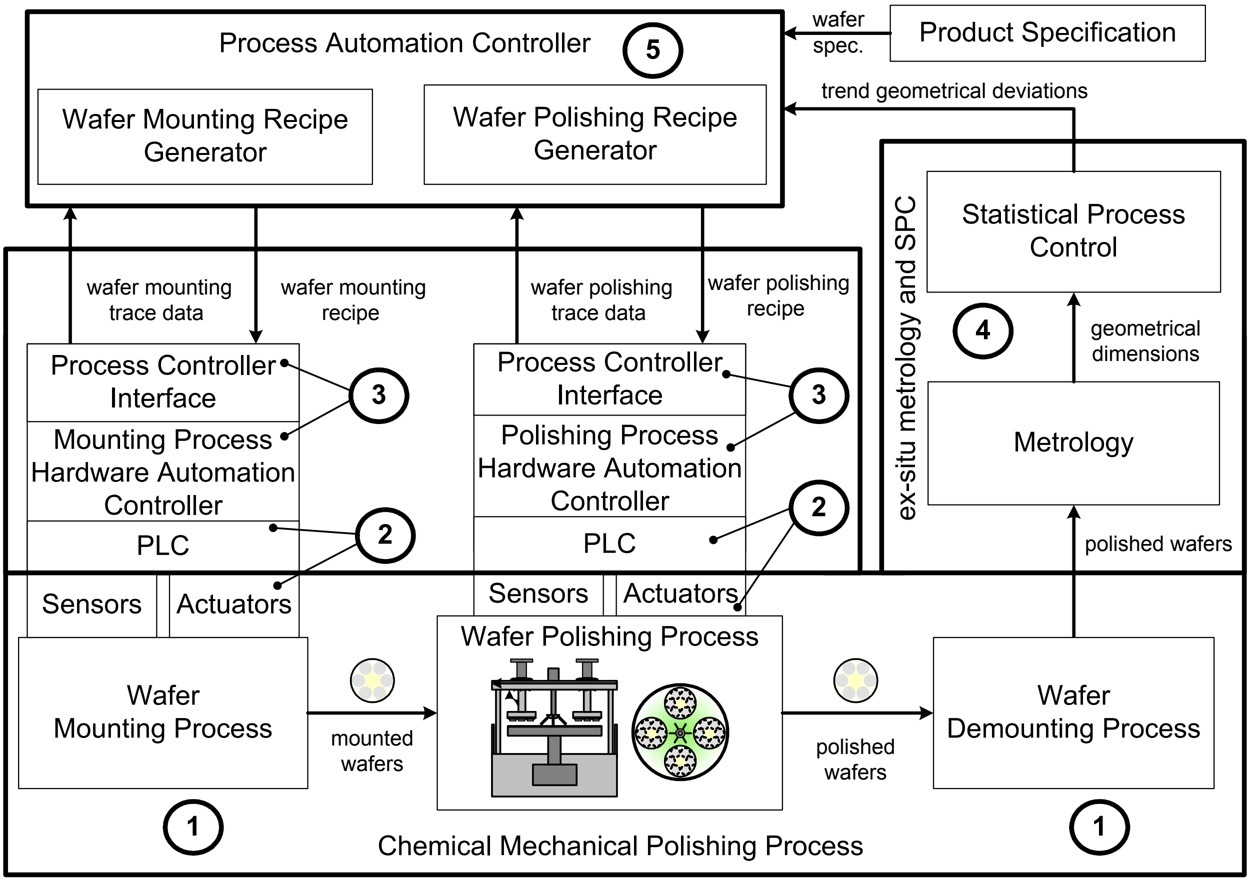


Figure 3.34: Functional groups1-5 of large volume wafer manufacturing CMP process machine

The diagnostic system requires the wafer mounting (section 3.1.2) and wafer polishing trace data (section 3.1.3) from the CMP process machine to diagnose the behavior of process and machine parameters during a particular process step. The diagnostic system requires the trace data, even if the CMP process machine is not processing, i.e. also during polishing pad renewal.

The diagnostic system requires the long-term different SPC trends of deviated geometrical indices, process control indices and the CMP process expertise knowledge to build the basis for diagnosing the most probable defect originator.

The diagnostic system should be able to represent the logic of defect origination as analyzed in section 3.2.4 based on the experience of CMP process expertise. It should provide mechanism to observe the latent defect contributors as the cause of a defect is not necessarily a particular observed process drift. It can also be a latent effect of an interdependent parameter (section 3.1.3), which comes suddenly to appearance and the reason for its occurrence has to be observed even more intensively. As discussed in section 3.1.3 the polishing pad characteristics changes depending upon the number of process runs it had undergone, the diagnostic system should adapt to the changing CMP process conditions and environment. This means that the diagnostic system should provide a mechanism to represent the time dependencies of CMP process and machine parameters to predict the time dependent origination of a particular defect.

The diagnostic system should be able to provide the mechanisms to integrate all known parameters to observe individually their behavior during a process run to correlate and interpret the interactions of these parameters. The diagnostic system should be able to model the strategies of most probable occurrences and appearances as described in section 3.3.1 table 3.4 and section 3.3.2 table 3.5, to use these strategies to recognize the non-trivial coherence among the defect originators and the CMP process and machine parameters.

The diagnostic system should provide a mechanism to classify (section 3.2.4) an observed occurrence, after waiting a certain number of repetitions of this occurrence, to correlate this with the parameters, which can be responsible for the origination of a new defect.

The diagnostic system should provide information about the observations, about the known causes of defects (section 3.2.4) and about other parameter drifts (section 3.3.1 table 3.4 and section 3.3.2 table 3.5), which are not directly related to this particular defect but occur whenever this defect occurs.

3.5 Summary

Chapter 3 shows the mechanical and chemical aspects of CMP process and machine parameters (section 3.1), their influence, interdependencies and role during the CMP process. Sections 3.2.1 and 3.2.2 show the geometrical aspects of the wafer surface flatness, which are specified by the IC manufacturers as product specification. The wafers thus, manufactured should be conform to these specifications. The deviations of these specifications lead to undesired wafer topographies and can be represented as defect classes (section 3.2.4). To control the geometrical deviations during CMP process for the studied CMP process machine, the corresponding process control indices (section 3.2.3) are analyzed and mapped to the geometrical indices (section 3.2.1). In section, 3.3 the CMP process and machine parameters, which influence the wafer geometry are analyzed and based on the knowledge of CMP process expertise the correlation of these parameters to wafer geometry defects is established (sections 3.3.1 and 3.3.2). The problem domain and the production environment in which the diagnostic system should be deployed is analyzed in section 3.4.

4 Requirement specifications on a diagnostic system for defect analysis

4.1 Requirements on a diagnostic system to analyze defects during CMP process

Based on the currently applied approaches to control CMP process (chapter 2, section 2.3), the theoretical analysis and the problem domain analysis, done in chapter 3, a diagnostic system for defect analysis for the CMP process and CMP process machine should satisfy following requirements.

- **Stability, availability** **R 1**

Due to a very high technical availability of the CMP process machine the deployed diagnostic system should have undergone a long-term availability and stability test according to the test specifications in the production environment. The diagnostic system should not intervene in the decisions of CMP process automation controller due to its high availability.

- **Machine downtime** **R 2**

It should provide drifts and shifts of the process and machine parameters during the CMP process machine downtime.

- **Adaptability to the changing process characteristics** **R 3**

The diagnostic system should adapt and acclimatize to the changing process environment. The CMP process machine with time adapts itself to the changing process characteristics during CMP process.

- **Model temporal information** **R 4**

The diagnostic system should explicitly adapt to the time representation and the property changes of process and machine parameters in this regard.

- **Cause detection** **R 5**

To diagnose the defects, it is becoming very important to detect the cause of the defects at a very early stage of the process to reduce the long CMP process machine downtime.

- **Reliability, expert's knowledge** **R 6**

The information flow, required for the reliability of diagnostic system and for the establishment of the correlation patterns during the CMP process, should be provided by the CMP process expertise in the production environment. This includes all the process steps and the machine parameters, which are required for the analysis to recognize the non-trivial coherence among the process steps and the related parameters that could be responsible for the origination of a defect.

- **Defect localization, classification and evaluation** **R 7**

The defect localization at a very early stage (i.e. the area, the type and the cause in all its details to avoid its occurrence), its classification, evaluation, and the decision of a reaction is required.

- **Performance** **R 8**

Faster detection of the defect sources is based upon the coordinate availability, defect classifications, defect patterns and the defect pictures (localization of defects).

- **In-situ diagnostic system** **R 9**

The detection of origination of defects and their classification should be done during the wafer manufacturing and the corresponding corrective actions should be taken in-situ to reduce the risk for the occurrence of defects during the wafer production.

- **Repetitive defect detection** **R 10**

Detection of repetitive defect sources to improve the process steps by reducing the influence of these sources in a particular process step.

- **Process and machine yield, throughput** **R 11**

It should determine and detect the trend of defect densities during CMP processing as early as possible to improve the process and machine yield by avoiding the origination of defects at a very early stage during CMP processing.

- **Test and applicability** **R 12**

The agent based diagnostic system should suffice the long-term tests, its applicability, and the practicability in the production environment and it should be checked against the above requirements.

4.2 Summary

The main objective of the research work is to develop an agent based diagnostic system for defect analysis during CMP process for the studied CMP process machine. The main aim of the research work is to:

1. Detect the origination of defects at a very early stage during the wafer manufacturing process
2. Reduce the defect densities
3. Reduce the unscheduled downtime of the CMP process machine
4. Improve the reliability and accuracy of the process run by in-situ observation of the CMP process
5. Provide the CMP process automation controller with information about the possible process drifts and shifts
6. Provide the corresponding corrective actions to the process engineer
7. Ask the process engineer to improve the process step characteristics by repetitive defect detection during a particular process step
8. Reduce the risk of defect occurrence
9. Adapt to the changing CMP processing characteristics and environment
10. Observe explicitly the changing properties of process and machine parameters with time

The agent concept supports here the requirement of not intervening in the decisions of CMP process automation controller and it operates independently.

5 Design and development of the agent based diagnostic system for defect analysis during CMP

5.1 Introduction

The consolidated findings, as discussed in chapters 2, 3 and 4, lead to the conclusion that the interaction dynamics of process and machine parameters during CMP process are very complex. Many physical models of the CMP process have been developed to understand and observe the chemical and mechanical behavior of this process in the laboratories, which builds the basis to make wafer-manufacturing process more robust. The step from the laboratory to wafer manufacturing is not very easy, as the behavior of process and machine parameters is different in production environment, compared to that under the laboratory conditions. For example, under the laboratory conditions two or three "perfect" wafers having no geometrical deviations can be produced. But when these conditions are transferred over to production environment, it is not practically possible to maintain the laboratory conditions, because the process and machine parameter characteristics changes with time. These changes are not only due to the wearing and tearing of machine parts, pad deformation, slurry and DI water contamination, blocked nozzles (slurry supply, wax dispensing), unplanned CMP process machine downtime, wafer crash, stochastic errors and operating errors. It is also due to the interactions among the known parameters and due to sudden influence of latent parameters, which were not observed under laboratory conditions. It is therefore necessary to develop a model describing the complete behavior of the CMP process at a particular time under production environment in coherence with the behavior of influencing process and machine parameters at that time.

In this chapter the complete design of agent based diagnostic system for defect analysis based on the requirements discussed in chapter 4, and the correlations between defect classes and process and machine parameters as discussed in chapter 3, is developed.

5.2 Model design basic approach

Chapter 3, section 3.1 describes the different physical models to understand the mechanical and chemical components of the CMP process. The only possibility to observe the studied CMP process machine and its periphery is to build an empirical model of its behavioral patterns [Wendt 1989]. The *behavioral pattern* of the CMP process machine is characterized by the information generated during a particular processing state (productive, standby, unscheduled downtime, scheduled downtime, non-scheduled time and engineering [SEMI E10 2001, SEMI E30 2003, SEMI E58 2001]):

$$\boldsymbol{BP}(t) = f(\boldsymbol{I}(t)) \qquad 5.1$$

Where $\boldsymbol{BP}(t)$ is the behavioral pattern characteristics of CMP processing machine during a particular processing state $t_{process\ state\ start} \le t \le t_{process\ state\ end}$ or a particular processing state transition $t_{state\ transition\ start} \le t \le t_{state\ transition\ end}$. $\boldsymbol{I}(t)$ represents the vector space of information characteristics generated by the CMP process machine (figure 5.1) during processing state or processing state transition. Where $I_1(t),\dots I_n(t)$ are the linearly independent vectors in the vector space $\boldsymbol{I}(t)$:

$$\boldsymbol{I}(t) = \{I_1(t),\dots,I_i(t),\dots I_n(t)\} \qquad 5.2$$

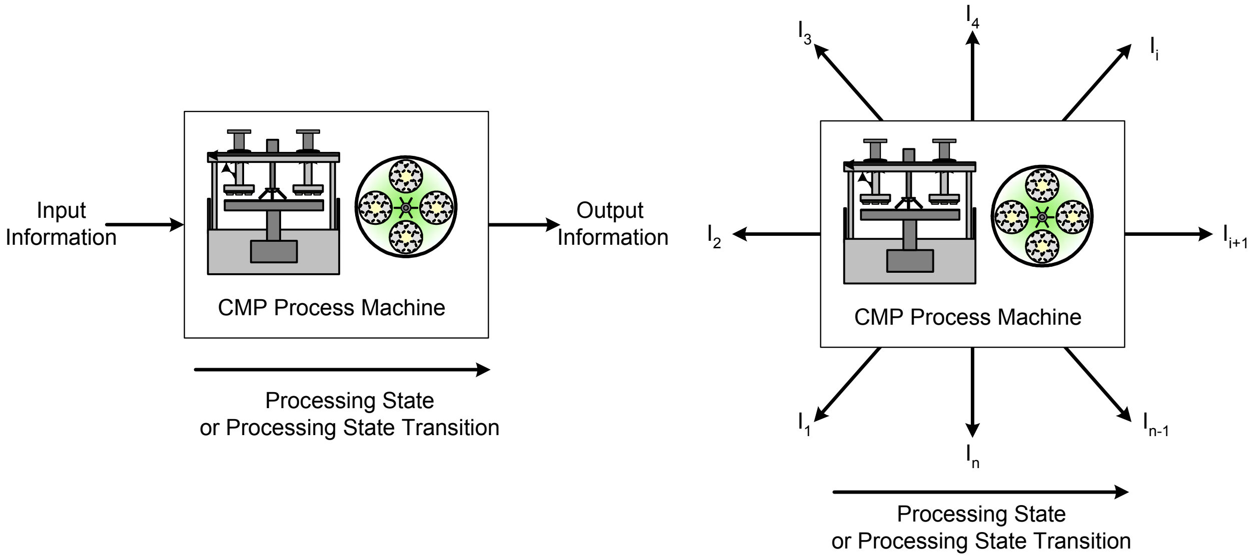


Figure 5.1: CMP process machine receives and generates information during a processing state or processing state transition

The *generated information* is the dynamical characteristics of process and machine parameters under observation during a particular time interval (i.e. duration of a processing state or processing state transition):

$$\boldsymbol{I}(t) = f(\boldsymbol{PT}(t), \boldsymbol{M}(t)) \tag{5.3}$$

$$\boldsymbol{PT}(t) = \{pt_1(t), \ldots, pt_i(t), \ldots pt_n(t)\} \tag{5.4}$$

$$\boldsymbol{M}(t) = \{m_1(t), \ldots, m_i(t), \ldots m_n(t)\} \tag{5.5}$$

Where $pt_i(t)$ and $m_i(t)$ are linearly independent vectors in the vector spaces $\boldsymbol{PT}(t)$ and $\boldsymbol{M}(t)$, respectively representing the dynamic characteristics of process and machine parameters during a particular processing state or processing state transition. The *dynamical characteristics* [Wendt 1989] ($pt_i(t)$, $m_i(t)$) of a particular process or machine parameter is the set of numerical values acquired periodically, i.e. sampled in a defined time interval (sampling rate [SEMI E5 2000]) or non-periodically (event triggered) during a processing state or a processing state transition:

$$pt_i(t) = \{pt_i(t_0), \ldots, pt_i(t_i), \ldots pt_i(t_n)\}; \quad t_0 \le t \le t_n \tag{5.6}$$

$$m_i(t) = \{m_i(t_0), \ldots, m_i(t_i), \ldots m_i(t_n)\}; \quad t_0 \le t \le t_n \tag{5.7}$$

Where t_0 is the start time, t_n is the end time and $\Delta t = t_n - t_0$ is the duration of a particular processing state or processing state transition. The *behavior* $\boldsymbol{B}(t_0)$ of the CMP process machine is a set of all observed process and machine parameter values at time t_0 and their correlation to the expected values during a processing state or processing state transition. It describes the functional coherence between the actual dynamical characteristics and the expected characteristics of the observed process and machine parameters (see chapter 3, sections 3.3.1 and 3.3.2):

$$\boldsymbol{B}(t_0) = f(\boldsymbol{PT}(t_0), \boldsymbol{M}(t_0)) \mapsto f(\boldsymbol{E}(t_0)) \tag{5.8}$$

The *expected characteristics* of process and machine parameters are the correlation between the:

- Measured process control and geometrical indices (chapter 3, sections 3.2.1, 3.2.2 and 3.2.3) of the manufactured wafers and the observed process and machine parameter characteristics at time t_0 and

- Expected empirical characteristics of process and machine parameters determined during the study of physical models and the observed process and machine parameter characteristics at time t_0

Thus, the behavioral pattern is a set of all behaviors observed during a particular processing state or processing state transition and can be represented as a n-dimensional behavioral pattern space with ascertainable behaviors as its dimensions. Every space axes is represented by a particular physical behavior of the CMP process machine in a defined time interval (Δt), which is the duration of processing state or processing state transition.

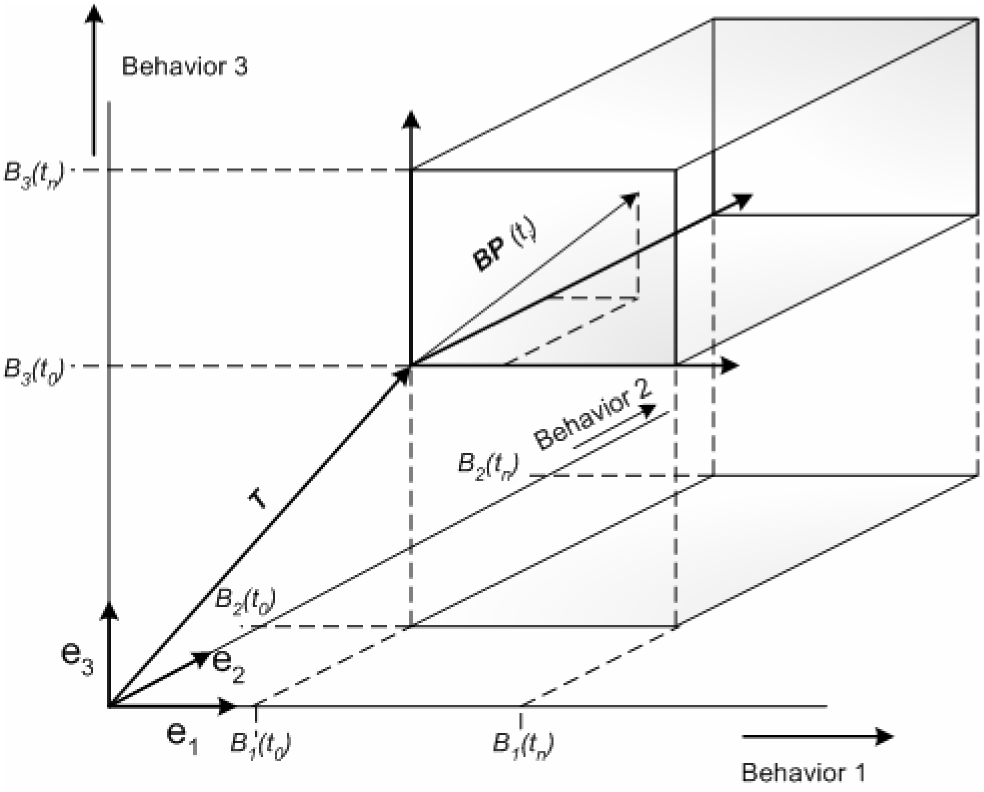


Figure 5.2: Creation of a three dimensional behavioral pattern space of CMP process machine during a particular processing state or processing state transition

Figure 5.2 shows the three dimensional behavioral pattern space depicting the three behavior-axes orthogonal to each other, the transformation vector ***T*** and a particular behavioral pattern at time t_i ***BP***(t_i) in the Cartesian coordinate system. The mathematical representation of orthogonality of the behavior-axes is achieved by applying cross product on unit vectors as given by the equation 5.9 [Oberholthaus 1995]:

$$e_1 \times e_2 = e_3;\ e_2 \times e_3 = e_4;\ \ldots;\ e_{n-1} \times e_n = e_1;\ e_n \times e_1 = e_2; \tag{5.9}$$

Where $e_1 = \begin{bmatrix} 1 \\ 0 \\ \cdots \\ 0 \end{bmatrix}; e_2 = \begin{bmatrix} 0 \\ 1 \\ \cdots \\ 0 \end{bmatrix}; e_n = \begin{bmatrix} 0 \\ 0 \\ \cdots \\ 1 \end{bmatrix}$ are the unit vectors.

The new behavior of CMP process machine requires an increment of n-dimensional behavioral pattern space. It is therefore necessary to position the new behavior in the present structure of behavioral pattern space (i.e. to define a new unit vector, the origin of the behavior-axis and its normed segmentation), so that the extended cross product of unit vectors can be applied as given by the equation 5.10 [Oberholthaus 1995]:

$$\ldots;\ e_{n-1}\times e_n = e_{n+1};\ e_n\times e_{n+1} = e_{n+2};\ \ldots;\ e_{n+i-1}\times e_{n+i} = e_1;\ e_{n+i}\times e_1 = e_2 \tag{5.10}$$

The model of behavioral patterns of the CMP processing machine and its periphery builds the basis to observe, classify, and localize the origination of defects during the CMP processing.

5.3 Problem domain modeling

In this section, based on section 5.2, at first the CMP process machine model is developed describing the n-dimensional process space. Any deviation of the linearly independent behavioral pattern characteristics in the CMP process space can lead to defect origination. The second part of this section deals with the development of correlation model between the behavioral pattern characteristics of CMP process machine and the defect classes. The problem domain modeling approach is shown in figure 5.3.

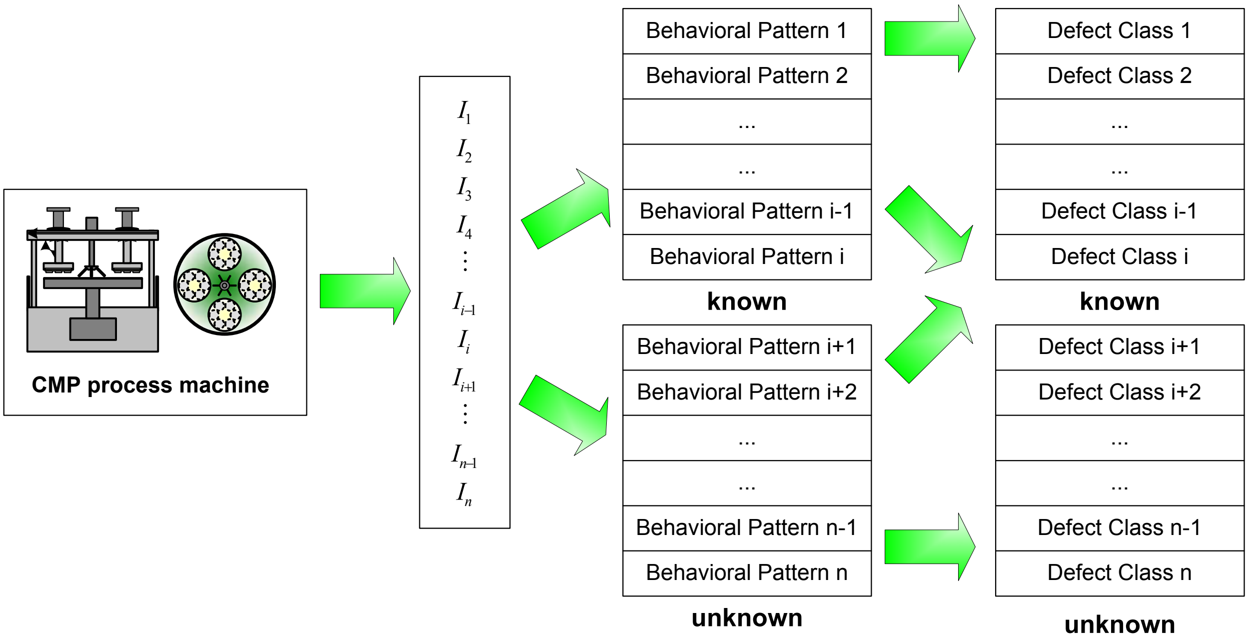


Figure 5.3: Problem domain model

Figure 5.3 shows the generated information characterized by the known and unknown behavioral patterns of the CMP process machine. The known behavioral patterns can be correlated to the corresponding known defect classes. The unknown behavioral patterns as well as the unknown defect classes can be discovered during the observation of CMP process machine. The CMP process therefore, requires a very thorough observation and process expertise to understand and determine the correlation between the behavioral patterns and the defect origination. The correlations are continuously subjected to dynamical changes as they depend upon different combinations of behavioral patterns leading to new perceptions and combinations of their behavioral characteristics and hence resulting in discovery of new defect classes.

5.3.1 Development of CMP process machine model

The CMP process machine in the production environment follows a particular behavioral pattern during a processing state or processing state transition [SEMI E10 2001, SEMI E30 2003, SEMI E58 2001] and provides continuously information about itself and its surroundings. As discussed in chapter 3, section 3.4 the different sensors, actuators, control parameters, the empirical characteristics of CMP process machine parts and the whole process technology are the main sources responsible for information generation. These sources are represented by the process and machine parameters as discussed in section 5.2. These process and machine parameters generate the information in terms of the numerical values, which they take during a particular processing state or processing state transition. The set of all behavioral pattern characteristics during different processing states (productive, standby, unscheduled downtime, scheduled downtime, non-scheduled time and engineering) and processing state transitions describes the complete process space of the CMP process machine as shown in figure 5.4.

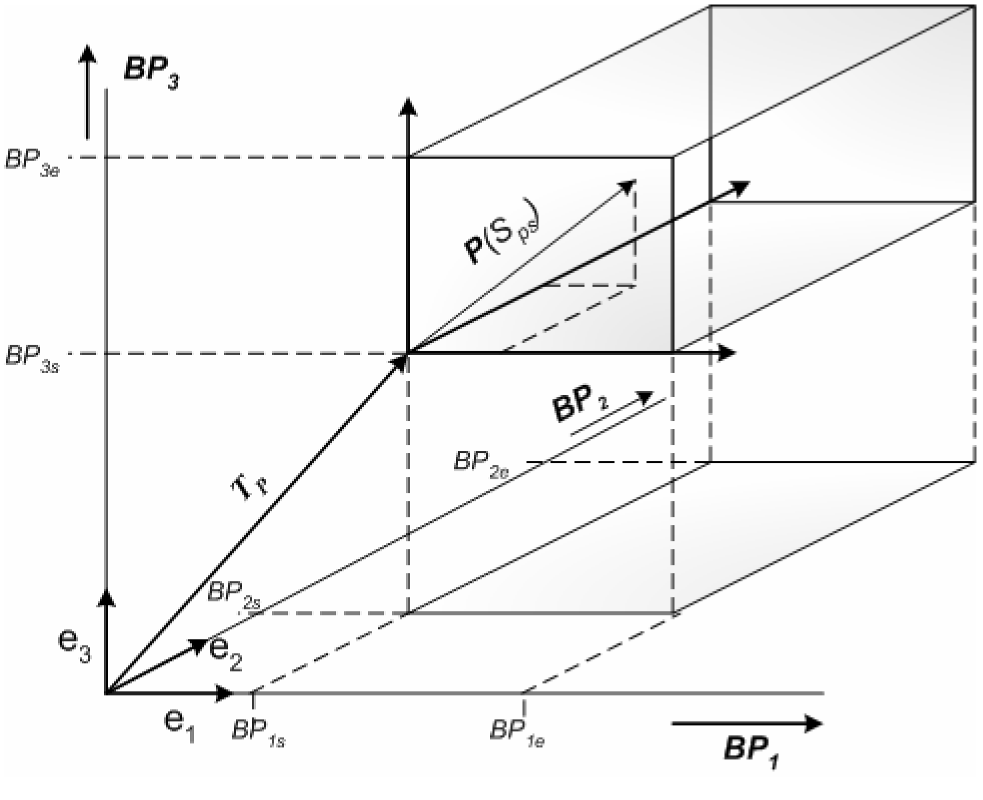


Figure 5.4: Three dimensional process space of CMP process machine

Figure 5.4 shows the three dimensional process space of the CMP process machine with the behavioral pattern characteristics $\mathbf{BP}_1$, $\mathbf{BP}_2$ and $\mathbf{BP}_3$ as orthogonal axes, $\mathbf{T_P}$ as transformation vector and $\mathbf{P}(S_{ps})$ as CMP process vector in a particular processing state S_{ps} or processing state transition S_{pt}. It is given by the equation 5.11:

$$\mathbf{P}(S_{ps}) = f(\mathbf{BP}); \text{ where } \mathbf{BP} = \{\mathbf{BP}_1, \mathbf{BP}_2, \ldots, \mathbf{BP}_i, \mathbf{BP}_{i+1}, \ldots, \mathbf{BP}_n\} \qquad 5.11$$

The n-dimensional CMP process space $\mathbf{P}^n$ is determined by analyzing the CMP process and machine information during a particular processing state or processing state transition. The process and machine information is provided by CMP process automation controller as discussed in chapter 3, section 3.4. Figure 5.5 shows the different steps required for determining the CMP process space. At first in figure 5.5 (1), the behaviors of different process and machine parameters are determined by analyzing the process and machine parameters based on equation 5.6, 5.7 and 5.8 during a process state or process state transition. The behavioral pattern space is determined by observing the behaviors of process and machine parameters at time (t_i) during processing state or processing state transition figure 5.5 (2). The CMP process space figure 5.5 (3) is determined by analyzing and observing all the behavioral pattern characteristics in different processing states and processing state transitions as given by the equation 5.11.

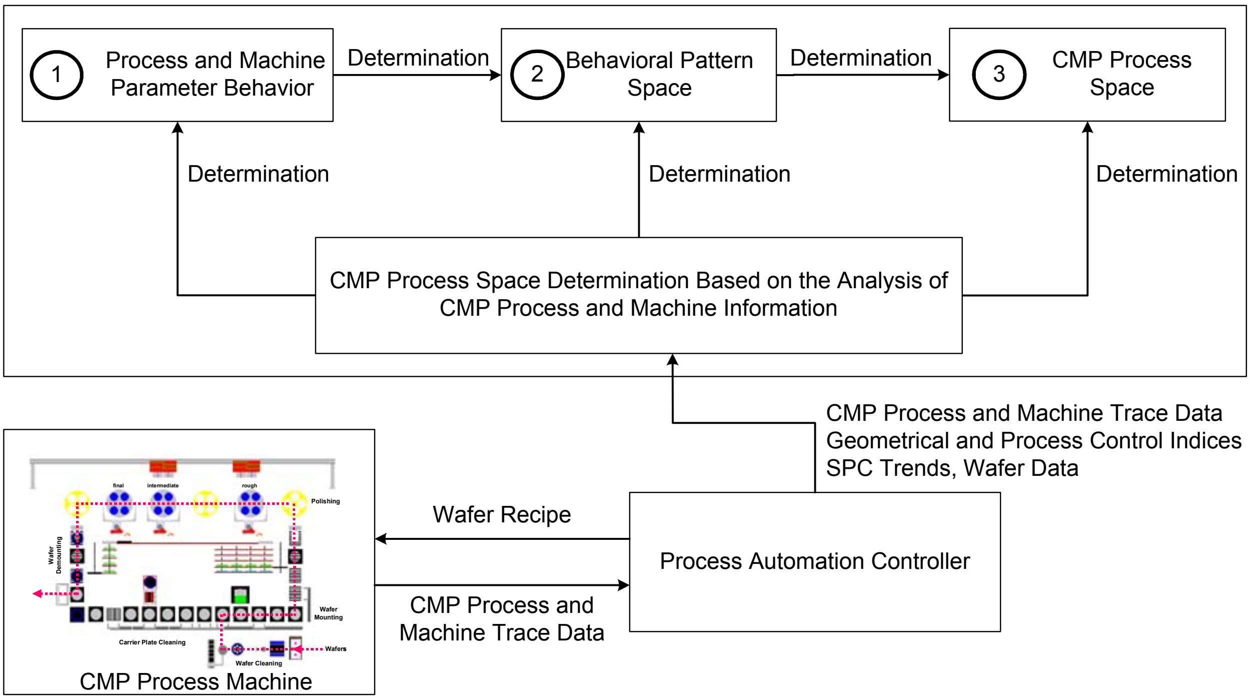


Figure 5.5: Determination of CMP process space

The CMP process machine states are finite and therefore, the behavioral pattern characteristics in a particular state can be correlated between the observed and the expected process and machine parameters values. Deviations of these parameters provide the information about the behavioral change of CMP process leading to the origination of defects. Therefore, the analysis of the behavioral patterns in the production environment includes behavioral pattern interpretation of the CMP process and the functional coherence between the current behavior and the actual behavior to detect the origination of defects. The influencing process and machine parameters, as described in chapter 3, section 3.3 characterize the behavioral pattern of the process machine. In chapter 3, sections 3.1.2 and 3.1.3 the different behavioral pattern characteristics during CMP process are analyzed, e.g. during the CMP process the behavioral characteristics of polishing plate, polishing pad, slurry, the rotating carrier plates and the pressure unit are discussed.

5.3.2 Development of the correlation model

The drift or shift of CMP process vector in the CMP process space can occur due to change in behavioral pattern characteristics of the CMP process machine. This behavioral pattern change, which is the deviation between the expected behavioral pattern characteristics and the current behavioral pattern characteristic, can be the cause of defect origination. Figure

5.6 shows the behavioral pattern characteristics and the defect classes related to different process steps during CMP processing. Any point in the n-dimensional CMP process space $\boldsymbol{P}^n$ can be assigned to defect classes, which have been discussed in chapter 3, section 3.2.4. The defects associated to defect classes are classified based on the measured deviations of process control indices or measured geometrical indices determined by the ex-situ geometrical measurements of manufactured wafers. The measured process control and geometrical indices provide the information about the most probable influence of the process and machine parameters responsible for the defect origination. On the other hand, a particular behavioral pattern characteristics is dependent upon the set of behaviors during a particular processing state or processing state transition, which is further influenced by the process and machine parameters. Change in a particular behavior of the CMP process machine can result in a change of behavioral pattern characteristics, which further influences the deviation of CMP process vector $\boldsymbol{P}(S_{ps})$ equation 5.11 in the n-dimensional CMP process space $\boldsymbol{P}^n$. Therefore, the observed drift or shift of CMP process vector $\boldsymbol{P}(S_{ps})$ influences the wafer geometry directly. The observed drift and shift of the CMP process vector $\boldsymbol{P}(S_{ps})$ in the n-dimensional CMP process space $\boldsymbol{P}^n$ can have many contributors. The exact sources of these contributors can be the interdependencies among the behavioral pattern characteristics themselves or some other behavioral pattern characteristics showing a deviation having indirect influence on this process vector drift. It can also be the combination of all involved behavioral pattern characteristics. For Example the behavioral pattern characteristics deviation during wafer mounting process influences the behavioral pattern characteristics during polishing, hence resulting in deviation of measured process control indices or geometrical indices and the contributors to this deviations can be the behavioral pattern characteristics drift during wafer mounting process as well as during wafer polishing process. The exact cause of defect origination can therefore have many contributors influencing directly or indirectly the CMP process vector $\boldsymbol{P}(S_{ps})$ in the n-dimensional CMP process space $\boldsymbol{P}^n$.

The deviations or drift and shift of CMP process vector can be represented by linearly independent, mutually exclusive and exhaustive set of defect class vectors $D_1, \ldots, D_d$ (figure 5.6) building the d-dimensional defect class vector space $\boldsymbol{D}$ (i.e. a set of non-overlapping defect class vectors covering the whole defect class vector space $\boldsymbol{D}$) given by equation 5.12:

$$\boldsymbol{D} = \{D_1, D_2, \ldots, D_b, D_{b+1}, D_{b+2}, \ldots, D_c, D_{c+1}, D_{c+2}, \ldots, D_d\} \qquad 5.12$$

Where, the defect class vector space $\boldsymbol{D}$ is a linear subspace of CMP process $\boldsymbol{P}^n$. A particular defect class D_d can have all behavioral pattern characteristics involved for its origination and is given by the equation 5.13:

$$D_d = f(\boldsymbol{BP}); \text{ where } \boldsymbol{BP} = \{\boldsymbol{BP}_1, \boldsymbol{BP}_2, \ldots, \boldsymbol{BP}_i, \boldsymbol{BP}_{i+1}, \ldots, \boldsymbol{BP}_n\} \qquad 5.13$$

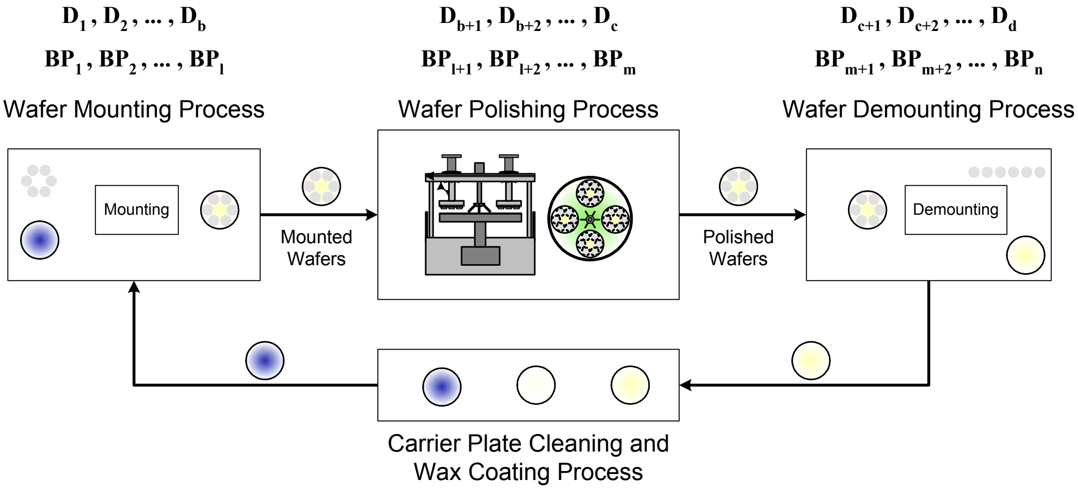


Figure 5.6: Chemical Mechanical Polishing process showing the behavioral patterns and defect classes

The ascertainment of the contributors is done by correlating the expected behavioral pattern characteristics and the actual behavioral pattern characteristics of CMP process machine, where the influence of all process and machine parameters is investigated. The result therefore, can be that all established behavioral pattern characteristics involved are potential contributors of the defect origination, belonging to a defect class, represented by the behavioral pattern characteristics vector ***BP***. The classification and specification of defect classes is done using basic probability theory [Leang 1997], which is the basic principle of Bayesian theory [Finetti 1974]. The Bayesian theory is well developed and has a well-formalized procedure for implementing diagnostic systems [Leang 1997]. The defect classes $\omega_l, 1 \le l \le \boldsymbol{D}$ with known probability distributions and a priori probabilities $p(\omega_l)$ build the d-dimensional defect class vector space ***D***. The sum of probabilities of all defect class vectors in the defect class vector space ***D*** is given by the equation 5.14:

$$\sum_{l=1}^{\boldsymbol{D}} p(\omega_l) = 1 \qquad 5.14$$

The behavioral pattern characteristics vector ***BP*** representing the behavioral pattern characteristics of the CMP process machine, responsible for defect origination in d-dimensional space $\boldsymbol{R^d}$, belongs to the defect class ω_l with the conditional probability $f(\boldsymbol{BP}|\,\omega_l)$. Using Bayes theorem, ***BP*** can be assigned to the defect class regions by minimizing the conditional error probability $C_l(\boldsymbol{BP})$ is given by the equation:

$$C_l(\boldsymbol{BP}) = \sum_{j=1, j \ne l}^{\boldsymbol{D}} p(\omega_j | \boldsymbol{BP}) \qquad 5.15$$

Where applying Bayes theorem $p(\omega_j | \boldsymbol{BP})$ is given by the equation:

$$p(\omega_j | \boldsymbol{BP}) = \frac{f(\boldsymbol{BP} | \omega_j) \bullet \mathrm{p}(\omega_j)}{\sum_{k=1}^{\boldsymbol{D}} f(\boldsymbol{BP} | \omega_k) \bullet \mathrm{p}(\omega_k)} \qquad 5.16$$

Where the $p(\omega_j|\,\boldsymbol{BP})$ is the conditional probability of defect class determined from conditional probabilities of behavior pattern characteristics $f(\boldsymbol{BP}|\,\omega_j)$ and prior probabilities of defect classes $p(\omega_j)$ and the optimal error probability e^* is given by minimizing the conditional error probability $C_l\,(\boldsymbol{BP})$:

$$e^* = \min_{l=1,\dots\boldsymbol{D}} C_l(\boldsymbol{BP}) = 1 - \max_{l=1,\dots,\boldsymbol{D}} p(\omega_l | \boldsymbol{BP}) \qquad 5.17$$

The behavioral pattern characteristics are mapped to the defect class ω_0, when the optimal error probability is greater than the specified threshold conditional probability value "C_a":

$$\boldsymbol{BP} \xrightarrow{d} \omega_0, \text{ when } e^* > C_a \left(C_a = \text{threshold}\right) \tag{5.18}$$

The pattern characteristics are mapped to the defect class ω_l, when the conditional probability $p(\omega_l| \boldsymbol{BP})$ satisfies the following equation:

$$\boldsymbol{BP} \xrightarrow{d} \omega_l, \text{ when } p\left(\omega_l \middle| \boldsymbol{BP}\right) = \max_{j=1,\ldots,\boldsymbol{D}} p\left(\omega_j \middle| \boldsymbol{BP}\right) \geq 1 - C_a \tag{5.19}$$

Figure 5.7 shows the mappings of behavioral pattern characteristics in d-dimensional space $\boldsymbol{R}^d$ to the defect class regions $\Omega_A \cup \Omega_R$:

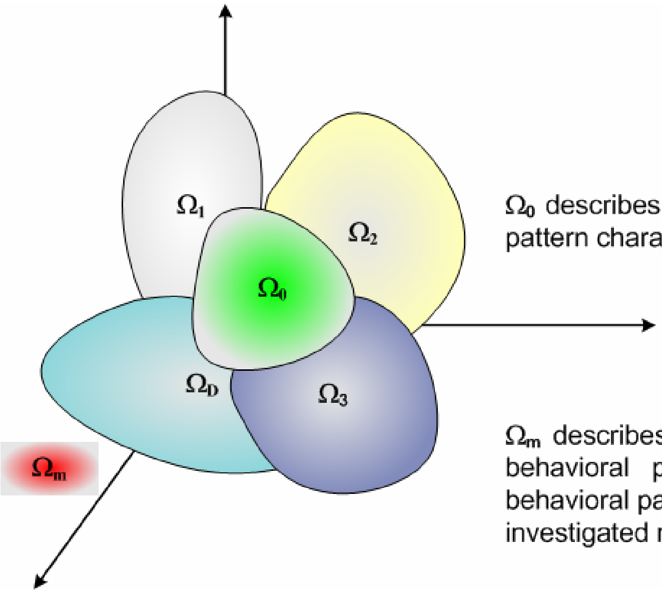
$$\boldsymbol{R}^d = \Omega_A \cup \Omega_R \tag{5.20}$$

Where $\Omega_A = \Omega_1 \cup \Omega_2 \cup \Omega_3 \ldots \cup \Omega_D$ set of all classified defect class regions with known behavioral pattern characteristics, responsible for the origination of defects and

$$\Omega_R = \Omega_0 \cup \Omega_m \text{ and } \Omega_0 \cap \Omega_D = \Phi \tag{5.21}$$

Where the defect class region Ω_0 contains a set of all unclassified defects and the defect class region Ω_m contains a set of all unknown behavioral pattern characteristics.

The correlation between the observed behavioral pattern characteristics and the probable regions of defect classes in the production environment is thus established using Bayesian theory as shown in the figure 5.7. The assignment of behavioral pattern characteristics to the defect classes in the corresponding regions build the basis to represent the defect origination characteristics for establishing diagnosis in the knowledge base.



Ω_0 describes defect class region, where the behavioral pattern characteristics of unclassified defects are found

Ω_m describes defect class region, where the unknown behavioral pattern characteristics are found. These behavioral pattern characteristics are to be observed and investigated more thoroughly.

Figure 5.7: Mapping of behavioral pattern characteristics to different defect class regions

5.4 Defect evaluation system design

The defect evaluation (DE) system consists of communication control component, defect evaluation front door component and defect evaluation component as shown in the figure 5.8. The encapsulated operational functionalities are accessed by services provided by these components. The defect evaluation system through its *communication control* *component* can be easily integrated and adapted in the manufacturing facilities or processing machines by just configuring an instance of it for the required communication.

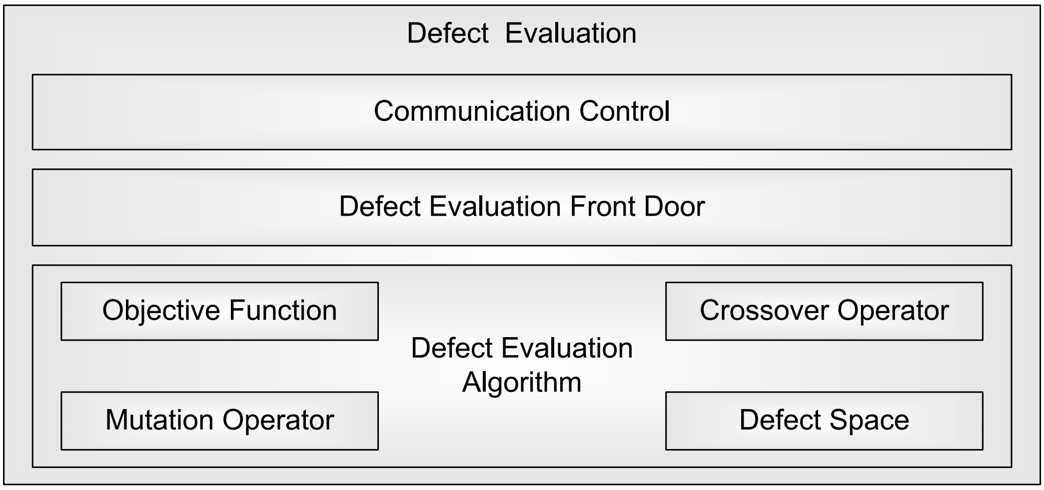


Figure 5.8: Design of defect evaluation system

The *defect evaluation front door component* encapsulates the *defect evaluation algorithm component* completely. It provides the services, which can be called by any other system to start defect evaluation. It provides the mechanism to interpret the list of defect classes, list of behavioral pattern characteristics and list of parameters for the defect evaluation algorithm component. It converts these lists to the corresponding objects, as required by the defect evaluation component and is responsible to start the defect evaluation algorithm. The defect evaluation algorithm component provides the list of evaluated objects to defect evaluation front door component, which further interprets these objects and converts them into the list of defect classes correlated to the list of responsible behavioral pattern characteristics. The *defect evaluation algorithm component* provides the services for defect evaluation front door component to start, tune, configure and stop the defect evaluation algorithm.

- **Defect evaluation algorithm**

The correlation between the defect classes in d-dimensional space $\boldsymbol{R}^d$ and the behavioral pattern characteristics in n-dimensional space is evaluated using genetic algorithms. As the search space for the defect classes is d-dimensional and the corresponding search space for behavioral pattern characteristics is n-dimensional, where *dim n* > *dim d*. This implies that the origination of a particular defect class has to be localized, classified in d-dimensional space and the cause or causes of its origination is/are to be searched in n-dimensional CMP process space. The genetic algorithms [Rechenberg 1973, Holland 1975, Michalewicz 1994] provide a multi-directional stochastic search method using natural evolutionary process operating on the number of possible combinations of defect classes in d-dimensional space and their originators behavioral pattern characteristics in n-dimensional space, to find the potential solution space of defect class combinations and their originators. It employs *heuristics* such as *selection* of behavioral pattern characteristics and defect classes, *crossover* generating different combinations of behavioral pattern characteristics and defect classes and *mutation* for evolving and extending the search space for optimal correlation combinations. Figure 5.9 shows a composite genome, also known as *genome* or *chromosome* representing the defect classes. Every defect class is defined as a *gene*, which refers to a list of behavioral pattern characteristics randomly assigned to it. The behavioral pattern characteristics in the referred list are not necessarily responsible for the origination of defects associated to this defect class. Every genome therefore, represents a potential correlation between the defect classes and the behavioral pattern characteristics. The genomes undergo crossover to generate further potential solutions, known as *population* of a *generation*. An evolution process run on a population of genomes corresponds to a search through a space of potential correlations between the defect classes and behavioral pattern characteristics.

In every generation, the combination of best, intermediate and worst potential solutions builds the basis for further exploration and exploitation of potential solutions. The further exploitation is done by using *mutation* operator, a probability with which a characteristic of gene is changed. The crossover and mutation probabilities decrease, as the search space increases (i.e. the number of generations). A particular potential solution (genome) is evaluated using *objective function* to distinguish between two potential solutions. The objective function plays the role of environment during the evolution process. The objective function used here is based on the Bayesian theory (equations 5.15 - 5.19). Figure 5.9 depicts the genetic representation of the potential correlation between the defect classes and the behavioral pattern characteristics. The initial population is created by randomly assigning the behavioral pattern characteristics to different defect classes. As it is possible, that one particular behavioral pattern characteristic can be responsible for one or more defect classes therefore, a particular behavioral pattern characteristic can appear in two different lists or in worst case, all the defect classes can have the list of all possible behavior pattern characteristics. The conditional probability equation 5.15 $C_l(\boldsymbol{BP})$ of every defect class in the genome is evaluated and if the equation 5.19 is satisfied, the corresponding gene in the genome is assigned a very high score.

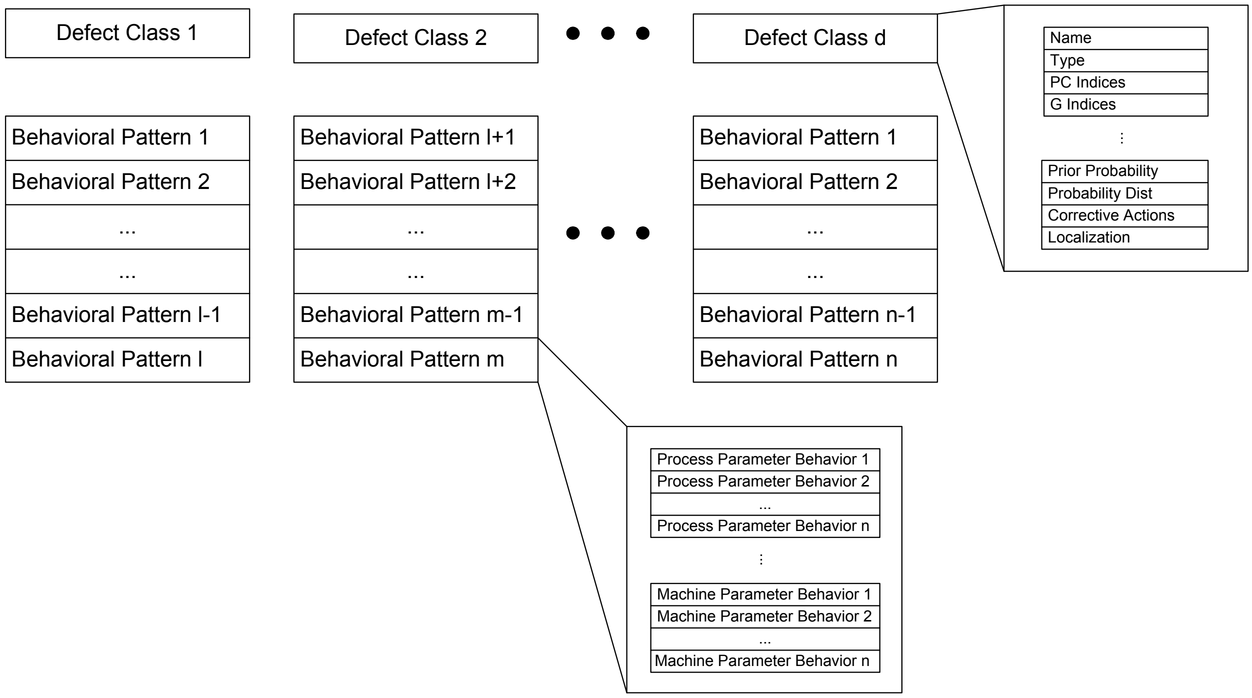


Figure 5.9: A composite genome representing defect classes referring to a list of most probable behavioral pattern characteristics and the related parameters

The score of every gene i.e. defect class is added at the end and the maximum score qualifies a particular genome to be the best in a generation. During multi-directional search it is possible to find a genome with only one gene (i.e. a defect class) referring to a list of behavioral pattern characteristics responsible for its origination. This particular genome is weighted with a very high score and if it survives during the evolution process then most probably a unique defect class is discovered with its contributors. Random combinations of best, intermediate and bad genomes in a generation are used to explore the further potential correlations between the defect classes and the behavioral pattern characteristics. The genetic algorithm terminates after a specified time or it finds the optimal combination of defect classes and its originators earlier than the specified time. The evaluated defect classes are assigned to the corresponding defect class regions having a-prior probabilities and the correlated behavioral pattern characteristics as shown in the figure 5.10.

The indefinite defect classes are assigned to the defect class region Ω_0 and the unknown behavioral pattern characteristics are assigned to the defect class region Ω_m. The defect class regions are subjected to very thorough observations and investigations during CMP process and the continuous corrections and optimizations are done by the expertise of the process engineer in the production environment. The defect classes and the related behavioral pattern characteristics thus detected build the basis for diagnostic system.

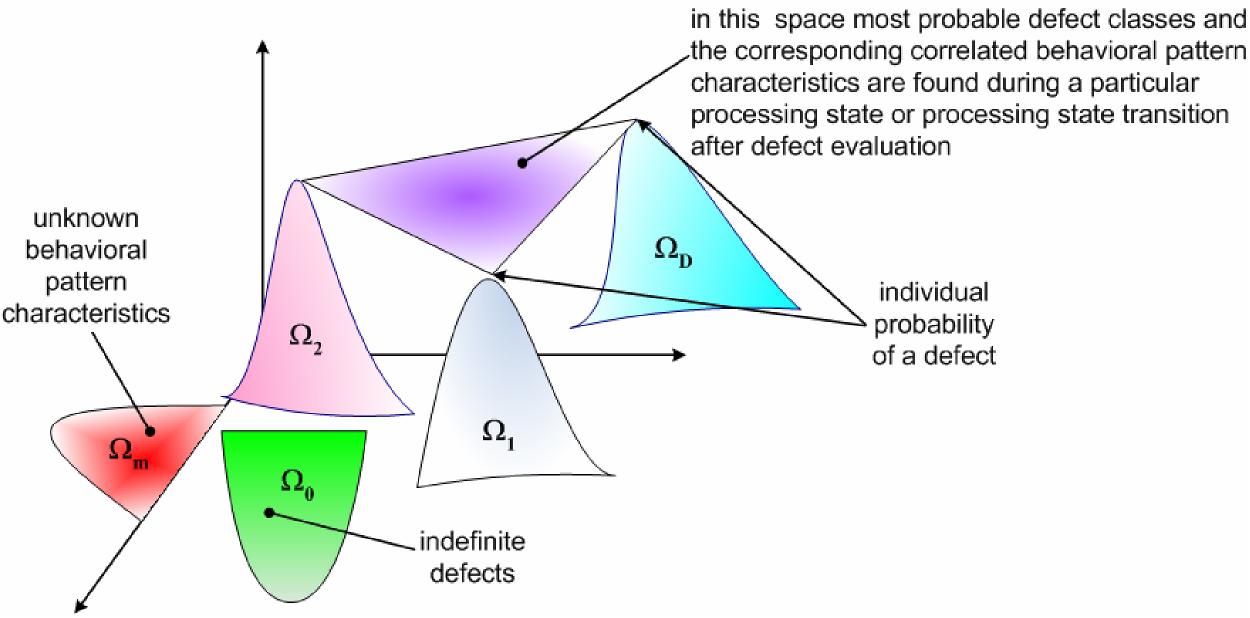


Figure 5.10: The regions of evaluated defect classes and the most related behavioral pattern characteristics responsible for their origination

5.5 Architectural artifacts and diagnostic system design

Defect classes and corresponding correlated behavioral pattern characteristics, discussed in section 5.4, provide the basis for in-situ defect detection during the CMP process. To establish the in-situ defect analysis mechanism, a diagnostic system, providing time dependant operational and dynamic inferences about the CMP process vector characteristics drift (see equation 5.11 section 5.3.1) during CMP process is used. The representation of CMP process space knowledge is embodied completely in the diagnostic system (knowledge model [Schilstra 2001]) to immediately analyze the CMP process vector characteristics and provide the analyzed information to process engineer. The data required to analyze the CMP process vector are provided by the CMP process machine during processing state or processing state transition, so that the inference engine of diagnostic system can interpret the data and provide its results to the CMP process automation controller or to the process engineer. A particular defect class can have many behavioral pattern characteristics of CMP process vector, responsible for its origination during a particular processing state or processing state transition, therefore different combinations of knowledge representation of the CMP process vector are modeled separately to observe the corresponding influence during defect origination. The CMP process vector characteristics are observed during a processing state or processing state transition. These characteristics depend upon the different behavioral pattern characteristics during the current state, the time elapsed during the current state and its behavior during previous processing states or processing state transitions. The design of the diagnostic system for defect analysis includes not only the knowledge representation of the CMP process vector, but also the time dependency and adaptability of CMP process vector to its production environment. In the next sections, the time dependency, environment adaptability, knowledge based system and the behavioral pattern characteristics representation of CMP process vector, required for design of diagnostic system for defect analysis, are discussed.

5.5.1 Temporal representation of CMP process vector

The CMP process vector characteristics represented by behavioral pattern characteristics in n-dimensional CMP process space (section 5.3.1) has an additional independent dimension i.e. time, which has an autonomous status and exists independently [Gamper 1996] of changes during the CMP processing. The CMP process vector characteristics can be viewed using *independent time theory* and *dependent time theory* [Lin Y 1991, Gamper 1996]. From the independent time theory point of view the surveillance of CMP process vector is done by observing the behavioral pattern characteristics undergoing different forms of changes that occur during a processing state or processing state transition with time. The observed behavioral pattern characteristic changes are related to the independent time (i.e. the time continues irrespective of the behavioral pattern characteristic changes) and the propositions for these changes are valid only during the associated time space, which can be a collection of discrete time points or time intervals. It means, that each behavioral pattern characteristics change (depending upon the propositions) has an associated time, over which it is true.

From the dependent time theory view, the observation of the CMP process vector requires a time dependent logical analysis of behavioral pattern characteristic changes prior to a discrete time point or time interval, when this change will take place. It means, when a time point or a time interval is reached the corresponding change (based on the time dependent logical consequences) in behavioral pattern characteristics is expected. Exactly for the *defect origination*, it is important to scrutinize the logic of behavioral pattern characteristic changes before the time point is reached, where the occurrence of originating defect is unavoidable. The time dependency of the logic of behavioral pattern characteristics changes leads to the conclusion, that the explicit representation of *temporal* information of these changes is necessary as it provides information about the origination of drifts and shifts of CMP process vector.

The temporal representation of CMP process vector can have either an explicit time representation based on *time points* (also called instants [Gamper 1996]) or can be based on *time intervals* (also called time periods [Gamper 1996]) depending upon the performance of drift logic or change logic of behavioral pattern characteristics during CMP process. The time points and time intervals represent typical *primitive temporal objects* having positive duration and following temporal relations among each other such as:

- The relation between two time intervals, which can be: before, meets, starts, overlaps, during, finishes, equal, after, met, overlapped, finished, contains, started [source: Gamper 1996]
- The relation between a time point and a time interval can be: before, starts, during, finishes, after [source: Gamper 1996]
- The relation between a time interval and a time point can be: before, finished, contains, started, after [source: Gamper 1996]
- The relation between two time points: before, equal, after [source: Gamper 1996]

The above relations, which provide the past, current and eventually a list of (predicted) future values of information and a most probable explanation of a cause describe the temporal information of behavioral pattern characteristics, if and only if a behavioral pattern characteristics change is observed. *Temporal prediction* determines what might happen in the near future (i.e. prediction of a defect origination) where forward reasoning in time is done. *Temporal explanation* determines the happenings in past (i.e. cause of a particular defect) where backward reasoning in time is done. The temporal information of behavioral pattern characteristics is stored in the knowledge based system, which keeps the track of temporal information in order to maintain the validity of temporal predictions, temporal explanations and temporal reasoning facilities.

5.5.2 CMP process vector adaptability to production environment

During the CMP process, the behavioral pattern characteristics representing CMP process vector in n-dimensional CMP process space are in dynamical equilibrium and any shift or drift of these characteristics influences the CMP process vector resulting, in either a defect origination or shift of the established dynamical equilibrium point of the CMP process vector, without affecting the quality of the product. The temporal representation of the CMP process vector provides information about both defect origination and shift of the dynamical equilibrium. Therefore, when a particular drift or shift of the CMP process vector is observed then the temporal information of certain behavioral pattern characteristics most probably responsible for this drift, are investigated very thoroughly to distinguish between the defect origination and a shift of dynamical equilibrium. If the observed shift remains constant in a defined time interval then it is a shift of dynamical equilibrium of the CMP process vector. The reason for this particular shift e.g. can be the change of polishing pad properties or in general a temperature shift of the CMP process. As discussed in chapter 3, section 3.1.3 the properties of polishing pad change with the number of process runs it has undergone. To maintain the same product quality it is necessary for the CMP process machine to adapt to the changing process characteristics of polishing pad during CMP process. On the other hand, after a certain number of process runs a general temperature shift of CMP process is observed without affecting the product quality.

Another typical scenario, where the adaptability of the CMP process vector to the changing polishing characteristics of the studied CMP process is necessary, is after a fresh start of the CMP process machine or the start after the polishing pad is changed. The CMP process machine requires a certain number of process runs to stabilize itself after the fresh start, i.e. to reach a state of dynamical equilibrium. During CMP process, the CMP process vector adapts continuously to the changes of process and production environment in the CMP process space. This does not mean that the defect origination during this adaptation process is neglected. During adaptation process, the behavioral pattern characteristics are scrutinized very intensively. If there is an abrupt drift of a particular behavioral pattern, which is recorded and compared with the temporal information gathered in the past, immediately the logic and rules established for defect origination apply, and the behavioral pattern drift is observed. This drift is also observed even if the temporal logic and rules have not been established. The drift is in this case recorded and is provided to the CMP process engineers for its verification and validation.

The rules and logic for adaptability of the CMP process vector to the changing process and production environment in the CMP process space are established in the knowledge base system. The fine distinction between the defect origination and the shift of dynamical equilibrium of CMP process vector is done based on observations and the information provided by the CMP process expert, which then is implemented and tuned in the knowledge based system.

5.5.3 Design of diagnostic system

The drift and deviation of CMP process vector requires a mapping of it in a system, which provides the mechanism to interpret this deviation, its correlation and provides the diagnosis for this deviation. This section describes the knowledge base design, knowledge base architecture design and diagnostic system architecture design.

5.5.3.1 Design of knowledge base

The diagnostic system for defect analysis during CMP process uses knowledge base to analyze the cause of defect origination. For the dynamical analysis of unforeseen deviations of CMP process vector, it is necessary to have:

- The knowledge representation (i.e. system description) of the CMP process space (logic and rules)
- The temporal representation of the CMP process vector in the CMP process space (logic and rules)
- The adaptability of CMP process vector to the changing process and production environment in the CMP process space
- The definition of different diagnostic strategies (table 5.1) applied for the interpretation of unforeseen deviations of the CMP process vector. The interpretation of the detected deviation implies:
    - The analysis of the behavioral pattern characteristics based on different diagnostic strategies
    - The impact evaluation of the deviation on the current process run
    - The provision of the required corrective actions to avoid the defect origination

The different diagnostic strategies applied to diagnose technical systems in production environment are discussed in table 5.1. The combination of these strategies builds the basis for design of knowledge base to analyze the defect origination during CMP process.

Approach	Description	Requirements	Applications
Heuristic diagnostic systems	It uses statistical methods to establish the correlations between observations and diagnosis	Probabilities, security factors	Medicine and technical areas
Case based diagnostic systems	Corresponding information units of actual case are compared with already established known cases to diagnose multiple faults	Knowledge search with similar information content, such as expertise or experience in a special field	Medicine and service providers
Knowledge based diagnostic systems	The reusability of established information and knowledge builds the basis for knowledge based diagnostic systems characterizing the formal expert knowledge model	Knowledge base, methods to solve problems	Medicine, service providers and production and control engineering
Model based diagnostics systems	The model description of the system is predicted through simulating system behavior and comparing it with the operating mode of real system. The diagnostics process is activated immediately, when discrepancy between simulation and real operation mode is discovered	Model description	Production and control engineering, service providers (Traffic control systems, and diagnosis of digital integrated circuits)
Multi agent systems	During problem domain analysis recognized system components are modeled as acting and interacting autonomous units	Model description	Production and control engineering, service providers (robot controls, traffic control, Virtual reality)

Table 5.1: Different approaches to diagnose technical systems in production environment

5.5.3.2 Design of knowledge base architecture

The knowledge base architecture consists of system description component to describe CMP process space, correlation strategies component, planning component and defect classes component, as shown in the figure 5.11. All these components are accessed by services provided by them and they encapsulate their operational functionalities.

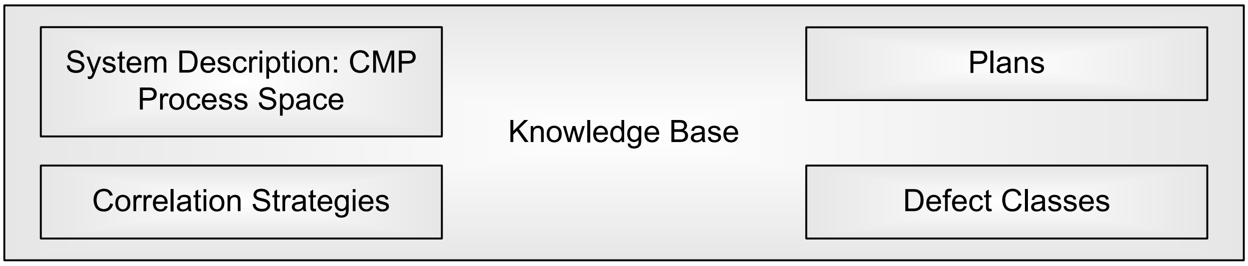


Figure 5.11: Knowledge base consists of system description component, correlation strategies component, planning component and defect classes component

The *system description* component provides the mechanisms discussed in table 5.1 to characterize and represent the CMP process space as described in section 5.3. The representation of behavioral pattern characteristics of CMP process vector, describing the CMP process space, is done by observing and analyzing the behavior of every process and machine parameter. The behavior of process and machine parameters is modeled based on:

- The mathematical analysis of parameters as discussed in chapter 3
- The observations of process and machine parameter behavior during CMP process
- The empirical behavior of individual process and machine parameters
- The process engineers expert knowledge

The influence (*symptoms*) of process and machine parameters during CMP process and the parameter interdependencies (*decision trees* and *diagnostic hierarchy*) is the basis for representing and formalizing (*rules* or *case based*) the diagnostic knowledge in the system description component. Thus building a CMP process space model, consisting of individual quanta of time dependent and process adaptable knowledge for each behavioral pattern characteristics, represented by the individual behavior of process and machine parameters. The time dependent and process adaptable knowledge is deployed either individually or in combination with others for diagnosing the CMP process vector deviation.

The *strategies* component provides the mechanism to:

- Interpret and correlate the symptoms
- Formalize the different combinations of decisions to conclude a particular diagnosis
- Employ correlation strategies and compute diagnoses during CMP process

Depending upon a particular symptom (CMP process vector deviation) and the involved behavioral pattern characteristics, which is further influenced by the behavior of process and machine parameters, a particular strategy is defined which correlates the correspondence between the CMP process vector deviation and the interpretation of its causes. The approach here is to define the different correlation strategies for the detection of defect origination by observing the circumstances under which the deviation of CMP process vector takes place. The selection of the corresponding correlation strategy depends upon the time elapsed during the CMP process and the current state of the CMP process.

The *planning* component provides the mechanism of defining plans, consisting of a sequence of correlation strategies, to resolve the contradictions during the interpretation of CMP process vector deviation based on its observation during a particular processing state or processing state transition of CMP process machine. The defect origination during CMP process in a particular processing state or processing state transition can be due to the combination of deviations of different behavioral pattern characteristics of CMP process vector and it is possible that one of the behavioral pattern characteristics only appears to be responsible for a particular defect origination. Different plans combining different correlation strategy sequences provide the mechanism to resolve the detected contradictions and to distinguish between the responsible behavioral pattern characteristics and the ones, which only appear to be responsible for defect origination. The selection of a particular plan depends upon the observed behavioral pattern characteristics deviation of CMP process vector during a current processing state of the CMP process machine. The behavioral pattern characteristics of CMP process vector in the past thus provides the inference engine a plan containing sequences of correlation strategies to analyze the origination of defects and resolve conflicts.

The *defect classes* component provides the mechanism to assign and map the defects detected during the observation of CMP process vector to the corresponding defect classes. This is approved by the CMP process engineer or by the CMP process expertise as described in section 5.3.2, equations 5.20 – 5.22. It provides the mechanism to create, edit and update defect classes. All known defects associated to a defect class are saved in the knowledge base with all its origination details and the responsible process and machine parameters.. Certain behavioral pattern characteristics deviations of CMP process vector in the beginning cannot be associated to a particular defect class. In this case, this particular observation is saved separately. During the diagnosis corresponding deviations are observed and if there are more than ten repetitions, then the CMP process engineer or knowledge engineer classifies this observed deviation to a new defect class with all its origination details and the involved process and machine parameters. By certain observed behavioral pattern characteristics, it is sometimes difficult to assign the process and machine parameters, which are responsible for defect origination, these observations are also saved in this component, and special investigations are made to classify these defects by the CMP process expertise or by process engineer. This component provides the mechanism to save both known as well as unknown defects, the known and unknown (suspected) process and machine parameters, responsible for the origination of these defects. These defects, process and machine parameters require special observations during CMP processing and can provide some inference to the upcoming deviations.

5.5.3.3 Design of diagnostic system architecture

The Diagnostic system architecture encapsulates the knowledge base and provides the services to start the *inference engine*, which uses the system description component, strategies component, planning component and defect classes component encapsulated in the knowledge base. The inference engine component provides the mechanism to resolve conflicts and remove contradictions from extended logical (rules, decision trees and diagnostic hierarchy) interpretation of symptoms with integrity constraints using plans. The inference engine component uses the information, stored in the knowledge base, to diagnose the deviations. It follows the probability-based theoretical formulations as discussed in section 5.3.2 using Bayesian theorem given by equations 5.14 - 5.22. The deviations from expected characteristics represented by the equations 3.1 – 3.40 as discussed in chapter 3 and the empirical equations of process and machine parameters based on the observations made during CMP processing. This component provides the inferences during run time about most probable contributors, which are responsible for defect origination. To increase the performance of the inference engine during runtime, typical diagnostic scenarios are built up as cases in the inference engine component. A particular case is a collection of process parameters, machine parameters and known or unknown defect classes representing particular behavioral characteristics of CMP process vector. During the observation of the CMP process vector certain deviations of behavioral pattern characteristics are repeatable so that these deviations can be modeled as a case. The case model thus contains facts, which are asserted during observations and consultations with CMP process engineers to describe it, or there exists a particular behavioral pattern characteristics deviation situation. The CMP process vector deviation in a particular case is represented by vocabulary, similarity measure, adaptation knowledge, diagnostic profiles, inference set covering knowledge from the profiles and the set covering inference capabilities for multiple defects. During the CMP process run the CMP process vector deviations for a particular processing state or processing state transition is thus represented by a case model. The inference of a particular CMP process vector deviation during runtime is done by combining appropriate cases. If a particular deviation of the CMP process vector is observed and if a particular case is detected, then detailed analysis of responsible contributors for defect origination is considered. The case model is integrated into the inference engine component to improve the performance of the inference engine. The inference engine using the encapsulated knowledge base and the appropriate combinations of observed case models infers the CMP process vector deviation and its originators.

The diagnostic system through its *communication control component* can be easily integrated and adapted in the manufacturing facilities or processing machines by just configuring an instance of it for the required communication. Figure 5.12 shows the design of diagnostic system with all its components.

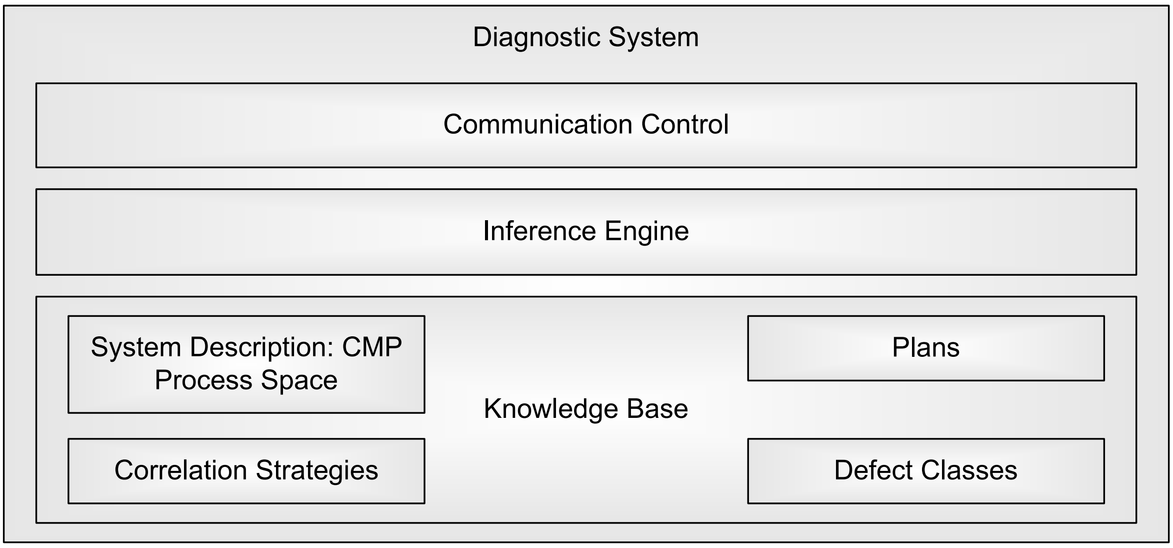


Figure 5.12: Diagnostic system architecture encapsulating a knowledge base, inference engine and communication control component

5.6 Design of the agent based diagnostic system

The realization and implementation of requirements R 1 - R 12 as described in chapter 4, section 4.1 necessitates the design of software mechanisms, which when deployed, must accomplish and fulfill the above requirements. The defect evaluation and the diagnostic system as designed in sections 5.4 and 5.5, individually satisfy part of these requirements and require a coordination mechanism so that when combined, the above requirements as a whole can be accomplished. This coordination thus required, needs a design of a software mechanism, which:

- Operates without any direct intervention of external resources such as humans and have a complete control over its actions and internal state
- Interacts with CMP process automation controller for data acquisition from CMP process machine or humans using a protocol, which can be understood by participants involved in communication

- Perceives in-situ the environment, which is the CMP process machine
- Does not intervene, control or influence directly the perceived environment, but provides the CMP process automation controller for CMP process machine, the corrective actions for the avoidance of originating defects
- Responds in a timely manner to changes that occur in it
- Does not only simply act in response to its environment, but also is able to exhibit goal-directed behavior by taking the initiative
- Interoperates and calls the internal services provided by defect evaluation components and diagnostic system components to detect the origination of defects by observing the CMP process vector and providing the results to CMP process automation controller, process engineer and CMP process expertise only when it detects a deviation of CMP process vector

This is achieved here by deploying the agent based software technologies and methodologies.

The agent communicates with the CMP process automation controller software for CMP process machine and provides the CMP process and machine parameters $\boldsymbol{PT}(t_0)$, $\boldsymbol{M}(t_0)$ to diagnostic system by calling the internal services provided by the diagnostic system. The diagnostic system starts the inference engine. When it detects a drift in behavioral pattern characteristics $\boldsymbol{BP}(t_0)$ of CMP process vector, the inference engine starts based on correlation strategy sequences to diagnose the cause of observed behavioral pattern characteristic drift by supposing, that all known or unknown defect classes saved in knowledge base, as a possible and plausible cause for this behavioral pattern characteristic drift. The correlation strategy at first in the inference engine authorizes every individual known or unknown defect class to prove its relevance and existence, i.e. its involvement in the observed behavioral pattern characteristics deviation. Every known or unknown defect class thus uses the corresponding inference mechanism, as it has been characterized and classified in the inference engine using the knowledge base, where all known origination details of the associated defects and related defect class, as described in section 5.5.3 “knowledge base design and knowledge base architecture”, is stored. Every individual defect class thus undergoes, based on the corresponding correlation strategies, an analysis and diagnosis mechanism and reports the analysis results individually to the inference engine. The inference engine evaluates these results to find the potential defect associated to this defect class responsible for this particular drift and reports this result to the agent. The agent depending upon the diagnostic results provides this information directly to the CMP process automation controller or to the CMP process engineer. The result includes the complete description of the originating defects in all its details. This means not only the known details about its origination but also the details about certain behavioral pattern characteristics, which were observed during the origination of a particular defect or it can be a complete new discovery of a CMP process behavioral pattern characteristics or a possible detection of a new defect class or of an unknown defect.

Based on these results and input of CMP process engineer, a defect evaluation cycle is started, either on the same machine where the defect analysis is running or on some other machine to separate the defect evaluation activity and diagnostic system for defect analysis activity. The defect evaluation in general requires more time; therefore, the agent starts these two activities separately to improve the performance of the in-situ diagnostic system for defect analysis. The agent provides the defect evaluation component as described in section 5.4, with behavioral pattern characteristics and the defect classes for the evaluation of results provided by the diagnostic system. The defect evaluation component thus evaluates the results and provides a defect class vector ***D***(t_0) and behavioral pattern characteristics vector ***BP***(t_0) to the agent, which further sends a message to the knowledge engineer to update the knowledge base. Figure 5.13 shows the design of agent based diagnostic system.

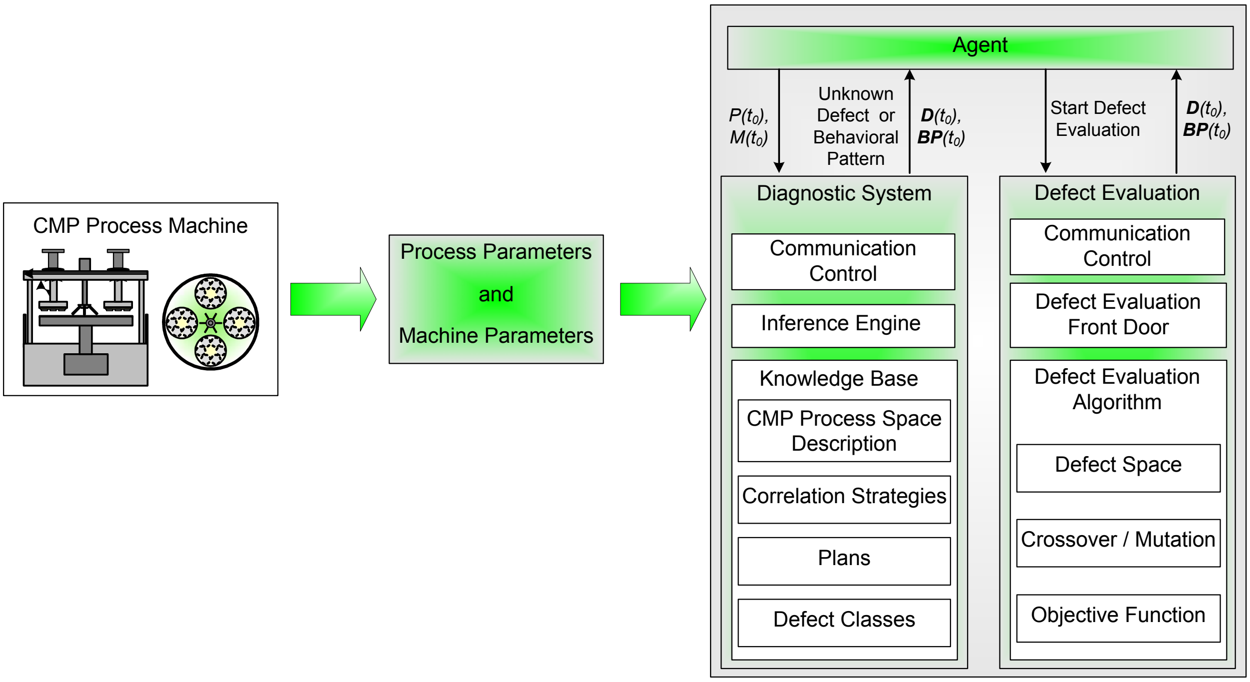


Figure 5.13: Design of agent based diagnostic system for defect analysis of studied CMP process machine

5.6.1 Design of agent based control

As described above the agent coordinates between the diagnostic system and defect evaluation system. It establishes the communication with CMP process automation controller and waits. The CMP process automation controller delivers a set of process and machine parameters during CMP processing state or processing state transition. The agent collects the process and machine parameter values and checks at first the syntax of the data set. If the data set is complete, it interprets these parameters and converts them into CMP process vector for the diagnostic system and for the defect evaluation system. The conversion for defect evaluation system is done only when it is required. The agent calls the service of diagnostic system to analyze the CMP process vector. The result of the analysis is provided back to the agent, which provides the diagnosis back to the CMP process automation controller and to the CMP process engineer only, if it detects a deviation in the behavioral pattern characteristics of CMP process vector. Otherwise, it waits for the next set of process and machine parameters.

In case of an unknown defect class origination or detection of a new behavioral pattern characteristics of a CMP process machine, the defect evaluation process can be started either automatically or initiated externally by the CMP process engineer. In this case, the agent converts the process and machine parameters in a process vector as required by the defect evaluation component and provide in addition the current defect vector space and the correlated behavioral pattern characteristics along with the unknown defect classes and the newly detected and not evaluated behavioral pattern characteristics to the defect evaluation component. The defect evaluation component provides the evaluated results back to the agent, which then sends a message to the knowledge engineer to update the diagnostic system. Figure 5.14 shows the design of an agent depicting the control activities it undergoes after receiving new process and machine parameters for starting a new defect evaluation.

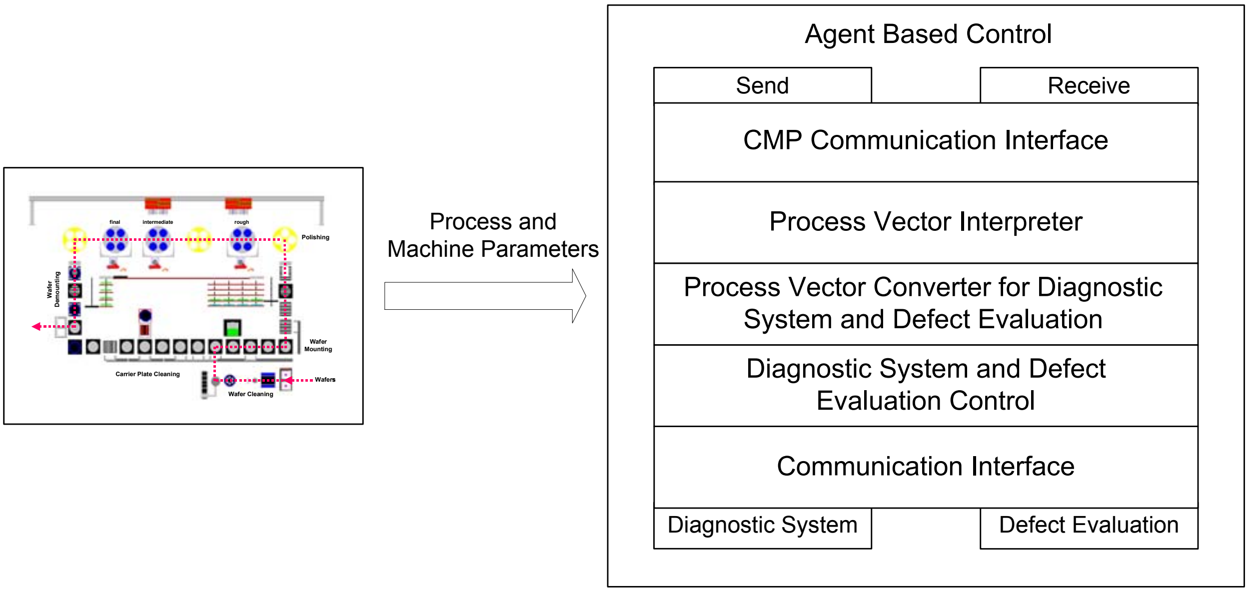


Figure 5.14: Agent showing the control activities, which it undergoes during diagnosis and defect evaluation process

5.6.2 Design of communication control component

The *Communication control* component is required to establish the internal communication between the defect evaluation system, diagnostic system and the agent or external communication between the agent and the manufacturing facilities. The communication control framework also provides a possibility to establish the communication among the internal components of a defect evaluation system, such as defect evaluation front door component and defect evaluation algorithm component or among the internal components of diagnostic system, such as the inference engine and the knowledge base. The communication control component facilitates a communication framework infrastructure, which interprets the incoming messages, converts these into the corresponding protocol, provides these to the internal components of defect evaluation system or diagnostic system, and sends an answer back to the manufacturing facility through the agent in the corresponding protocol. The communication layer uses a protocol, which is based on predefined international standards such as SECS/GEM, XML used in semiconductor manufacturing facilities to communicate with process, transport or metrology tools and DCOM, CORBA, TCP / IP, WSDL interfaces used in semiconductor manufacturing facilities for transmitting to and receiving data from manufacturing execution system and other applications in the manufacturing facilities.

A particular instance of communication controller can be configured for the application it is implemented. For example the diagnostic system only communicates externally with the agent by using the general services, provided by the communication framework such as connect, it connects to the agent and after the communication is established, they communicate with each other utilizing the services provided by them. The communication framework provides the basic services for all the applications such as to connect, disconnect, send, receive, events handling, exception handling, publish and subscribe. Depending upon the communication protocol the corresponding interpreter and converter for this protocol is provided by this component, which can be instantiated as required. In case in the manufacturing facility, a new protocol is used. An implementation of this is realized by mapping this protocol in a configuration file to the protocol provided by this component. Figure 5.15 shows a general overview of communication control component.

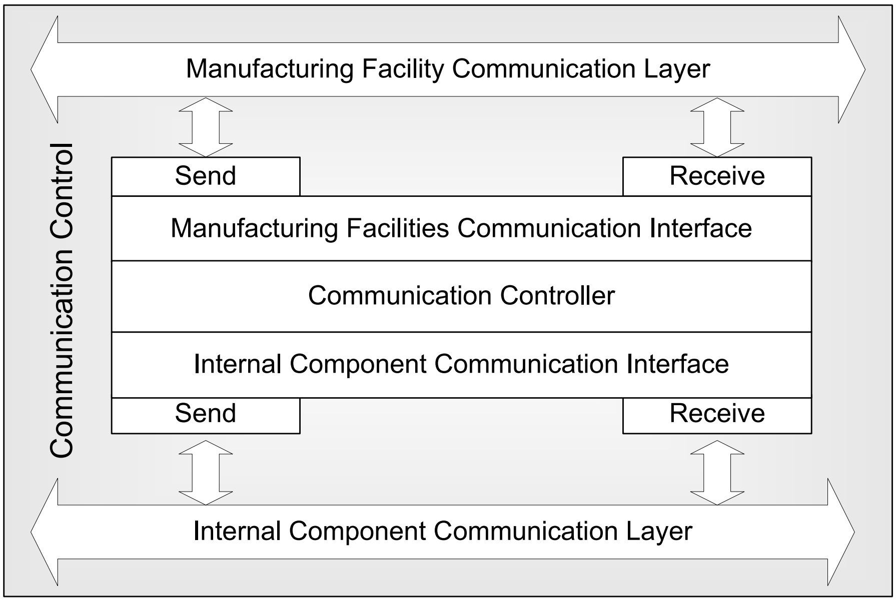


Figure 5.15: General overview of communication control component for defect evaluation system, diagnostic system and the agent

5.7 Enhancement of CMP process automation controller

The enhancement of CMP process automation controller for studied CMP process machine, which uses SPC as described in chapter 2 section 2.3.1 and chapter 3 section 3.4, can be achieved by integrating the agent based diagnostic system for defect analysis to improve the process quality and thus the product quality. The agent based diagnostic system is integrated directly in the CMP process control loop as shown in the figure 5.16. The CMP process automation controller provides the set of process and machine parameter values every 2-3 seconds through a session, which is established between the agent based diagnostic system and CMP process automation controller of studied CMP process machine through the communication control component. These process and machine parameter values are analyzed by the diagnostic system and the result, such as deviation of any behavioral pattern characteristics of CMP process machine, is sent back to the CMP process automation controller and to the process engineer. The CMP process automation controller, depending upon the process and machine parameter, calculates the new value for the parameter and downloads it to the CMP process machine automatically or ask the operator to make some corrective actions if necessary.

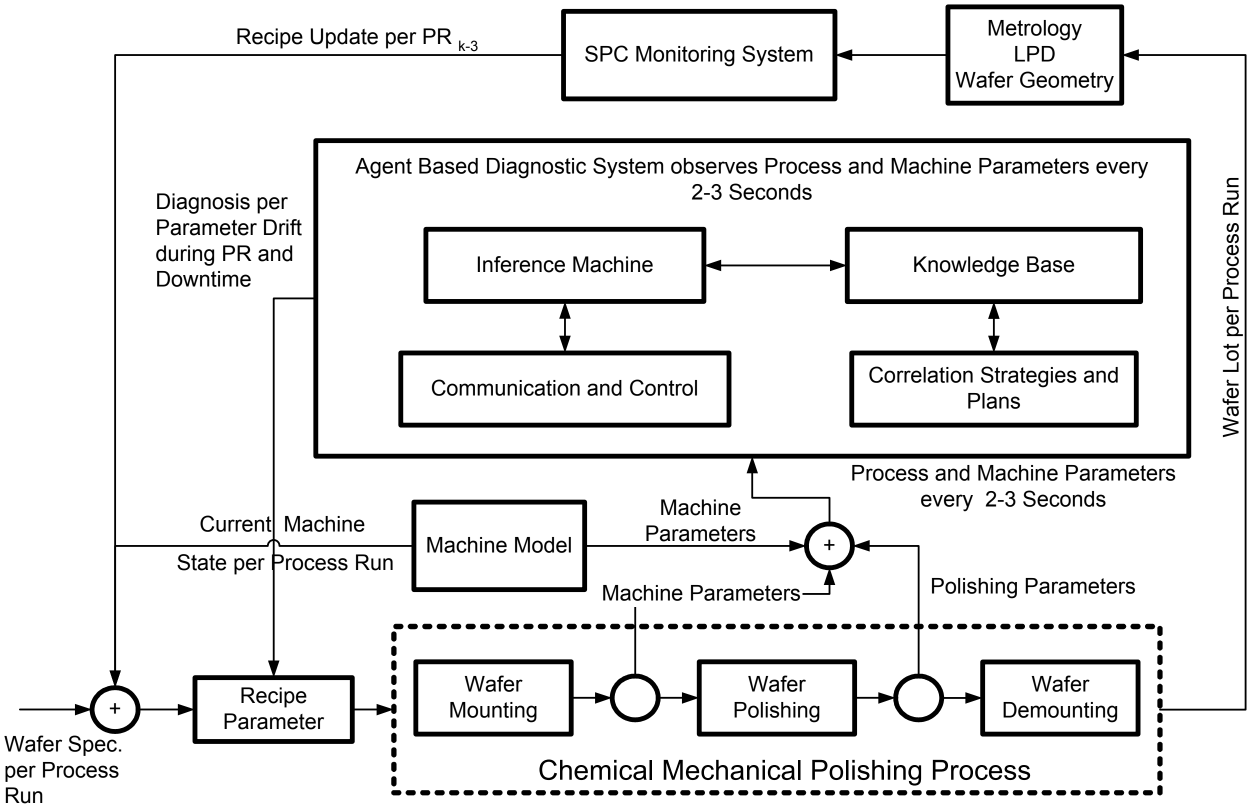


Figure 5.16: Enhancement of CMP process automation controller using agent based diagnostic system for defect analysis during CMP process

As described in chapter 3, section 3.4, the calculation of new process recipe for current process run depends upon the feedback of geometrical indices (chapter 3, sections 3.2.1 and 3.2.2) and process control indices (chapter 3, section 3.2.3) provided by ex-situ metrology tools for a complete wafer lot, after three process runs have been elapsed. This is only possible if there are many wafers, which have been measured without any interruption between the process runs. If there is an interruption between the process runs, the process and machine parameters are then subjected to the changed process conditions, which are then to be considered for the recipe calculation and the previously measured geometrical and process indices provide less information about the current state of CMP process machine.

The advantage of integrating agent based diagnostic system in the process control loop is that the correlation between the geometrical indices (chapter 3, sections 3.2.1 and 3.2.2), process control indices (chapter 3, section 3.2.3) and process and machine parameters is evaluated every 2-3 seconds. The evaluation is based on the process and machine parameters independent of the fact, in which processing state (productive, standby, unscheduled downtime, scheduled downtime, non-scheduled time, and engineering [SEMI E10 2001, SEMI E30 2003, SEMI E58 2001]) the CMP process machine is. The deviation in the behavioral pattern characteristics of the CMP process vector is detected at a very early stage, providing the CMP process automation controller to react not only after the process run, but also during the processing state. The agent based diagnostic system observes and analyzes the CMP process vector in all states also during the CMP process machine downtime, which means, that the defect analysis provides the CMP process automation controller enough information to regulate the process and machine parameters to reach the CMP processing steady state. Thus, the CMP process automation controller possesses enough information at any time to control and regulate the studied CMP process machine, this leads to the enhancement of the process control and process regulation capabilities of the current CMP process automation controller.

Figure 5.17 shows feed forward and feed backward process control loops during the wafer manufacturing process. When the process and machine parameters and the geometrical and the process control indices from the previous process step during wafer manufacturing process are also known, then the agent based diagnostic system after the analysis of these parameters provide control information to the CMP process automation controller to control and regulate the process to improve the product quality.

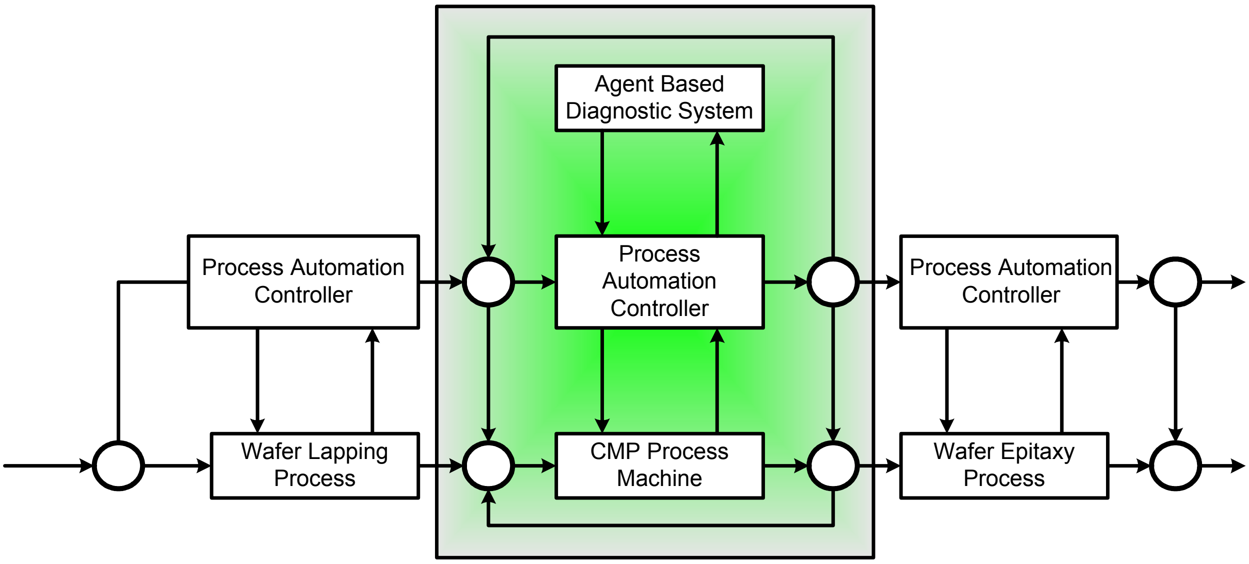


Figure 5.17: Feed forward and feed backward process control loops during the wafer manufacturing process

5.8 Summary

Chapter 5 provides the design of agent based diagnostic system for defect analysis during CMP process and thus building the basis for its implementation. Section 5.2 shows a mathematical model to describe the CMP process and builds the foundation for section 5.3, where CMP process model based on its behavioral pattern characteristics and the correlation model between the defect classes and behavioral pattern characteristics in production environment is developed. The known or unknown defect origination characteristic depends upon the behavioral pattern characteristic deviations of CMP process vector, the time and the CMP process state. The knowledge about behavioral pattern characteristics of CMP process vector increases with time. A defect evaluation and categorizing mechanism is thus provided in section 5.4. Section 5.5 deals with the design mechanisms to diagnose the origination of defects at a very early stage. The diagnostic system uses the temporal representation of CMP process vector, its adaptability to production environment, the knowledge base design and inference engine design, to detect the defect origination at a very early stage. The agent controls and coordinates the defect evaluation system and diagnostic system. The agent communicates with the CMP process automation controller and facilitates diagnostic system with CMP process vector as discussed in section 5.6. The agent based diagnostic system for defect analysis establishes in combination with CMP process automation controller a basis to observe the CMP process vector during processing and thus providing the CMP process engineer at a very early stage the CMP process vector deviations as discussed in section 5.7. The integration of agent based diagnostic system for defect analysis in the complete process control loop provides an advantage, that the process and machine parameters of previous process steps can also be taken into consideration which provide information to the CMP process automation controller how to regulate the current CMP process and machine parameters. The agent based diagnostic system for defect analysis predicts about the future behavioral characteristics of CMP process vector and provides this information to CMP process automation controller for the next CMP process run.

6 Implementation of the agent based diagnostic system for defect analysis during CMP process

The implementation of the agent based diagnostic system for defect analysis during the CMP process encompasses the implementation of a defect evaluation system. Further, it consists of implementation of mathematical and empirical description of CMP process space, defect classes and the inference engine in the knowledge base. Finally, the implementation of an agent for the coordination and communication among the components and the CMP process machine based on the design developed in chapter 5 is done.

6.1 CMP process space determination

For the representation and implementation of problem domain model in the knowledge base, the CMP process space is determined by observing, analyzing and examining the individual or combined influence of all process and machine parameters. Which means, the expected characteristics (chapter 5, section 5.2) and the dynamical characteristics (chapter 3, section 3.3) involved during a particular CMP processing state or processing state transition in the production environment. In this section the process and machine parameter behavior and behavioral patterns from the available process and machine trace data, geometrical and process control indices, SPC trends and wafer data provided by CMP process automation controller are observed, analyzed, examined and finally evaluated to represent them in the knowledge base as designed in chapter 5, section 5.3.1. In the next step the correlation between the expected and the dynamical process and machine parameters characteristics is established by observing the individual interdependencies of process and machine parameters with respect to each other or to geometrical and process control indices or to the observed SPC trends, based on the design in chapter 5, section 5.3.2. Thus observed correlations during a particular processing state or processing state transition are then mapped to the corresponding CMP process behavioral pattern characteristics in the knowledge base. The set of all known or unknown CMP process behavioral characteristics determine the CMP process space in the knowledge base.

6.1.1 Process and machine parameter behavior

A typical scenario during the study of CMP process machine in the production environment, is the polishing pad replacement, which is required due to the deformation (see chapter 3, section 3.1.3) the polishing pad undergoes. The continuous chemical and mechanical interactions are responsible for the pad deformation during a process run; influence the quality of CMP process and thus are responsible for increasing the density of origination of defects leading finally to its replacement. In this section, certain behavior patterns and their mathematical representations of process and machine parameters before and after the replacement of the polishing pad from the polishing plate to implement them in the knowledge base, are discussed. These patterns are typical representatives of the process and machine parameters observed in the production environment as shown in the figures 6.1 and 6.2. The characteristics, shown in the figures 6.1 and 6.2, are the average values during a particular process run taken by process and machine parameters. These average values are then observed during different process runs and the 6^{th} degree regression polynomials are evaluated to represent these characteristics in the knowledge base to follow these characteristics during diagnosing.

In figure 6.1 a the CMP process duration with respect to process run is observed, it shows that the polishing duration before the polishing pad replacement (i.e. from process run 534 till the process run counter is set to zero, when the polishing pad is renewed) increases and after the renewal it decreases, till a steady state is reached. The removal rate is directly influenced by the polishing pad deformation as discussed in chapter 3, section 3.1.3 equations 3.18 – 3.21. The change in the removal rate behavior, as depicted in the figure 6.1 b shows that before polishing pad replacement it decreases until approximately 10.5 µm/min. The removal rate is regulated by changing parameters such as polishing pressure, temperature or effective relative velocity between polishing pad and wafers.This shows a light increase in the removal rate as shown in the figure 6.1 b. The removal rate increases after the replacement of polishing pad up to 15 µm/min, till a steady state of 11.8 µm/min is reached. The removal rate influences directly the wafer geometry and thus plays a very important role for detecting the defect origination at a very early stage. The detection of its deviations during CMP process provide basic fundaments for the diagnostic system to observe the behavioral patterns of the parameters involved and to predict the origination of deviations in the next process runs, thus providing a feedback to CMP process automation controller.

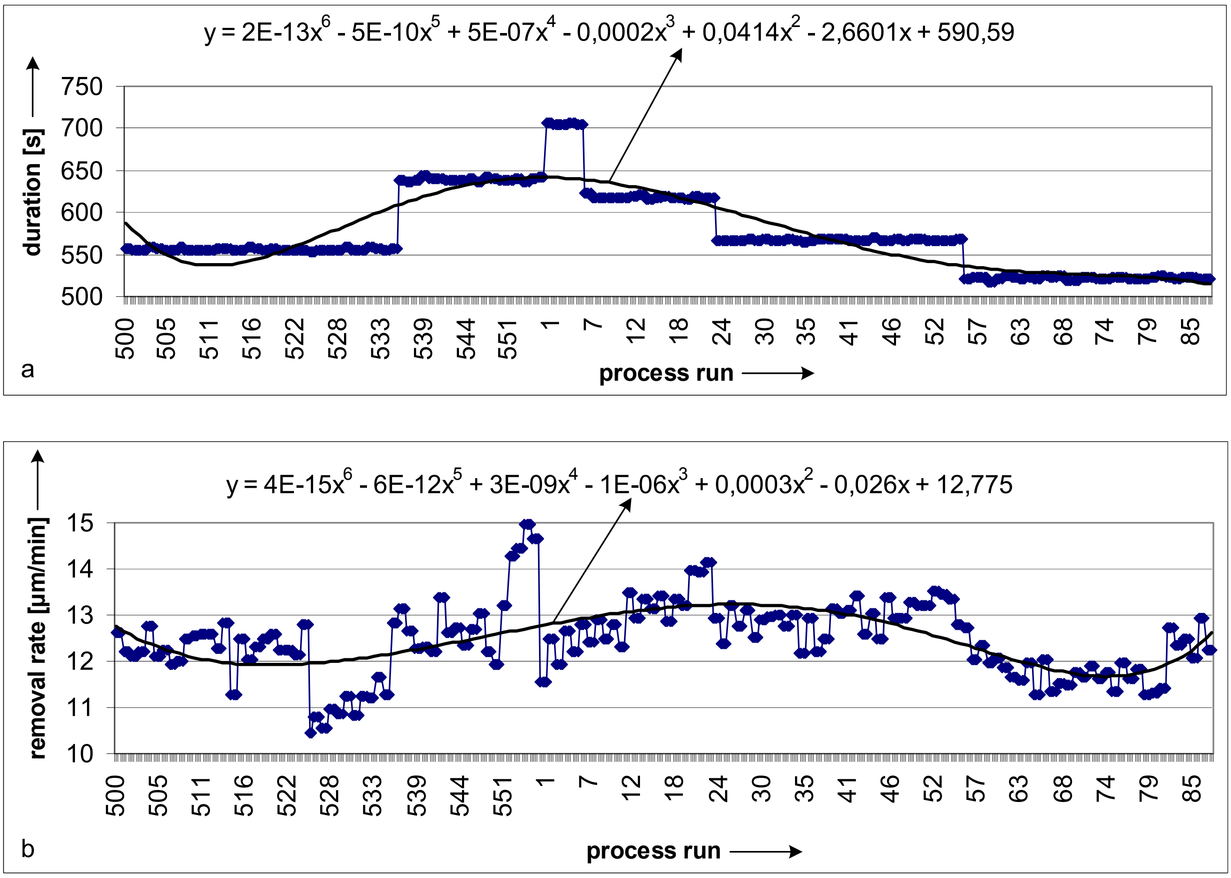


Figure 6.1: Parameter behaviors: process duration (a) and removal rate (b) with respect to process run before and after the exchange of polishing pad

Figure 6.2 a, depicts the oil bath temperature behavior, which is not directly controlled by the CMP process automation controller. This temperature is monitored and it provides the information about the health of the CMP process machine. The oil temperature sinks during the pad replacement process and provides information about the achievement of a steady state during the CMP process to the diagnostic system.

The slurry 3 behavior, as shown in the figure 6.2 b, during the whole CMP process run is controlled by the CMP process automation controller. Any change in its chemical or mechanical behavior, as discussed in chapter 3, section 3.1.3, equation 3.8, influences the removal rate, the process run duration, the geometrical indices and finally the quality of CMP process run. During the CMP process run, the CMP process automation controller controls the volume of this parameter and this value provides information about its viscoelastic characteristics to the diagnostic system. Before the polishing pad replacement, as shown in the figure 6.2 b, the average value per process run starts sinking down to approximately 0 liter and reaches a value of 8 liters during the steady state. During a particular process run the process and machine parameters, as discussed in chapter 3, section 3.3, take different values but show similar behavior as discussed here and provide considerable information to the diagnostic system to detect defect origination.

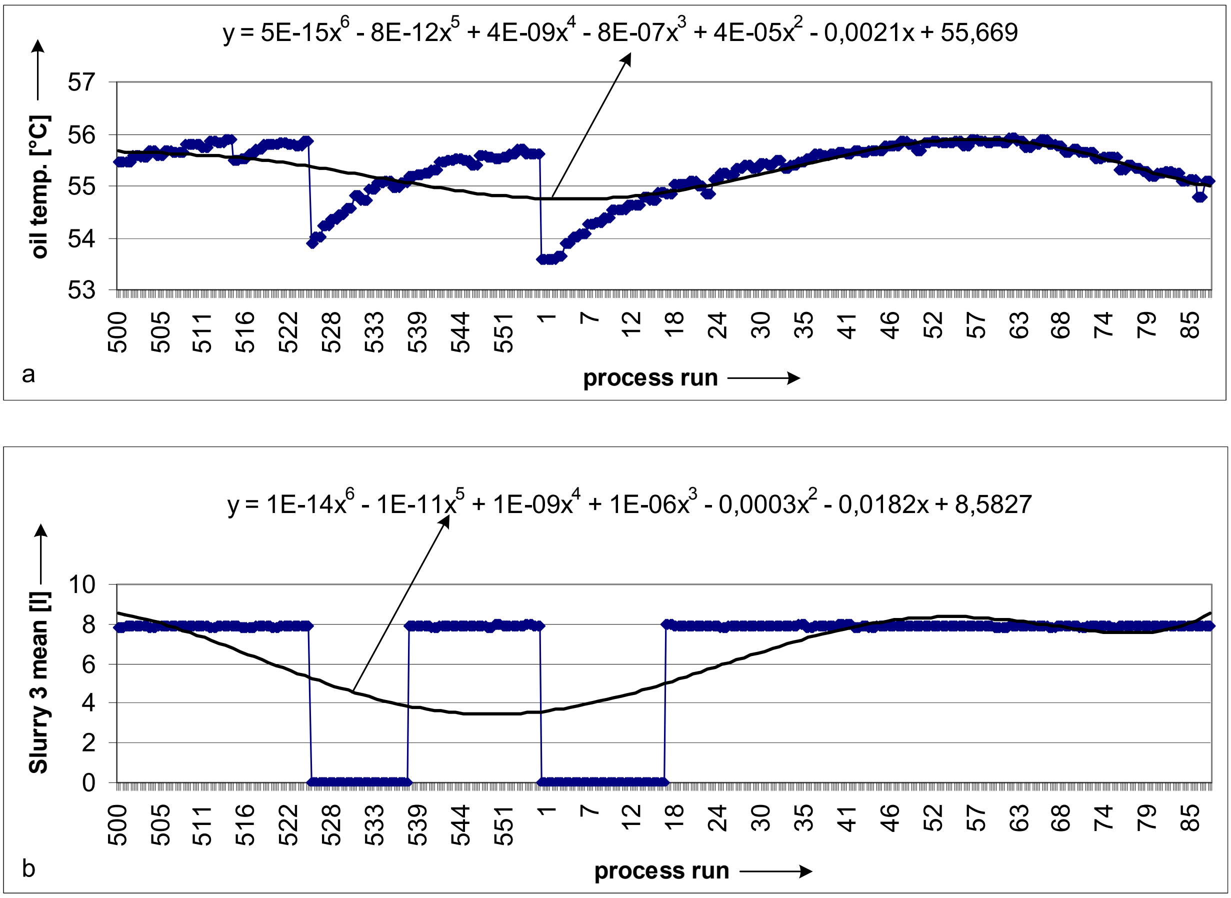


Figure 6.2: Parameter behaviors: oil bath temperature (a) and slurry 3 mean value (b) with respect to process run before and after the exchange of polishing pad

6.1.2 Mapping of the process and machine parameter behavior to the CMP process behavioral patterns

The different CMP process behavioral patterns in the production environment are characterized by the CMP process engineer or CMP process expertise based on the offline measurements made by the metrology tools, which provide information about the wafer flatness (see chapter 3, section 3.2) during a processing state or processing state transition. The geometrical indices and process control indices, thus evaluated, provide the exact information about the behavioral pattern characteristics of CMP process vector. In this section, the mapping between the CMP process and machine parameters behavior patterns and the corresponding geometrical and process control indices is made to determine the behavioral pattern characteristics of CMP process vector, which then is used as basis for describing the CMP process space in the knowledge base. The correlation between every process and machine parameter and evaluated geometrical and process control indices is established in the same pattern as it is described here for the process parameter “temperature of the polishing plate”. This parameter influences the process run duration, removal rate, the slurry flow directly and the oil bath temperature indirectly. Figure 6.3 a shows the behavioral pattern of polishing plate temperature, corresponding behavior of the process control index LT2-4 (figure 6.3 b) and that of geometrical index GFLR (figure 6.3 c) after the replacement of polishing pad, respectively.

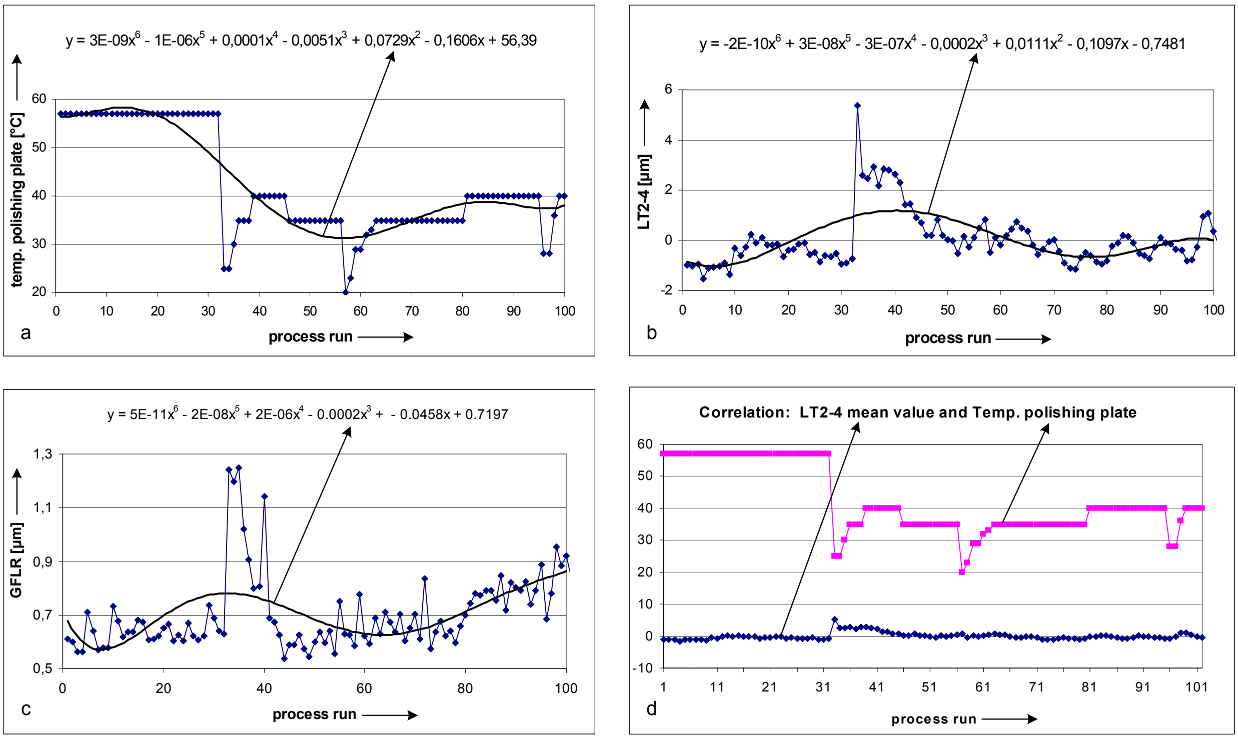


Figure 6.3: Parameter behaviors: polishing plate temperature (a), process control index behavior LT2-4 (b) geometrical index behavior GFLR (c) and correlation between the polishing plate temperature and process control index LT2-4 (d)

The correlation between polishing plate temperature and the process control index LT2-4 is shown in figure 6.3 d. The process control index LT2-4 and geometrical index GFLR are directly affected by the polishing plate temperature deviations thus providing the most probable symptoms to the diagnostic system. At the same time, the geometrical indices SFQR and GBIR and process control indices NLT2-4, E-2 and NLT3-5 (see chapter 3, section 3.2) in figure 6.4 a, and 6.4 b are influenced by the polishing plate temperature.

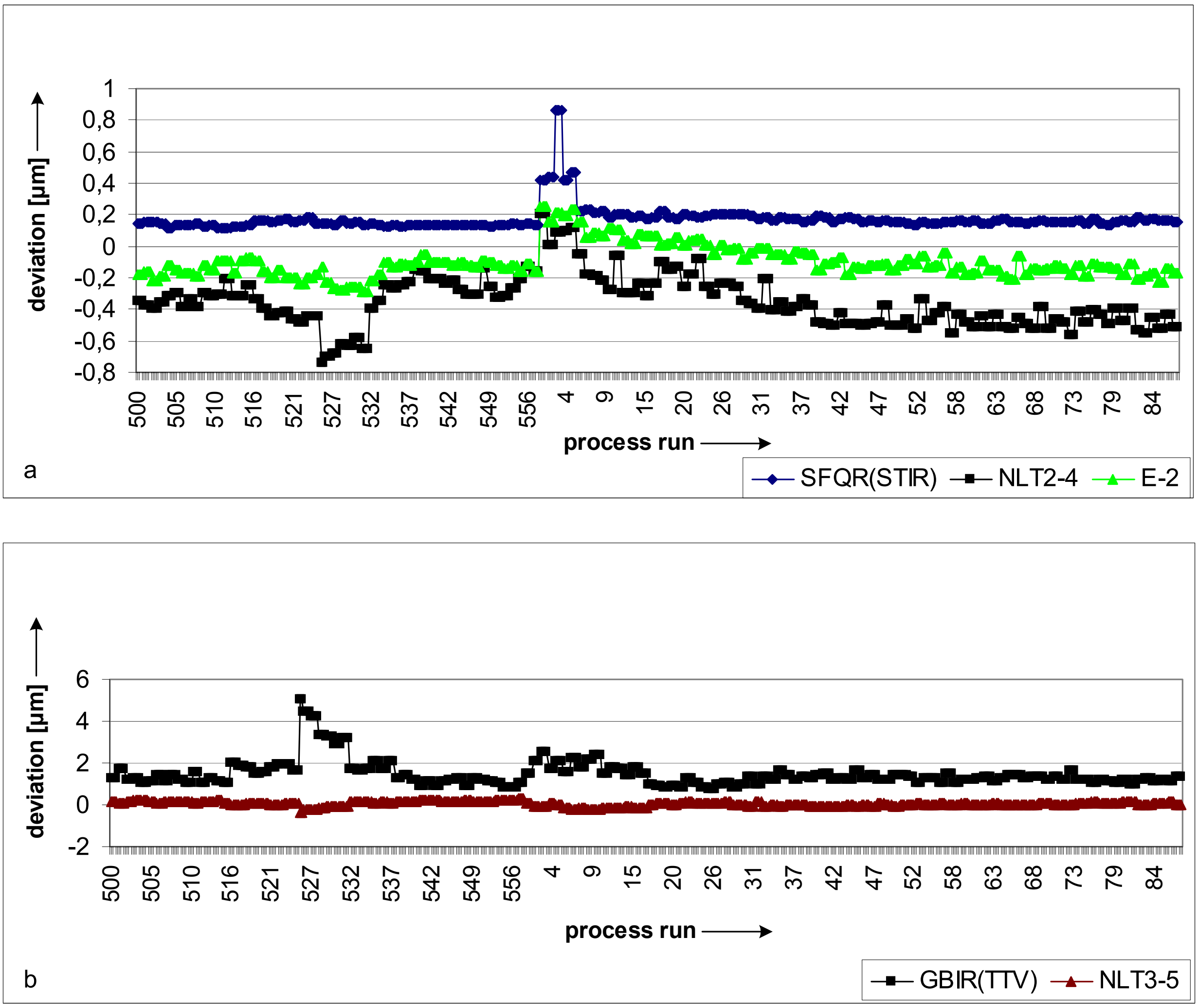


Figure 6.4: Correlation between geometrical, process control indices and polishing plate temperature (continued), geometrical index behavior SFQR, process control indices NLT2-4, E-2 (a), and geometrical index behavior GBIR (TTV) and process control index NLT3-5 (b)

The process and machine parameters behavior, as discussed in section 6.1.1, influence the geometrical and process control indices in the same manner as the polishing plate temperature discussed above. At the same time, these parameters influence each other during the CMP process. For example, the removal rate can be influenced by changing the pressure on the cylinder and by changing the relative velocity between cylinder head holding wafers and the polishing plate (chapter 3, section 3.1.3, Preston's equation 3.1 and the equations 3.2-3.5) and on the other hand the reduction of slurry flow increases the removal rate. All process and machine parameters, discussed in chapter 3, section 3.3 are thus observed during a particular CMP processing state or processing state transition as a whole not individually, thus representing one of the CMP process vector's behavioral pattern characteristics in the knowledge base. Any individual deviation of these parameters can be compensated by the deviations observed in other parameters during a process run, but a shift in the behavioral pattern characteristics of CMP process vector can lead to a particular defect origination. A set of all these characteristics during different processing states or processing state transitions represent the CMP process space in the knowledge base.

6.2 Implementation of defect evaluation system

For the geometrical dimensional conformance of manufactured wafer to DIN norms [DIN 50441/1 1991, DIN 50441/4 1991] and to tolerances specified by SEMI standard [SEMI M1 2002], the process engineering department at WSAG Burghausen has developed its own defect class catalogue (see chapter 3, section 3.2.4). The corrective actions are derived by the process engineers based on their experience, observations and the correlations between the defect classes and geometrical and process control indices (chapter 3, section 3.3) developed by them. The defect evaluation (DE) system incorporates the implementation of defect classes, based on the design discussed in chapter 5, section 5.4 along with responsible process and machine parameters as the basis to start with.

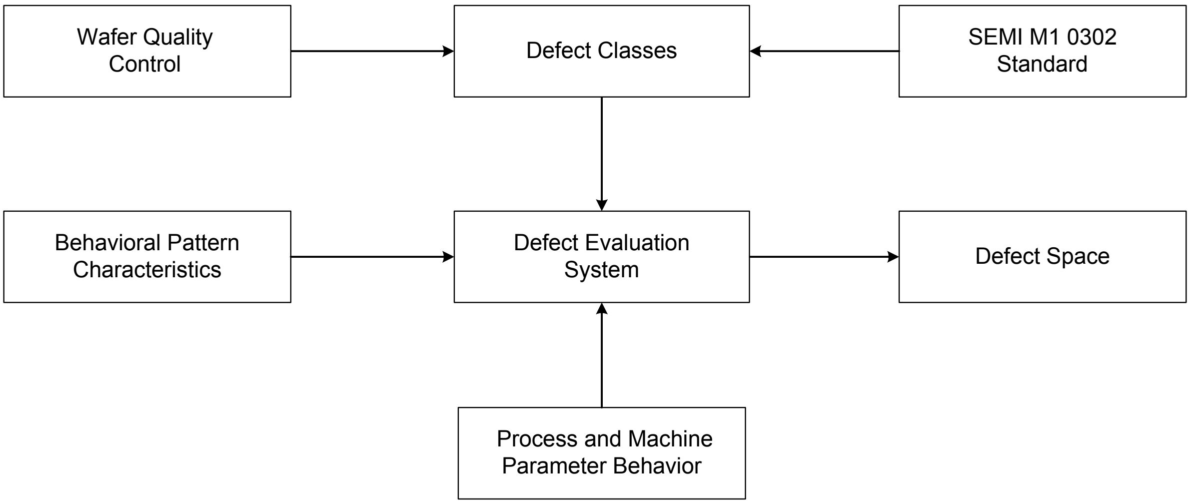


Figure 6.5: Implementation of defect evaluation system

Figure 6.5 shows the implementation of defect evaluation system. The agent provides a set of all behavioral pattern characteristics, a set of all defect classes and a set of all individual process and machine parameter behaviors after collecting them from knowledge base to the defect evaluation system. The implementation comprises instantiation of defect space, as a container object, containing defect class objects. A particular defect class object refers to a list of associated defects and its correlated behavioral pattern characteristic objects each of them refer further to a list of process and machine parameter behavior objects. All these objects are characterized by parameter component [Kumar 1998], a software package implemented for the CMP process automation controller in programming language Java^{TM} (Copyright © 1995-2003 Sun Microsystems, Inc) [Sun 1995-2003] at WSAG Burghausen. The parameter component provides mechanisms to define extend and characterize defect classes, behavioral pattern characteristics, or process and machine parameter behaviors using a parameter definition language (PDL) at any time. The stochastic character of the defect origination characteristics, the discovery of new behavioral pattern characteristics by process engineers or the changed limits of defect tolerances due to new revision of DIN norms or SEMI standards provided by wafer quality control department, enforce dynamic parameter enhancement of these classes during defect evaluation.

The defect evaluation is started by invoking the service “start defect evaluation” by the agent after providing the above parameters along with defect evaluation parameters to tune the defect evaluation algorithm as input. The defect evaluation system returns the defect class container, containing all defect class objects with all its references back to the agent, which further updates the knowledge base. Figure 6.6 shows the implementation of defect evaluation front door component and defect evaluation algorithm component as designed in chapter 5, section 5.4.

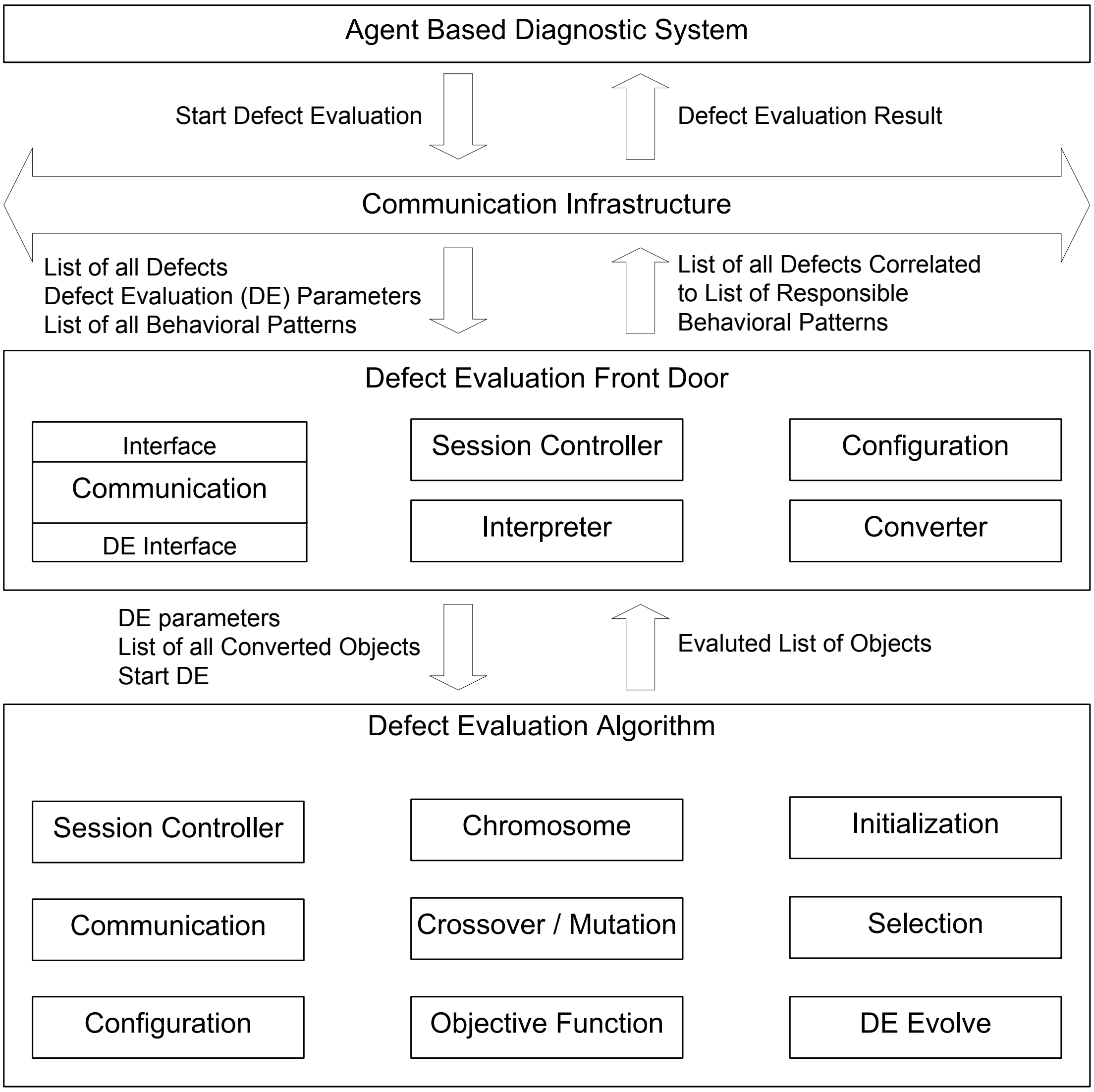


Figure 6.6: Implementation of defect evaluation front door and defect evaluation algorithm

The defect evaluation front door component encapsulates the defect evaluation algorithm component completely. This component therefore provides services to customize and to start defect evaluation algorithm component application. To establish this, it comprises implementation of:

- **Defect evaluation front door component**
  - This component owns, manages and instantiates the communication interface, session controller, interpreter, converter during run time and starts the defect evaluation algorithm component application. The component provides services to configure, to customize and to start defect evaluation algorithms. The component can start many defect evaluation algorithms with different parameter combinations depending upon the parameter settings by calling the service

provided by this component. The default mode is to start one defect evaluation algorithm with its corresponding parameters

- Communication interface: to communicate with defect evaluation algorithm component and agent, described later
- Encapsulated interpreter and converter: the interpreter object interprets the list of all defects, defect evaluation parameters, process and machine parameter behaviors and behavioral pattern characteristics based on the corresponding configuration, which provides the rules for parsing these lists. The converter converts these parsed objects in the object format as required by this component. After this component returns a new list of evaluated defect classes, these objects again interpret and convert objects back to the object lists as required by the manufacturing facility
- Session controller: the session controller object opens a session with the defect evaluation algorithm component to exchange information during computation. A typical session [EJB^{TM} 1998] object is not shared among multiple clients (here defect evaluation front door component instantiating many defect evaluation algorithms see later) as it isolates the needs of this component from the rest of the world. The session object is transaction-aware, updates shared data, is relatively short-lived and is removed when either the session controller or the defect evaluation algorithm component application crashes. The session controller has to re-establish a new session object to continue computation if required

- **Defect evaluation algorithm component**
  - The front door defect evaluation component manager starts defect evaluation algorithm component application, which then provides services to start different instances of defect evaluation algorithms in the distributed environment, if the “number of algorithm parameter” is other than one. The defect evaluation front door session controller (in this case client) opens a session with defect evaluation algorithm session controller (here server) using the configuration for a number of sessions, which depends upon the number of started defect evaluation algorithms. The agent can start different defect evaluation algorithms with corresponding crossover, mutation strategies having different selection and objective functions to search solution space for the potential combinations of process and machine parameter behaviors and behavioral pattern characteristics responsible for defect origination. The defect evaluation algorithm component at first initializes the genetic algorithm (figure 6.6), which evaluates the defect classes by instantiating a list genome having defect classes as genes, each gene is assigned a list of behavioral pattern characteristics generated at random, setting the crossover probability, mutation probability, computation duration, the selection function and the objective function. The implementation of genetic algorithm as designed in chapter 5, section 5.4, used to evaluate defect classes is based on the C++ library “GAlib” version 2.4.5, developed by Matthew Wall [Wall 1996] MIT in 1996. After the initialization the DE evolve class is instantiated and the defect evaluation algorithm is started [Wall 1996]. The evaluated results are then returned back to defect evaluation front door component per session, which passes the results back to the starting entity

6.3 Implementation of agent based diagnostic system

6.3.1 Implementation of diagnostic system

The implementation of the diagnostic system for defect analysis (see chapter 5, sections 5.5) consists of:

- Implementation of knowledge base (chapter 5, sections 5.5.3.1 and 5.5.3.2), i.e. the representation of CMP process space in the knowledge base using rules, decision trees, symptoms, diagnosis and diagnostic hierarchies
- Implementation of temporal representation of CMP process vector (chapter 5, section 5.5.1) in the knowledge base
- Implementation of CMP process vector adaptability to production environment (chapter 5, section 5.5.2)
- The implementation of inference engine component for the in-situ analysis of behavioral pattern characteristics (chapter 5, section 5.5.3.3) representing the CMP process vector

➢ **Implementation of CMP process space representation in the knowledge base**

The implementation of CMP process space representation as designed in chapter 5 and as observed in section 6.1, is done with SOLVATIO® version 2.2.3 developed by IISY AG Germany [SOLVATIO® 2002]. The software provides knowledge based solutions for automated error diagnosis. The knowledge base development kit is implemented in programming language LISP and provides a runtime diagnostic system communication interface in Java™ (Copyright © 1995-2003 Sun Microsystems, Inc) [Sun 1995-2003] to communicate with the agent (section 6.3.2), which further communicates with CMP process machine in the production environment. Figure 6.7 shows the implementation of CMP process space in the knowledge base; it includes the implementation of process and machine parameter behavior (equations 3.1 – 3.40, chapter 3, section 3.1.3 and 3.2) in the production environment. It describes the representation of complete material flow logistics (chapter 3, section 3.1.1) in the production environment of the studied CMP process machine in the knowledge base. The wafer on its way to CMP process undergoes different process steps, performed by the process resources sequentially and during this it is continuously under the influence of changing process and machine parameter behaviors, which determine its quality. The process resources are represented in the knowledge base as question class hierarchy [SOLVATIO® 2002], which is extended by symptom hierarchy by adding the corresponding process and machine parameters as symptom interpretations to these classes. Process resources such as polishing plate, polishing pad extend the symptom hierarchy of CMP process space, as shown in figures 6.7 and 6.8. The set of symptoms (here process and machine parameters) are grouped into two categories based on their time dependencies:

- Time independent symptoms
- Time dependent symptoms: here the values of process and machine parameters are saved from the beginning of the CMP process to observe the time dependent changes of the properties of process and machine parameters

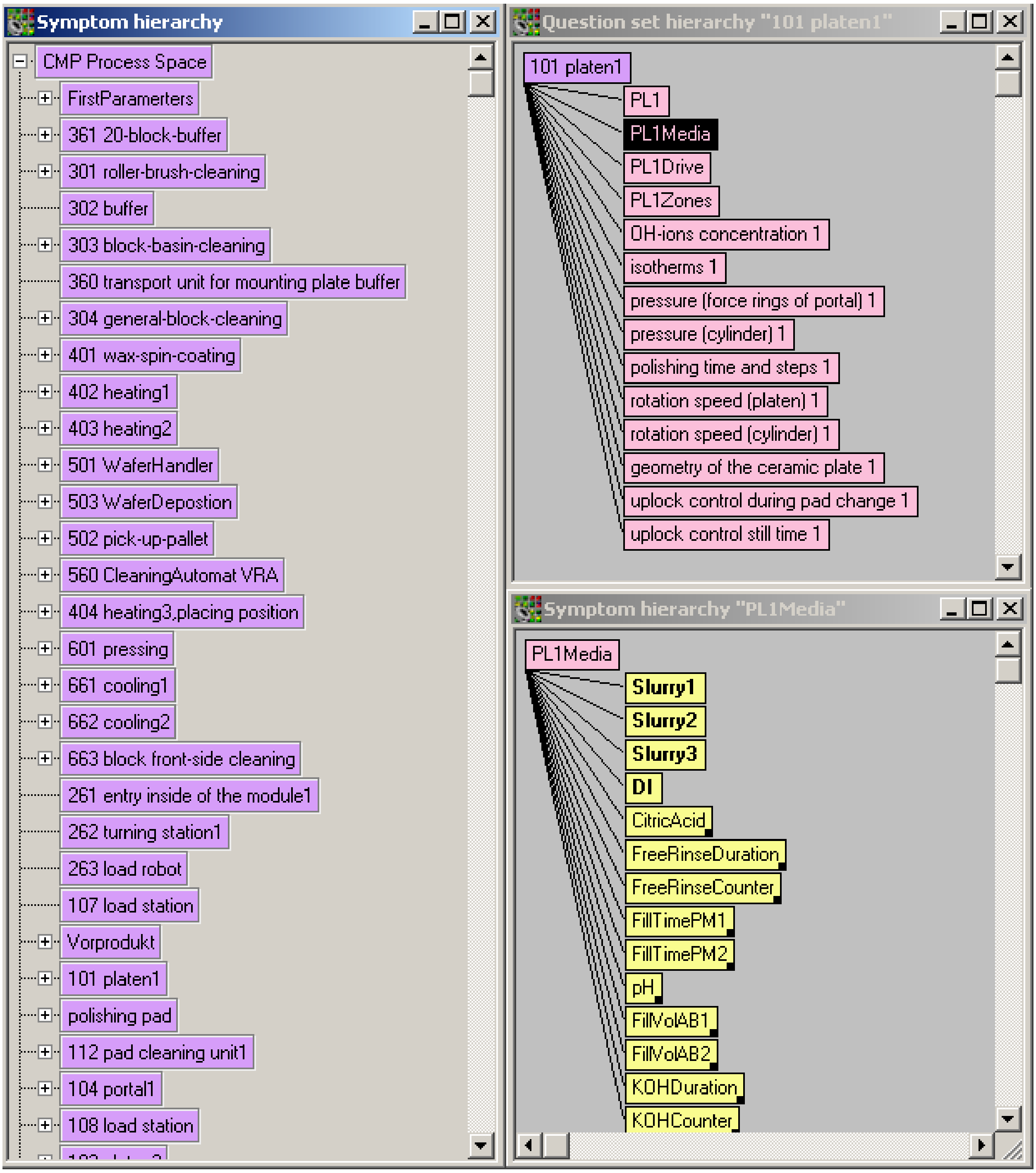


Figure 6.7: Implementation of CMP process space in the knowledge base using question set hierarchy with symptom hierarchy as its extension

The properties of polishing pad figure 6.8 are further described by a set of symptoms such as its “porosity, chemical resistance, thickness and texture, specific gravity, compressibility, hardness, pore diameter and slurry transportation”, also discussed in chapter 3, section 3.1.3, to observe the pad behavior during CMP process. The representation of polishing plate properties, such as “PL1Media” (figure 6.7) and “PL1, PL1Zones and PL1Drive”, as shown in figure 6.8, in the knowledge base provide the symptoms for the diagnostic system during the defect origination phase by indicating a deviation in the corresponding behavioral pattern characteristic, which is responsible for the observation of the behavior of CMP polishing plate.

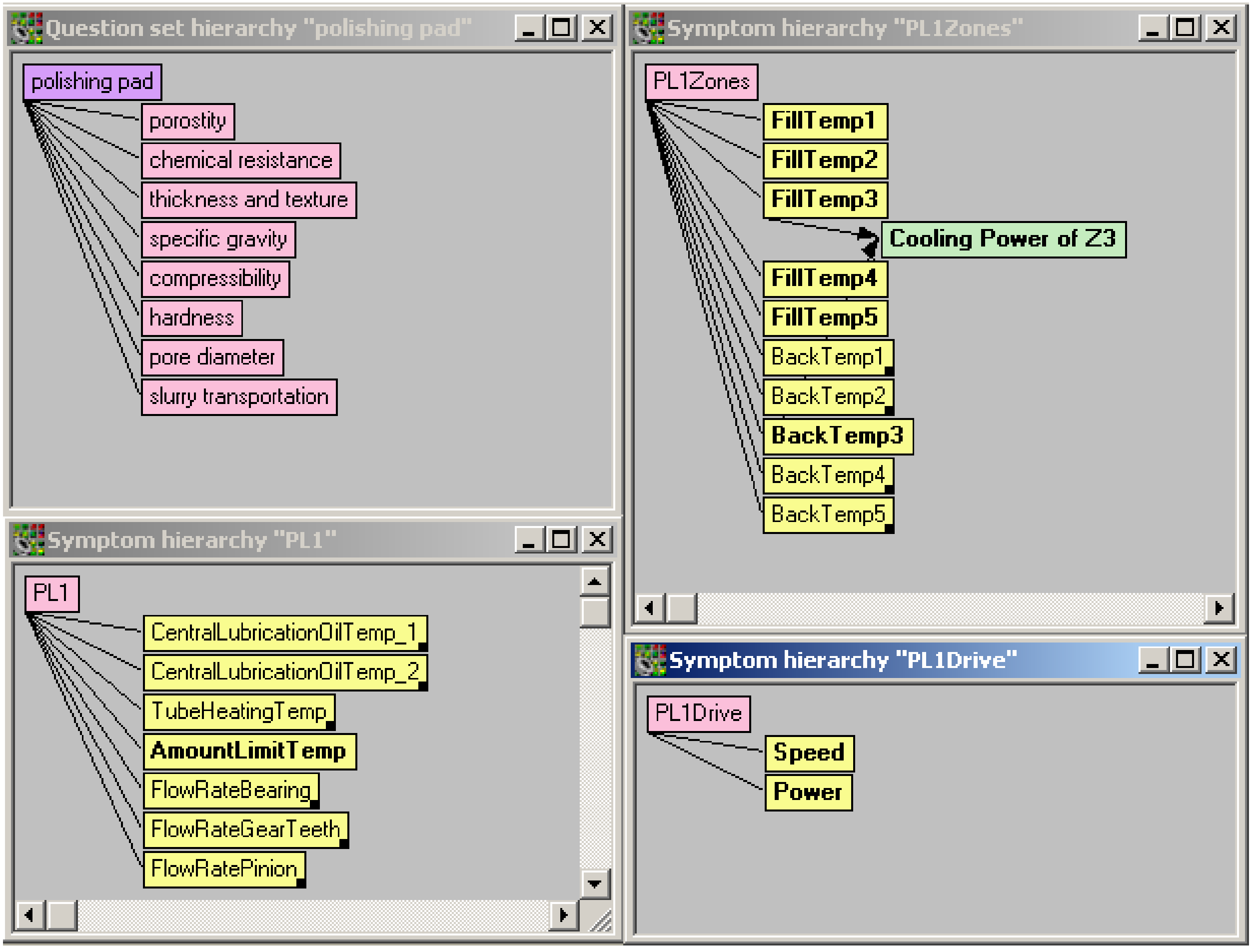


Figure 6.8: Implementation of the polishing pad and polishing plate properties as symptoms in the knowledge base

- **Temporal representation of CMP process vector**

The implementation of time dependent symptoms of CMP process vector (i.e. time referenced behavioral pattern characteristics) and the influencing time dependent process and machine parameters is accomplished in the knowledge base. This is done by implementing the diagnostic rules (i.e. logic operators), conditions and evaluation mechanisms, provided by the knowledge base SOLVATIO® for every symptom, the relationship among primitive temporal objects, the corresponding temporal prediction and the temporal explanation, as discussed in chapter 5, section 5.5.1. The rules and conditions check the coherence of these objects during run time and they provide information about their temporal consistency. The temporal consistency implies checking of new values of a particular process and machine parameter influencing behavioral pattern characteristics, with respect to its past values in the knowledge base, propagating the temporal prediction and providing the temporal explanation by localizing assertions responsible for possible inconsistencies. These temporal inconsistencies provide information about the time dependent changes of the corresponding behavioral pattern characteristics, process and machine parameter behaviors, thus indicating the origination of defect characteristics with a temporal prediction and explanation, which alerts the process engineer, knowledge engineer or the operator to take further corrective actions to avoid the origination of defects. Figure 6.9 and 6.10 show two examples of temporal reasoning implementation. In figure 6.9 the rules for temporal object relationships, as described in chapter 5, section 5.5.1 are implemented using the “FROM, TO” representation, such as “FROM before 16 seconds TO now” for the “increase or decrease of speed by 5 rpm”. The temporal relationship for the parameters, discussed in chapter 3, section 3.3.2, are established to observe their relative shifts and drifts during CMP process.

Derivation of LT2-4:

```
? (P4)  IF              Speed INCREASES 5 rpm [ FROM before 16 Seconds TO Now ]
                OR      Speed DECREASES 5 rpm [ FROM before 16 Seconds TO Now ]
        AND             StepChangeUnLoadV1 holds since 6 sessions
                OR      StepChangedRinseV1 holds since 6 sessions
                OR      StepChangedSoftpolV1 holds since 6 sessions
                OR      StepChangedRemovalStepV1 holds since 26 sessions

? (P4)  IF      Cooling Power of Z3 INCREASES 5 ° C  [ FROM before 24 Seconds TO Now ]
        OR      Cooling Power of Z3 DECREASES 5 ° C [ FROM before 24 Seconds TO Now ]

? (P4)  IF      RemovalStepV1 HOLDS SINCE [ SINCE before 20 Sessions ]
        AND     Slurry1 > 0 l [ Now ]
        AND     Slurry1 = 0 l [ before 1 Session ]
        AND     NOT     Slurry1 IS BETWEEN 0 l AND 0 l [ FROM before 6 Sessions TO before 1 Session ]
        AND             RemovalStepV1 = ESTABLISHED

? (P4)  IF      RemovalStepV1 HOLDS SINCE [ SINCE before 20 Sessions ]
        AND     Slurry2 = 0 l [ before 1 Session ]
        AND     Slurry2 > 0 l [ Now ]
        AND     NOT     Slurry2 IS BETWEEN 0 l AND 0 l [ FROM before 6 Sessions TO before 1 Session ]
        AND             RemovalStepV1 = ESTABLISHED

? (P4)  IF              RemovalStepV1 HOLDS SINCE [ SINCE before 8 Sessions ]
                AND     RemovalStepV1 = ESTABLISHED
        AND             Slurry3 INCREASES 0.5 l [ FROM before 1 Session TO Now ]
                OR      Slurry3 DECREASES 0.5 l [ FROM before 1 Session TO Now ]

? (P4)  IF              RemovalStepV1 HOLDS SINCE [ SINCE before 20 Sessions ]
                AND     RemovalStepV1 = ESTABLISHED
                AND     Slurry1 > 0 l [ Now ]
        AND                     Slurry1 DECREASES 0.15 l [ FROM before 1 Session TO Now ]
                AND     NOT     Slurry1 DECREASES 0.7 l [ FROM before 1 Session TO Now ]
                OR              Slurry1 INCREASES 0.15 l [ FROM before 1 Session TO Now ]

? (P4)  IF              RemovalStepV1 = ESTABLISHED
                AND     RemovalStepV1 HOLDS SINCE [ SINCE before 20 Sessions ]
                AND     Slurry2 > 0 l [ Now ]
        AND                             Slurry2 INCREASES 0.2 l [ FROM before 1 Session TO Now ]
                        OR      NOT     Slurry2 DECREASES 1.5 l [ FROM before 1 Session TO Now ]
                        AND             Slurry2 DECREASES 0.2 l [ FROM before 1 Session TO Now ]
```

Figure 6.9: Implementation of temporal reasoning and process adaptability rules to observe the process control index Linear Taper LT2-4

- **Implementation of CMP process vector adaptability to the changing process conditions in the production environment**

The implementation of the adaptability of CMP process vector to the changing process and production environment during the CMP process is accomplished by defining individually for each process step in the production environment the duration it requires, to achieve the steady state. The behavioral pattern characteristics observation during every process step and the process engineer’s experience provide the steady state behavior of the CMP process machine during these steps. Figures 6.9 and 6.10 show two examples of adaptability implementation, where the process step “RemovalStepV1 HOLDS SINCE [SINCE before 20 sessions]” (figure 6.9) or “StepChangedRemoval-StepV1 holds since 26 sessions” (figure 6.10). The logic operator “HOLDS SINCE” can be set to the observed duration for the adaptation of CMP process vector in the production environment during a particular process step.

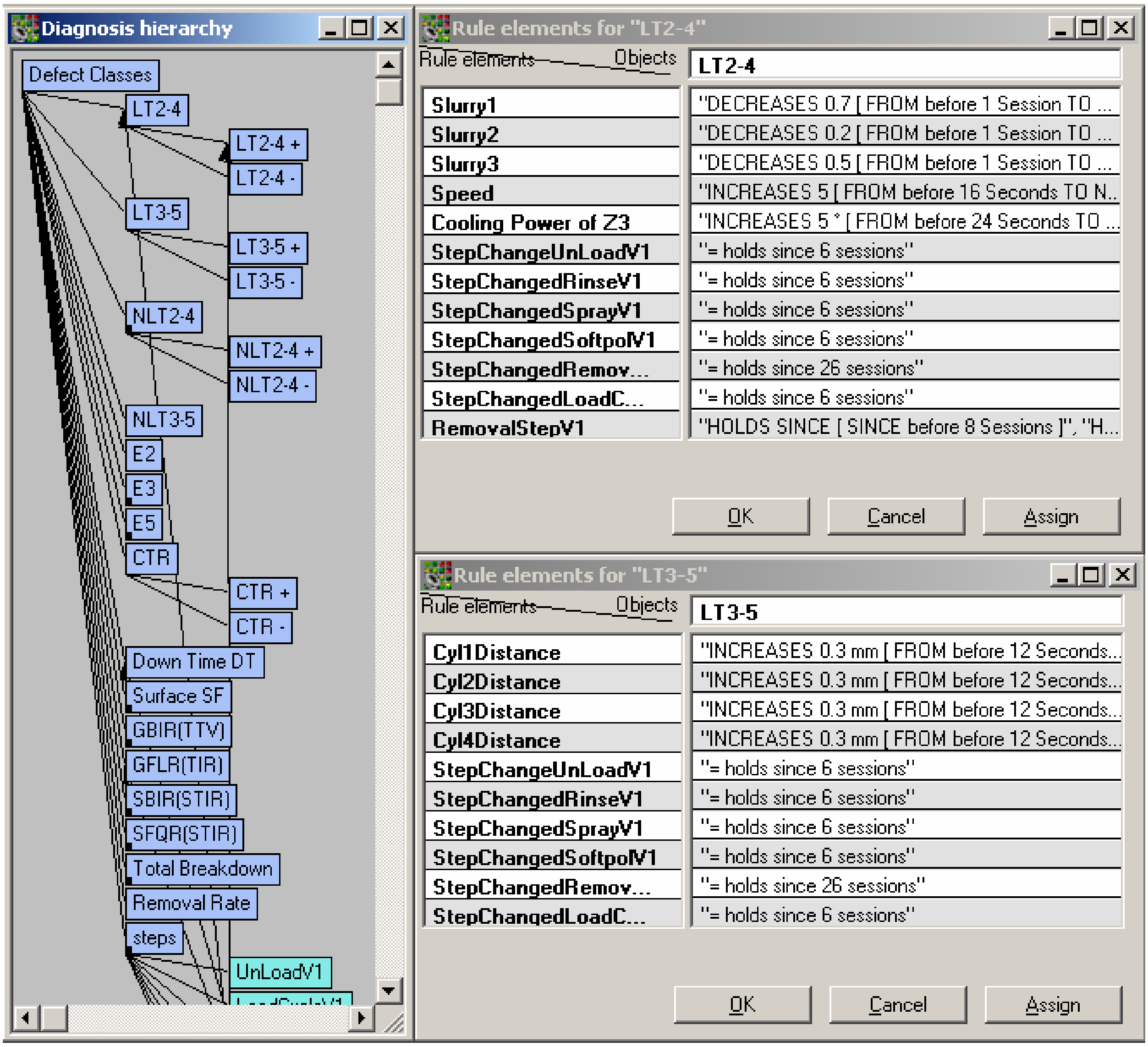
Derivation of Removal Rate:

```
? (P4)  IF            Speed INCREASES 5 rpm [ FROM before 16 Seconds TO Now ]
                OR    Speed DECREASES 5 rpm [ FROM before 16 Seconds TO Now ]
        AND           StepChangedRemovalStepV1 holds since 26 sessions
                OR    StepChangedSoftpolV1 holds since 6 sessions
                OR    StepChangedRinseV1 holds since 6 sessions
                OR    StepChangeUnLoadV1 holds since 6 sessions

? (P4)  IF            Power INCREASES 4 kW [ FROM before 12 Seconds TO Now ]
                OR    Power DECREASES 4 kW [ FROM before 12 Seconds TO Now ]
        AND           StepChangeUnLoadV1 holds since 6 sessions
                OR    StepChangedRemovalStepV1 holds since 26 sessions
                OR    StepChangedRinseV1 holds since 6 sessions
                OR    StepChangedSoftpolV1 holds since 6 sessions

? (P4)  IF            Cyl4Power DECREASES 50 kW [ FROM before 12 Seconds TO Now ]
                OR    Cyl1Power DECREASES 50 kW [ FROM before 12 Seconds TO Now ]
                OR    Cyl2Power DECREASES 50 kW [ FROM before 12 Seconds TO Now ]
                OR    Cyl3Power DECREASES 50 kW [ FROM before 12 Seconds TO Now ]
        AND           StepChangedRemovalStepV1 holds since 26 sessions
                OR    StepChangedSoftpolV1 holds since 6 sessions
                OR    StepChangedRinseV1 holds since 6 sessions

? (P4)  IF            StepChangedRemovalStepV1 holds since 26 sessions
                OR    StepChangedSoftpolV1 holds since 6 sessions
                OR    StepChangedRinseV1 holds since 6 sessions
        AND           Cyl1Power INCREASES 50 kW [ FROM before 12 Seconds TO Now ]
                OR    Cyl2Power INCREASES 50 kW [ FROM before 12 Seconds TO Now ]
                OR    Cyl3Power INCREASES 50 kW [ FROM before 12 Seconds TO Now ]
                OR    Cyl4Power INCREASES 50 kW [ FROM before 12 Seconds TO Now ]
```

Figure 6.10: Implementation of temporal reasoning and process adaptability rules to observe removal rate behavior during CMP process

- **Implementation of diagnostic derivations for defect analysis**

The defect classes origination due to the deviation of geometrical and process control indices, as discussed in chapter 3, section 3.2.4, build the basis for diagnostic derivations for these deviations, the cause for these deviations are most likely the changes in behavioral pattern characteristics, which further depend upon the changes in process and machine parameter behavior combinations. In the knowledge base, these indices are represented by diagnosis hierarchy as shown in the figure 6.11. Figures 6.9 and 6.10 show the rules implemented to derive the deviation of process control index Linear Taper LT2-4 (figure 6.9) and that of Removal Rate (figure 6.10). The symptom interpretations combined with heuristics provide origination probability of a deviation. The heuristic knowledge is derived from expertise of CMP process engineers. The different strategies and plans are developed for the inference engine based on the evaluations of expert's knowledge about how strongly the symptoms or lack of symptoms influences a particular final diagnosis. These strategies and plans are entered in the knowledge base [SOLVATIO® 2002] using heuristic derivation rules such as "a priori occurrence probability of a diagnosis, a priori rules, heuristic derivations and implementation of Bayesian theorem (equations 5.14-5.22, chapter 5, section 5.3.2)". Figure 6.11 shows some of the rule elements for process control index LT2-4 and LT3-5 as an example.



Rule elements / Objects	LT2-4
Slurry1	"DECREASES 0.7 [FROM before 1 Session TO ...
Slurry2	"DECREASES 0.2 [FROM before 1 Session TO ...
Slurry3	"DECREASES 0.5 [FROM before 1 Session TO ...
Speed	"INCREASES 5 [FROM before 16 Seconds TO N...
Cooling Power of Z3	"INCREASES 5 ° [FROM before 24 Seconds TO ...
StepChangeUnLoadV1	"= holds since 6 sessions"
StepChangedRinseV1	"= holds since 6 sessions"
StepChangedSprayV1	"= holds since 6 sessions"
StepChangedSoftpolV1	"= holds since 6 sessions"
StepChangedRemov...	"= holds since 26 sessions"
StepChangedLoadC...	"= holds since 6 sessions"
RemovalStepV1	"HOLDS SINCE [SINCE before 8 Sessions]", "H...

Rule elements / Objects	LT3-5
Cyl1Distance	"INCREASES 0.3 mm [FROM before 12 Seconds...
Cyl2Distance	"INCREASES 0.3 mm [FROM before 12 Seconds...
Cyl3Distance	"INCREASES 0.3 mm [FROM before 12 Seconds...
Cyl4Distance	"INCREASES 0.3 mm [FROM before 12 Seconds...
StepChangeUnLoadV1	"= holds since 6 sessions"
StepChangedRinseV1	"= holds since 6 sessions"
StepChangedSprayV1	"= holds since 6 sessions"
StepChangedSoftpolV1	"= holds since 6 sessions"
StepChangedRemov...	"= holds since 26 sessions"
StepChangedLoadC...	"= holds since 6 sessions"

Figure 6.11: Implementation of geometrical and process control indices as diagnosis hierarchy in the knowledge base

- **Implementation of inference engine for in-situ analysis of CMP process vector**

The inference engine component, responsible for in-situ interpretation of changes in CMP process vector, consists of implementation of algorithms, which use the planning and strategy components of the knowledge base to resolve the potential conflicts and contradictions about the involvement of particular behavioral pattern characteristics during a particular CMP processing state or processing state transition. The derivation graphs as shown in figure 6.12 provide different plans to evaluate a particular deviation of behavioral pattern characteristics (i.e. deviation of CMP process vector, leading to a particular diagnosis).

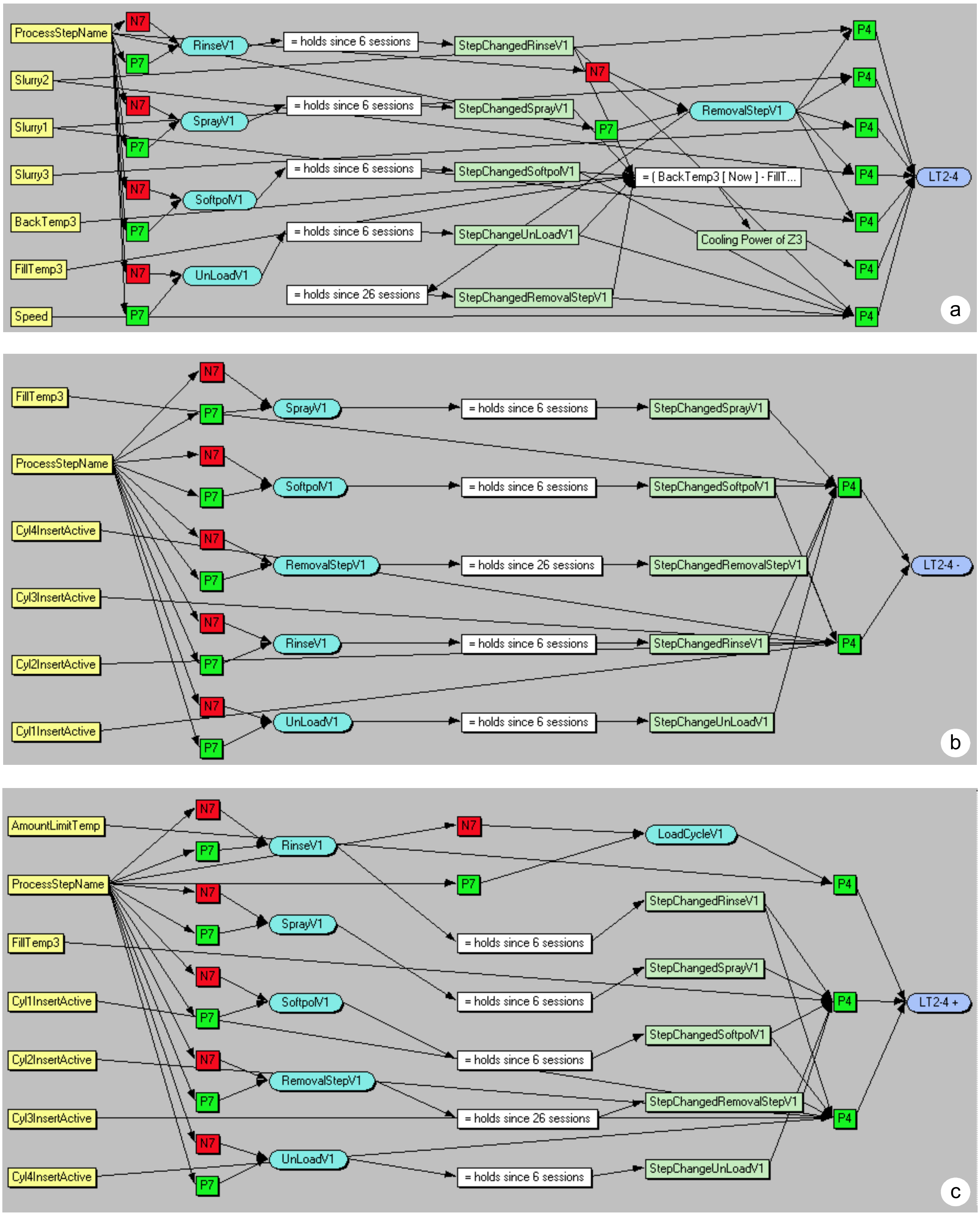


Figure 6.12 Derivation graphs for process control index a) Linear Taper LT2-4, b) negative Linear Taper LT2-4- and c) positive Linear Taper LT2-4+

For example in figure 6.12 a, the Linear Taper LT2-4 can have many paths for its origination. The variation of the volume of process parameter “Slurry1”, “Slurry2” and “Slurry3”, which is the mixture of the composition “Slurry1” and “Slurry2”, leads to the deviations of process control index LT2-4 and the geometrical index GFLR (TIR). Thus, both of these indices deviate simultaneously and to resolve this conflict, at the same time the changes in process parameter “BackTemp3” and “FillTemp3” are observed. The combination of all these observations leads to the conclusion, that process control index LT2-4 is deviating from its normal course. The process parameter “FillTemp3” is also involved in diagnosing process control indices LT2-4- and LT2-4+, as shown in figures 6.12 b, and 6.12 c. Therefore, the inference engine checks all possible strategies and follows the plans to resolve the conflicts to provide most probable involved behavioral pattern characteristics and the related process and machine parameter behaviors for the origination of defects.

6.3.2 Implementation of agent based control

The coordination and control of defect evaluation system and the diagnostic system is achieved by an agent, which also on other hand establishes communication with CMP process machine to collect in-situ process and machine parameter information to accomplish in-situ diagnostics.

Figure 6.13 shows an agent as designed in chapter 5, sections 5.6, 5.6.1 and 5.6.2 communicating with CMP process automation controller through socket interface [Napper 1998] using TCP/IP protocol and with diagnostic system for defect analysis and defect evaluation system using Java^{TM} Remote Method Invocation (RMI) [Sun 1995-2003]. The RMI facilitates distributed computing by invoking remote Java^{TM} objects of diagnostic system for defect analysis and defect evaluation running on different hosts. The agent thus can start the diagnostic system for defect analysis and defect evaluation simultaneously or individually by providing the required information.

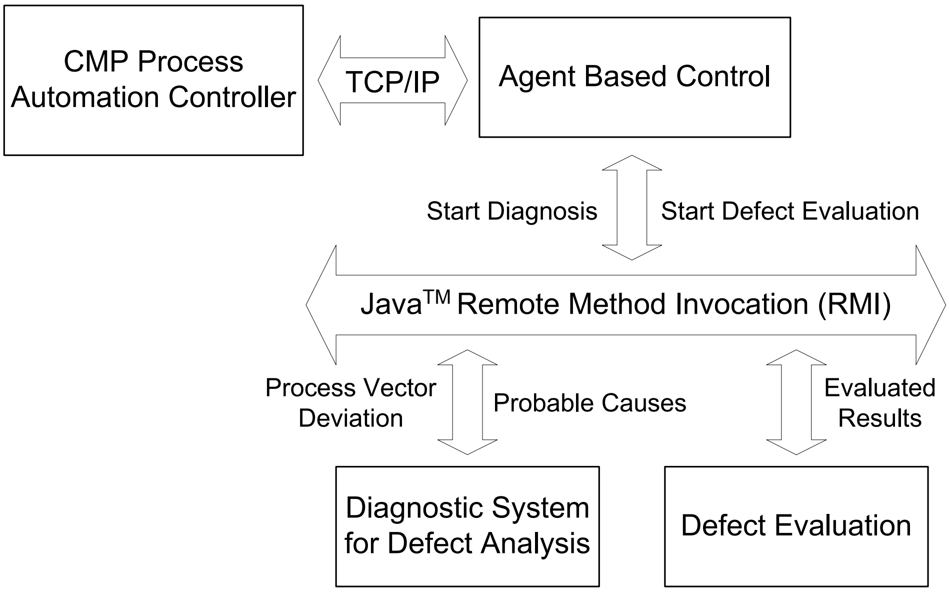


Figure 6.13: Implementation of agent communicating with CMP process automation controller, diagnostic system for defect analysis and defect evaluation system

- **Agent based control**

After starting and establishing the communication with diagnostic system for defect analysis, defect evaluation and CMP process automation controller, the agent enters the state waiting for messages (i.e. it is inactive). As the CMP process automation controller sends a new set of process and machine parameter values, the agent is immediately active, as shown in the activity diagram [Booch 1999] in figure 6.14.

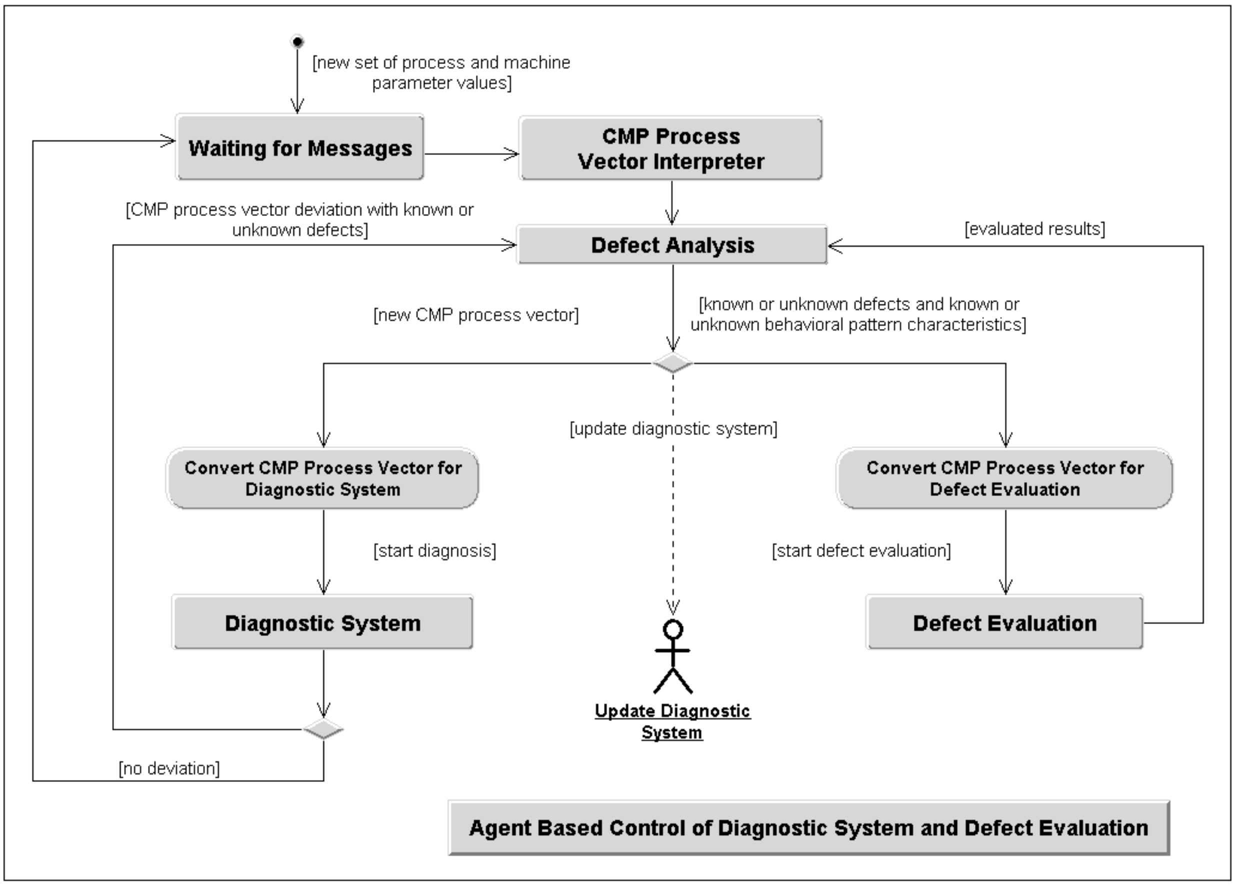


Figure 6.14: Implementation of agent based control for diagnostic system and defect evaluation

The agent interprets the new set of process and machine parameters and it generates a new CMP process vector. The diagnosis is started after the interpretation and conversion of process and machine parameters into the CMP process vector for the diagnostic system. The conversion encompasses the mapping of the process and machine parameters to the variables defined in the knowledge base. The diagnostic system extracts the process and machine parameter values from the CMP process vector and sets correspondingly the knowledge base variables. The inference engine component uses then the plans, strategies and rules as implemented in section 6.3 and evaluates the results. If there is a deviation of CMP process vector and its cause is not explicitly known, the agent or process engineer can start exclusively the defect evaluation. In this case, the agent collects the set of all defect classes, behavioral pattern characteristics, process parameter behaviors, machine parameter behaviors, and provides these to the defect evaluation system, which returns after evaluation the results back to the agent. The process engineer at first analyzes and reviews the evaluated results and then he carries out the diagnostic system update explicitly. The agent thus coordinates and controls both the defect evaluation system and the diagnostic system.

6.3.3 Implementation of communication control component

The defect evaluation system, the diagnostic system for defect analysis and the agent require communication mechanisms to exchange data among each other and internally, as designed in chapter 5, sections 5.4, 5.5 and 5.6. For this reason, a design pattern for communication control component is developed and implemented as a package. All these systems therefore implement this package and define their scope of usage accordingly. Figure 6.15 shows an implementation example of communication control component as a package for the agent. It includes the implementation of communication controller, which is instantiated by the agent and is responsible for establishing communication with defect evaluation, diagnostic system through Java^{TM} RMI and with CMP process machine using socket and TCP/IP protocol. Further the agent instantiates a session controller as shown in the class diagram [Booch 1999] figure 6.15, which opens a session with defect evaluation and diagnostic system to accomplish a secure data exchange between them, after the communication is established. The communication control component implemented for defect evaluation system has an additional implementation of Java^{TM} Native Interface (JNI) to establish communication with C++ environment to start the defect algorithms.

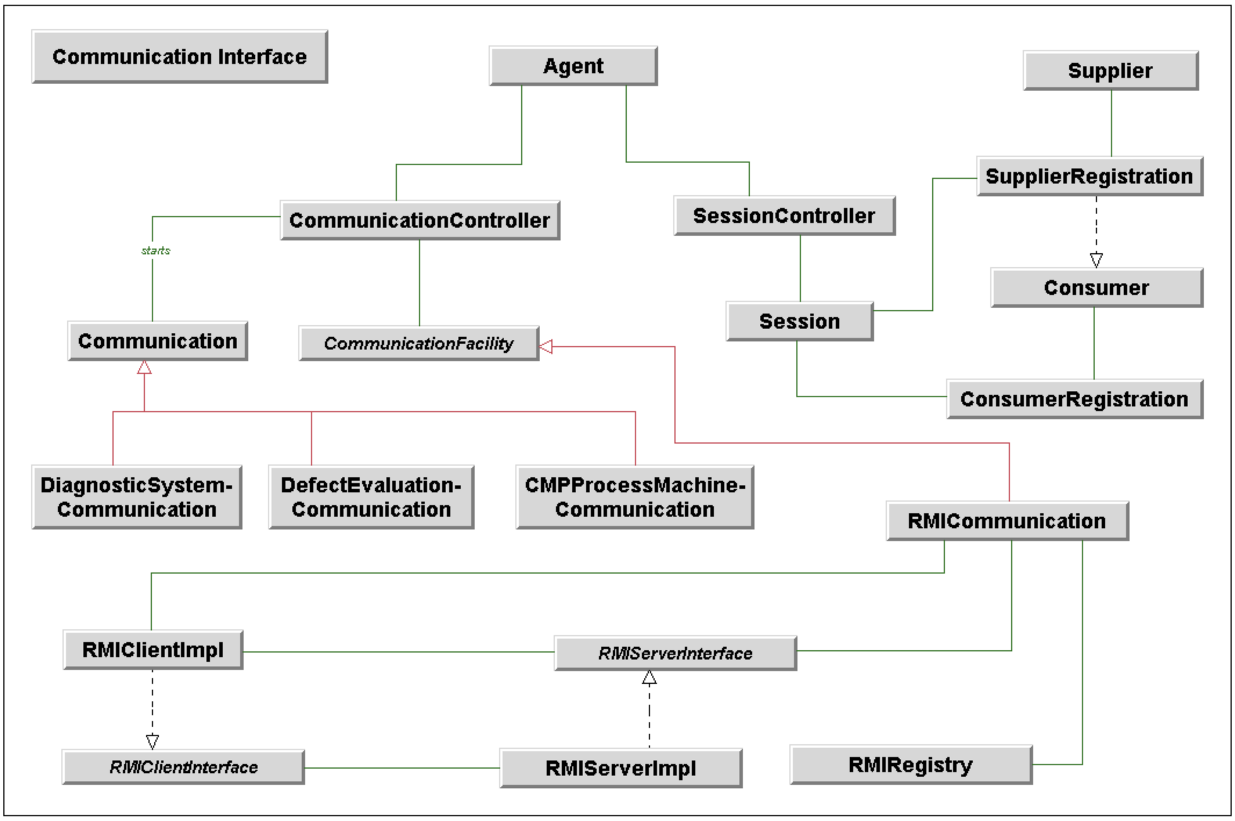


Figure 6.15: Implementation of communication control component as a package for agent as an example

6.3.4 System integration

The defect evaluation system and diagnostic system for defect analysis are independent applications; both of them provide services to be invoked by other applications. The agent establishes communication with both applications and invokes the services for starting defect evaluation or starting diagnostic system thus taking control of these applications. The data required by these applications is collected by the agent and provided accordingly to them, when corresponding services are invoked. Figure 6.16 shows the complete agent based diagnostic system for defect analysis application from the view of process engineer or any manufacturing facility application.

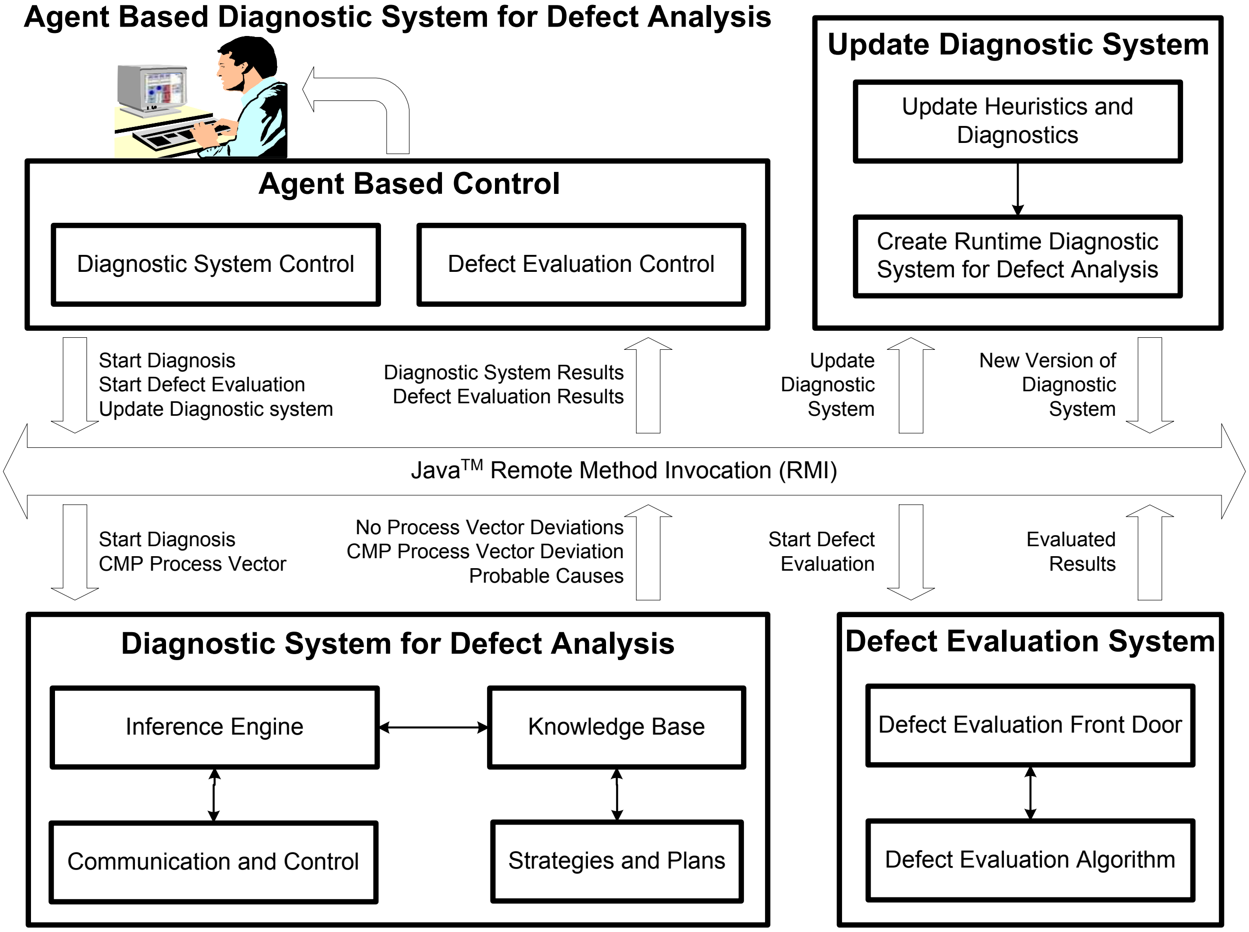


Figure 6.16: Integration of agent based control, diagnostic system for defect analysis, defect evaluation system and update mechanism of diagnostic system

The updating of diagnostic system is integrated only at a message level as shown in figure 6.14. After the defect evaluation, the agent sends a message to the knowledge engineer to update the diagnostic system and provides all the details for the update, i.e. the list of all defect classes referring to the behavioral pattern characteristics and the corresponding process and parameter behaviors. The knowledge engineer updates the knowledge base and generates a new run time updated version of the diagnostic system for defect analysis, which is then automatically used during the next cycle of defect analysis.

- **Implementation of CMP process automation controller enhancement using agent based diagnostic system for defect analysis during CMP process**

The integration of CMP process automation controller and agent based diagnostic system for defect analysis is established using sockets to exchange data between the two applications. In addition to sockets, Java^{TM} RMI can also be used by the CMP process automation controller to invoke the services provided by the agent and exchange data. The CMP process automation controller provides every 2-3 seconds (chapter 5, section 5.7) the process and machine parameter values to the agent, which analyzes and provides results back to the process engineer, who then investigates and validates the results and optimizes the inference strategies and plans in the knowledge base. The agent can be completely integrated in the feed back and feed forward control loops of CMP process automation controller, thus enhancing it by detecting the deviations at a very early stage and supporting CMP process automation controller to take actions (regulate the process and machine parameters) against the origination of defects. The implemented agent based diagnostic system for defect analysis can also receive data from pre CMP process, analyze them and provide these to CMP process automation controller to calculate the new CMP recipe. It can further provide data to the post CMP process if required and thus it can be integrated in the production environment enhancing the current capabilities of CMP process automation controller additionally.

6.4 Summary

Chapter 6 provides the implementation of agent based diagnostic system for defect analysis during CMP process. For the representation of CMP process model in the knowledge base the different CMP process scenarios were investigated (section 6.1). The behavior of process and machine parameters (section 6.1.1) observed was characterized and mapped to the CMP process behavioral patterns (section 6.1.2). The defect classes, behavioral pattern characteristics, process and machine parameter behaviors, thus, observed were represented in the knowledge base SOLVATIO®. This system provides logic operators, rules, conditions, heuristics, decision trees and temporal reasoning (section 6.3.1) to implement symptom hierarchies and diagnosis hierarchies in the knowledge base. The symptom hierarchies, diagnosis hierarchies, strategies and plans are used by inference engine to resolve the conflicts between two contradictory diagnoses. The inference engine is used in-situ to diagnose the origination of deviations in CMP process vector during a CMP process run. The knowledge representation of CMP process space, along with inference engine and communication control component, builds the diagnostic system for defect analysis (section 6.3.1). The defect evaluation system, implemented in section 6.2, provides the possibility to detect and classify unknown defects and their causes. The list of current defect classes and the related behavioral pattern characteristics are then provided back to the agent. The agent provides these results to the CMP process engineer for approval, who finally decides to update the diagnostic system. Section 6.3.2 deals with the implementation of agent based control and communication control component. The communication control component is implemented by the diagnostic system for defect analysis, defect evaluation and by the agent to establish communications among themselves and with CMP process automation controller. The agent coordinates and controls (section 6.3.4) the data flow from CMP process automation controller to diagnostic system for defect analysis, from diagnostic system for defect analysis to defect evaluation system and vice versa, builds together with all these systems an “agent based diagnostic system for defect analysis” application.

7 System test and evaluation in the production environment

In this chapter the agent based diagnostic system for defect analysis is at first installed in the production environment, then tested and finally the applicability and practicability of agent based diagnostic system for defect analysis evaluated against the requirements, as discussed in chapter 4.

7.1 Integration in the production environment

The studied CMP process machine in the production environment is currently regulated by the CMP process automation controller, which communicates with CMP process data monitoring system to calculate a new process recipe for next process run (chapter 2, section 2.3.1). The CMP process automation controller writes every 2-3 seconds trace data in the CMP process run time information data file for every process run. For every process run, a new data file is created and the trace data is appended in this file. The trace data is provided to agent based diagnostic system for defect analysis through sockets using TCP/IP protocol. On the other hand, the CMP process controller still writes the trace data in the CMP process run time information data file per process run. Figure 7.1 shows the integration of agent based diagnostic system for diagnostic system in the production environment.

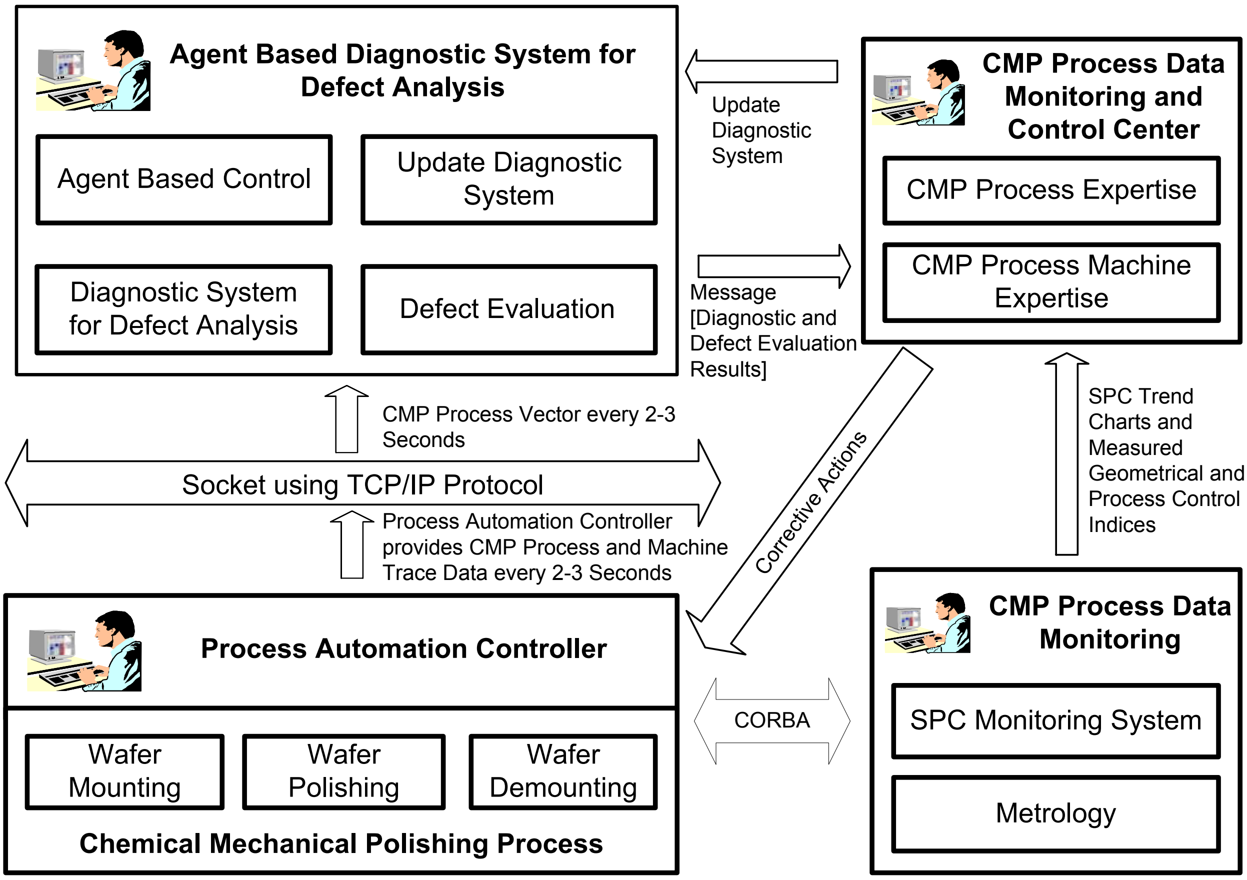


Figure 7.1: Integration of agent based diagnostic system for defect analysis in the production environment

The agent based diagnostic system analyzes the incoming trace data immediately and provides the diagnostic and defect evaluation results to CMP process data control center, where the CMP process machine expertise and CMP process expertise scrutinize these results and correlate them with the results provided by the CMP process data monitoring. Based on the results, the operator on the CMP process takes the corrective actions if required, on the other hand the CMP process machine expertise and CMP process expertise provide information to the CMP knowledge engineer to update the diagnostic system. The diagnostic system requires continuously the inputs of CMP process machine expertise and CMP process expertise to mature and then to provide suggestions for corrective actions directly to the CMP process operator.

7.2 Software quality assurance

➢ Testing of the application

To release the agent based diagnostic system for defect analysis in the production environment, following tests according to testing guidelines [Siegel 1996] were carried out:

- Unit test: the functional and operational tests for defect evaluation system, diagnostic system for defect analysis, agent based and communication control were carried out individually according to the software testing guidelines [Kumar 1999]. The anomalies detected were immediately corrected
- Integration test: at first, the agent and the diagnostic system were integrated together using communication control component. This was done to train the knowledge base to establish the diagnosis. This integration was tested until the diagnostic system started to provide reliable diagnosis. After this, the defect evaluation system was integrated to the agent based diagnostic system, using communication control component and the genetic algorithms were tuned to evaluate the defect classes
- System test: during this phase, the completely integrated system was tested under stress conditions to evaluate the diagnostic performance, defect evaluation performance and its real time behavior. The performance tests for diagnosis were carried out based on temporal reasoning (to test the time database capacity) and adaptability of the diagnostic system to continuously changing CMP process conditions and CMP process environment by providing around 50000 CMP process vectors for a single process run, in the real system its around 300 till 500 CMP process vectors. The performance of defect evaluation system was tested by incrementally increasing the defect classes, related behavioral pattern characteristics, and process and machine parameter behaviors, until the defect evaluation system reached the steady state
- Installation test: after the system test was successful, the installation routine for agent based diagnostic system for defect analysis was generated. This routine provides the different installation steps, which were to be carried out before the final release of the software. The tests involved software installation on a new computer and starting of the “agent based diagnostic system for defect analysis” application

➢ Installation

The agent based diagnostic system for defect analysis, after being thoroughly tested, is installed directly on the CMP process and machine expertise engineer’s computer at WSAG

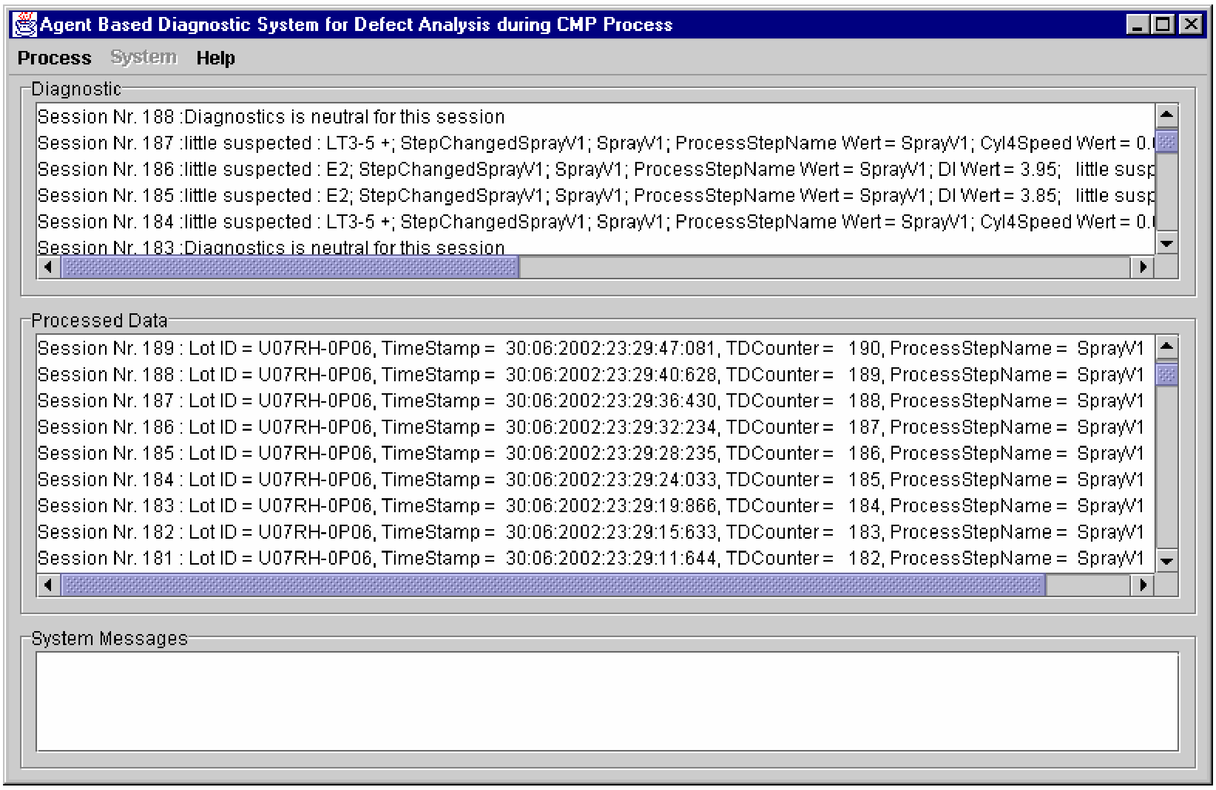
1997-2003 (figure 7.1). The requirement for the installation was to have the Java^{TM} run time environment on the machine and an Ethernet connection to the CMP process machine computer to establish the communication. The SOLVATIO® run time environment and defect evaluation algorithm applications required were also installed on the same computer. The agent based diagnostic system application when started establishes the communications with defect evaluation system, diagnostic system and CMP process automation controller in the background and informs the CMP process expertise if there are errors during initialization. The CMP process expertise then selects the actual updated diagnostic system and waits for the data from CMP process automation controller.

- **Run time testing and evaluation of results**

After the intensive testing and installation the behavior of the agent based diagnostic system for defect analysis during the CMP process was observed and tested in the production environment. The tests were targeted to verify the reliability of the deviations detected by the diagnostic system and its capability to provide the repeatability of the detected deviation.

The trace data is only available from the running CMP process machine in the production environment. Therefore, the tests and the results evaluated here are based on the observations made during the processing states and processing state transitions undergone by the CMP process machine, e.g. the observation of the polishing pad renewal process is only possible after approximately 120 process runs. On the other hand, the wear and tear behavior of the polishing pad and the dynamic adaptability of the diagnostic system to changing circumstances could be easily observed. During all the CMP processing states and the CMP processing state transitions there had been a continuous data flow from CMP process automation controller to the agent based diagnostic system for defect analysis.

The trace data, provided by the CMP process automation controller, is converted into CMP process vector and is provided directly to the diagnostic system by the agent. The diagnostic system analyzes the complete CMP process vector and displays the results in the graphical user interface, as shown in the figure 7.2 and at the same time, it saves only the detected deviations in a file for the CMP process engineer to observe them later. Figure 7.2 shows the deviations detected during the analysis of the CMP process vector during a particular process run. In this case the diagnostic system points out the most probable deviations of CMP process control indices, e.g. LT3-5+, E-2 (figure 7.2), the responsible behavioral pattern characteristics, process and machine parameters, the values taken by these parameters and the process steps during which this deviation is observed. The deviations thus observed are correlated later with the metrology results to verify and validate the observations made by the agent based diagnostic system for defect analysis.



```
Session Nr. 188 :Diagnostics is neutral for this session
Session Nr. 187 :little suspected : LT3-5 +; StepChangedSprayV1; SprayV1; ProcessStepName Wert = SprayV1; Cyl4Speed Wert = 0.
Session Nr. 186 :little suspected : E2; StepChangedSprayV1; SprayV1; ProcessStepName Wert = SprayV1; DI Wert = 3.95;   little susp
Session Nr. 185 :little suspected : E2; StepChangedSprayV1; SprayV1; ProcessStepName Wert = SprayV1; DI Wert = 3.85;   little susp
Session Nr. 184 :little suspected : LT3-5 +; StepChangedSprayV1; SprayV1; ProcessStepName Wert = SprayV1; Cyl4Speed Wert = 0.
Session Nr. 183 :Diagnostics is neutral for this session
```

```
Session Nr. 189 : Lot ID = U07RH-0P06, TimeStamp =  30:06:2002:23:29:47:081, TDCounter =   190, ProcessStepName =  SprayV1
Session Nr. 188 : Lot ID = U07RH-0P06, TimeStamp =  30:06:2002:23:29:40:628, TDCounter =   189, ProcessStepName =  SprayV1
Session Nr. 187 : Lot ID = U07RH-0P06, TimeStamp =  30:06:2002:23:29:36:430, TDCounter =   188, ProcessStepName =  SprayV1
Session Nr. 186 : Lot ID = U07RH-0P06, TimeStamp =  30:06:2002:23:29:32:234, TDCounter =   187, ProcessStepName =  SprayV1
Session Nr. 185 : Lot ID = U07RH-0P06, TimeStamp =  30:06:2002:23:29:28:235, TDCounter =   186, ProcessStepName =  SprayV1
Session Nr. 184 : Lot ID = U07RH-0P06, TimeStamp =  30:06:2002:23:29:24:033, TDCounter =   185, ProcessStepName =  SprayV1
Session Nr. 183 : Lot ID = U07RH-0P06, TimeStamp =  30:06:2002:23:29:19:866, TDCounter =   184, ProcessStepName =  SprayV1
Session Nr. 182 : Lot ID = U07RH-0P06, TimeStamp =  30:06:2002:23:29:15:633, TDCounter =   183, ProcessStepName =  SprayV1
Session Nr. 181 : Lot ID = U07RH-0P06, TimeStamp =  30:06:2002:23:29:11:644, TDCounter =   182, ProcessStepName =  SprayV1
```

Figure 7.2: Graphical user interface showing the observed CMP process vectors and the deviations detected by agent based diagnostic system for defect analysis

Figure 7.3 a, b and c show the number of defects detected during the different CMP process runs (18 till 155), where the CMP process machine had downtimes between the process runs 22-23, 26-27, 41-42, 54-57, 67-69, 124-125 and 149-151. The behavior of removal rate (figure 7.3 a), geometrical index GFLR (TIR) (figure 7.3 b) and process control index LT2-4 (figure 7.3 c) reflect the downtime behavior of the process machine, which is typical, as the feedback information for the CMP process automation controller after the CMP process machine downtime is not available. The CMP process machine requires a certain time to reach steady state. The recipe parameter values are calculated based on the measured values of previous CMP process runs, if the CMP machine downtime is less than 10 minutes. The longer CMP process machine downtime leads to empirical calculations of recipes based on the experience of CMP process expertise. The same behavior is also observed after the renewal of polishing pad. The CMP process automation controller, based on the new pad characteristics and the experience of the CMP process engineers, does the calculation of a new recipe.

The CMP process automation controller provides continuously trace data during the CMP process, even if the machine is down. The agent based diagnostic system for defect analysis analyzes this information and provides the behavior of all process and machine parameters to the CMP process engineer, who then can support the CMP process automation controller, either during the calculation of new recipes or by taking corrective actions. Thus, the agent based diagnostic system for defect analysis provides a continuous observation of CMP process machine.

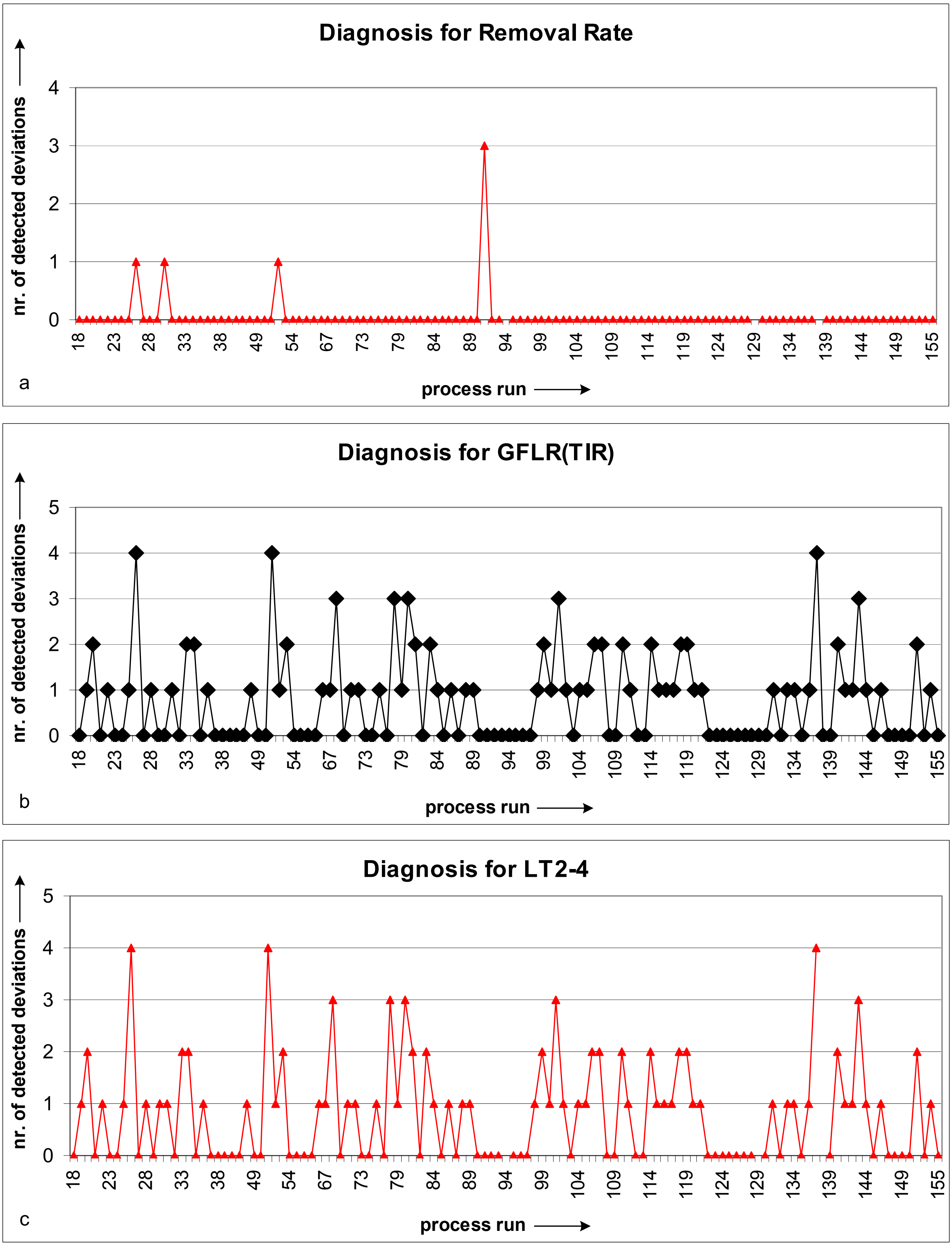


Figure 7.3: Number of detected defects or deviations of geometrical index and process control indices during process run 18-155

Figure 7.4 a and b show the corresponding measurements provided by the metrology department for geometrical index GFLR (TIR), process control index LT2-4 (figure 7.4 a) and removal rate (figure 7.4 b) during process runs 18-155. Comparing the figures it shows that, the agent based diagnostic system for defect analysis detects the origination of deviations in CMP process vectors at a very early stage and can provide this information to the CMP process engineer to take corrective actions.

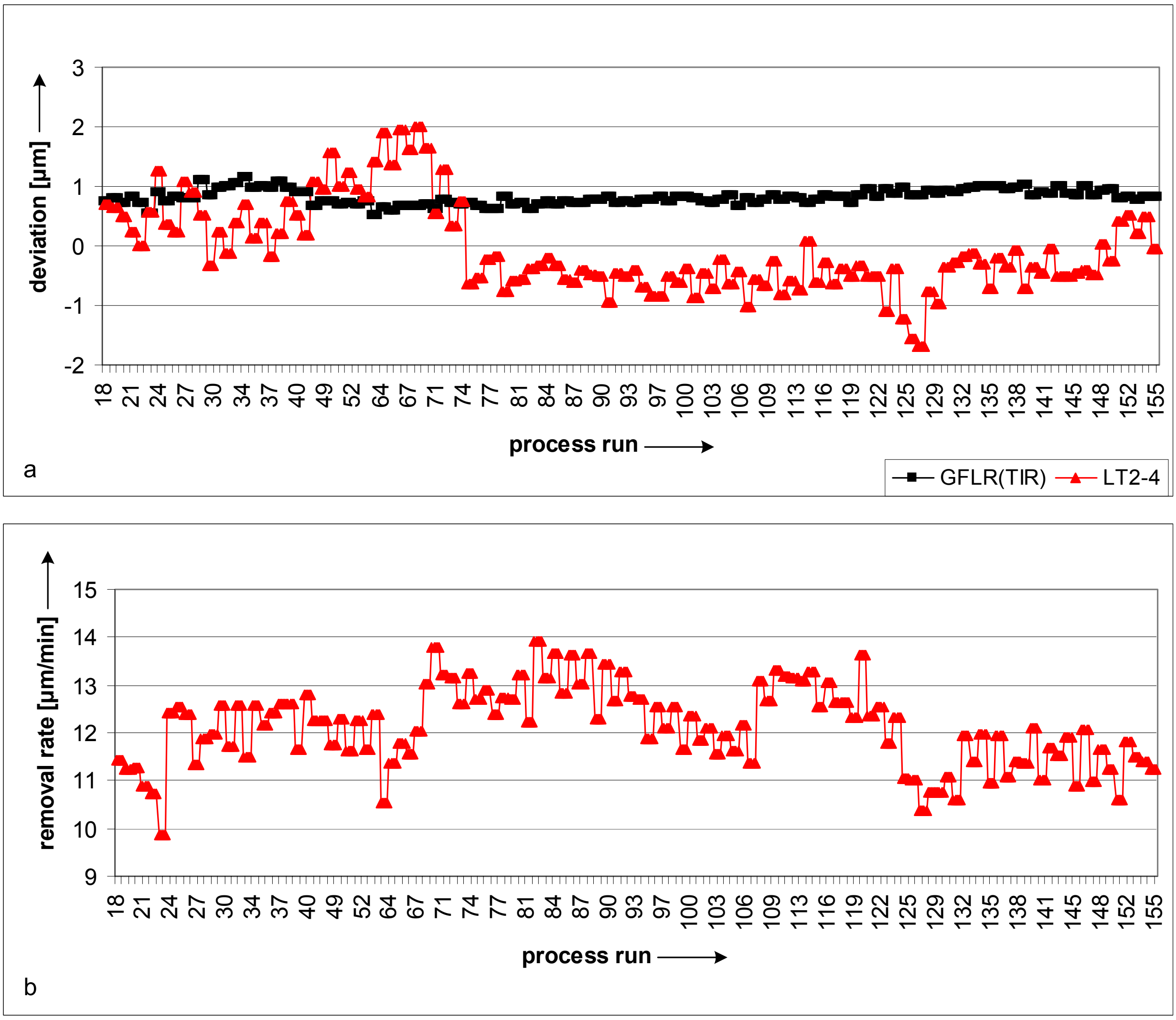


Figure 7.4: The characteristics of geometrical index GFLR, process control index LT2-4 and that of removal rate provided by metrology department

The timely difference between the two observations, figure 7.3 and figure 7.4, is more than 60 minutes, it means the agent based diagnostic system for defect analysis is in the position to detect the deviations earlier and during the process run at the same frequency as CMP process automation controller generates them. In this way, one can easily make predictions about the chemical and mechanical behavior of the CMP process machine.

The defect evaluation system provides the corresponding solutions in the background to evaluate the defect classes in the case of conflicts detected by the inference machine, which then were validated by CMP process expertise and CMP process machine expertise leading to the continuous improvement of in-situ diagnosis. It took almost a year to observe the different processing situations and to develop the corresponding interpretations for the knowledge base, where the defect evaluation system continuously provided the defect classes and related behavioral pattern characteristics to update the knowledge base. The defects and the related behavioral pattern characteristics, which were detected, but could not be assigned in the beginning, were stored in the knowledge database. They were taken into consideration every time, the defect evaluation was started, and then they were evaluated one after another. The detection of new defect classes lead to the simplification of the reasoning and inference mechanism in the diagnostic system.

7.3 Applicability and practicability evaluation

The agent based diagnostic system for defect analysis during CMP process developed and implemented within the scope of this work is implemented in Java^{TM} and ANSI C++. The software architecture is flexible, extendable and supports distributed computing, can be installed on heterogeneous platforms. The intensive testing of this software before it was installed in the production environment shows its high availability.

The main purpose of the agent based diagnostic system for defect analysis during CMP process is to detect not only the origination of defect at a very early stage, but also the exact characterization and localization of origin of these defects. This was achieved after long-term training of the inference engine in the diagnostic system and updating the knowledge base after every defect evaluation cycle. The inference engine provides exactly the cause, involved behavioral pattern characteristics, related process step and the involved process and machine parameter behaviors for the detected defect origination characteristics to the CMP process expertise, who can then further decide to take the corresponding corrective actions. Another challenge was the detection performance, detection reliability and the detection repeatability; this was achieved by very intensive observation of CMP process machine over a year and then implementation of these observations in the knowledge base using logic operators, rules, conditions, heuristics, conditional probabilities, and Bayesian theorem. In addition, the defect evaluation system enhanced the inference capability of the diagnostic system. The defect evaluation system provided the evaluation of defect classes by using genetic algorithm, which searches for the potential solution space for defect classes and related behavioral pattern characteristics in the CMP process space and provides a potential solution. This potential solution is then used to update the knowledge base thus simplifying the conflict resolution potential of the inference engine thus speeding up the inference cycles.

Another important factor was the time representation of the properties of CMP process and machine parameters and their adaptability to the changing CMP process and production environment. This was implemented by using temporal reasoning component provided by the knowledge base. It provides mechanisms to exactly track the time representation of behavioral pattern characteristics and process and machine parameter behaviors, during the analysis of the CMP process vector by the inference engine. At the same time, this time representation implementation adapts to the property changes occurring during a particular process run. It appears as if the diagnostic system synchronizes with the CMP process machine and reaches the steady state, as the CMP machine does in production environment.

The integration of an agent based diagnostic system for defect analysis during CMP process with CMP process controller in the production environment facilitates in-situ detection of origination of defects. Due to in-situ integration of agent based diagnostic system for defect analysis, it was possible to observe the machine downtime behavioral pattern characteristics of CMP process machine.

7.4 Summary

Chapter 7 shows the testability, the applicability and the practicability of the agent based diagnostic system for defect analysis during CMP process in the production environment. The software, as designed in chapter 5 and as implemented in chapter 6, is at first tested intensively (integration tests and system tests section 7.2) and then integrated (section 7.1) by installing the software on the computer of CMP process and machine expertise and then establishing communication with CMP process automation controller in the production environment through sockets. The run time testing (section 7.2) of the agent based diagnostic system for defect analysis shows that the detection of defect origination during a process run correlates with the observations provided by the offline metrology tool. Section 7.3 shows that the requirements R 1 – R 12, as discussed in chapter 4, section 4.1, are fulfilled by the agent based diagnostic system for defect analysis, during CMP process and the main objectives (chapter 4, section 4.2ing CMP process and the main objectives (chapter 4, section 4.2) of the research work are also achieved.

8 Conclusions and the future work

The rapidly changing technological characteristics of Integrated Circuits (i.e. their compactness and density) require a very high surface planarity and uniform surface topography of the starting substrate material (wafer). The IC manufacturers are demanding wafers with continuously decreasing defect densities, very tight tolerances and very short delivery times, from the wafer manufacturers. The in-situ defect detection, the real-time analysis of non-visual defects, the simultaneous differentiation of multiple defect types and the high capture rates of the detected defects are turning out to be the major challenges for the wafer manufacturers. The current wafer manufacturing process is very complex and has already a very high technical and organizational availability.

As a final step in the manufacturing process of wafers, CMP process has emerged as a critical technology for achieving the required global planarization. The high complexity of the CMP process makes the localization (i.e. to find out the defected area, the type and the cause) and control of the process and machine parameters responsible for defect origination during a process run very difficult. This leads to intolerable machine downtimes, caused by the time-consuming defect localization procedures. The deductions of corrective actions and the establishment of correlations between the detected defects and the process parameters are mostly based on the long year CMP process experience of the process engineers.

The state of the art to analyze the investigated defects is to correlate these defects with the drifts and shifts of process and machine parameters offline, i.e. after the defects are already there. To avoid the undesired defect origination and machine downtimes, different process control approaches currently deployed were investigated. At first, the process control approaches deployed for CMP process were examined. Then the research was extended to evaluate the process control approaches for other process machines in the semiconductor manufacturing facility, such as Plasma Etch process machine, CVD process machine and photolithographic process machine. The investigations showed, that the deployed process control approaches did not detect the origination of defects during processing. However, for the Plasma Etch process and CVD process machines, it was possible to detect defects with additional integration of impedance sensors. Nevertheless, none of the process control approaches showed the adaptability to continuously changing process and production characteristics in the production environment. The time representation of the properties of process and machine parameters was not implemented by the investigated process control algorithms, and none of them provided much information about the chemistry of the CMP process.

Within the scope of this work, the theoretical and problem domain analysis of CMP process was carried out systematically to understand the CMP fundamentals, based on physical models in conjunction with experimental data, provided by the wafer manufacturing facility (WSAG 1997-2003, Germany). The theoretical analysis showed, that the steady state of CMP process machine is a dynamical balance between the mechanical actions at pad and wafer surface, chemical actions of slurry weakening the atomic or molecular layer of the wafer surface, and the slurry particles along with the pad asperities responsible for the final removal of material from the wafer surface. Any drift or shift of this dynamical balance leads to origination of defects, which are then correlated to the geometrical measurements provided by ex-situ metrology. The wafer surface quality (specified by geometrical and process control indices) is an indication of the expected yield and the reliability of the CMP process. Every wafer thus produced by the CMP process is measured and checked against the geometrical specifications (DIN 50441/1, DIN 50441/4, SEMI M1 2002). The deviations of the specified geometrical and process control indices lead to undesired defects. These defects can have many probable process and machine parameters as their causes. The determination of the exact source of the defect originator becomes very complicated. Thus, the behavior of all process and machine parameters from the beginning of the CMP process in all its processing states should be observed and the exact influence of all these parameters should be known. It becomes even more complicated to find out the unknown influence of the known parameters.

The consolidated findings lead to the conclusion, that the interaction dynamics of process and machine parameters during CMP process requires a system, which observes all the process and machine parameter behaviors from the beginning of the CMP process. The system has to learn the CMP process behavior to predict, to localize, to represent and to provide the possible corrective actions in order to avoid the occurrence of defects during CMP process.

The core of the research work is to develop and implement an agent based diagnostic system for defect analysis during CMP process for the studied CMP process machine. The system should detect the origination of defects at a very early stage during the wafer manufacturing process. It should reduce the defect densities, improve the reliability and accuracy of the process run by in-situ observation of the CMP process, provide the corresponding corrective actions to the process engineer, reduce the risk of defect occurrence, adapt to the changing CMP processing characteristics and environment and observe explicitly the changing time-dependent properties of process and machine parameters.

To achieve this at first a mathematical model to describe CMP process was developed. This model was used as basis to describe the process and machine parameter behaviors and the behavioral pattern characteristics of CMP process. Further, it was used to build the correlation model between the defect classes and behavioral pattern characteristics in production environment. To evaluate and categorize the detected known or unknown defects, a defect evaluation system was designed. This component uses genetic algorithms to classify defects and the related CMP behavioral pattern characteristics. In the next step, a complete design of diagnostic system was developed with an in-built knowledge base and inference machine to diagnose the observations. The diagnostic system design included the time representation of the process and machine parameter properties using temporal reasoning, as well as the adaptability of observed process and machine parameters to the continuously changing CMP process and production characteristics. The design of the agent that controls and coordinates both the defect evaluation system and diagnostic system was developed as next. A framework was designed to establish communication between the defect evaluation system, the diagnostic system and the agent. The agent shall establish the communication with the CMP process automation controller to facilitate the diagnostic system with CMP process vector. The design facilitates the agent based diagnostic system to be integrated into the complete process control loop.

After the completion of the design, the whole system was implemented in small steps, which included at first the representation of CMP process space in the knowledge base SOLVATIO®. The representation in knowledge base was done by a very thorough observation of CMP process, involved process and machine parameters and the corresponding observed defects during different processing states and processing state transitions. Thus every known or unknown defect, the related behavioral pattern characteristics and process and machine parameter behaviors were described in the knowledge base, using logic operators, rules, conditions, heuristics, decision trees, temporal reasoning to implement symptom hierarchies and diagnosis hierarchies in the knowledge base. The symptom hierarchies, diagnosis hierarchies, strategies and plans were used by the inference engine to resolve conflicts between two contradictory diagnoses. The inference engine is used in-situ to diagnose the origination of deviations in CMP process vector during a CMP process run. The defect evaluation system was implemented to detect and classify unknown defects, their causes and to update the current defect classes and the related behavioral pattern characteristics in the knowledge base. The agent collected the trace data from CMP process automation controller, it provided this data to diagnostic system in case of conflicts, which the inference engine could not resolve, and it started the defect evaluation. The agent provided the evaluated defect classes to CMP process expertise for verification and validation and then finally updating the diagnostic system.

After the system was deployed in the production environment, it took over a year of training for the diagnostic system to detect the origination of defects at a very early stage, to exactly localize and characterize the origination of these defects, to achieve high defect detection reliability and repeatability and to increase its detection performance. After this learning process, the system provides exactly the cause, involved behavioral pattern characteristics, related process step, the involved process parameter and machine parameter behaviors for the detected defect origination characteristics to the CMP process expertise. Its integration with CMP process controller in the production environment facilitates in-situ detection of the origination of defects.

The main objective of this work, was to optimize and improve only the Chemical Mechanical Polishing process. Further research work is required to observe the wafer mounting process. Many causes, which were not detected during CMP process, have their origination during wafer mounting process. So that the diagnostic system observing wafer mounting process can provide data to the diagnostic system observing CMP process through communication among the two agents. The wafer mounting process is a very critical and sensitive area regarding particle contamination and the surface uniformity required during mounting process. The software framework developed and implemented here can be easily deployed for the wafer mounting process but it is necessary to do very intensive study of the wafer mounting process for its representation in the knowledge base. Further research work is required to develop self-learning diagnostic system to replace the currently implemented defect evaluation system.

Additional research work will be required to enhance the developed knowledge base by implementing the detailed representation of the behavioral pattern characteristics of polishing pad, slurry and abrasives.

9 Zusammenfassung und Ausblick

Die sich schnell ändernden technologischen Eigenschaften von integrierten Schaltungen (d.h. ihre Kompaktheit und Dichte) erfordern eine sehr hohe Oberflächenebenheit und eine konstante Oberflächentopographie des benötigten Substratmaterials (Wafer). Die IC-Hersteller verlangen Wafer mit ständig abnehmenden Defektdichten, sehr enge Toleranzen und sehr kurze Lieferzeiten von den Wafer-Herstellern. Die in-situ Defekterkennung, die Echtzeitanalyse von nichtoptischen Defekten, die simultane Unterscheidung von mehrfachen Defekttypen und die hohen Erfassungsraten von ermittelten Defekten erweisen sich als die größten Herausforderungen für die Wafer-Hersteller. Der gegenwärtige Waferherstellungsprozess ist sehr komplex und hat bereits eine sehr hohe technische und organisatorische Verfügbarkeit.

Als abschließender Schritt im Waferherstellungsverfahren hat sich der CMP-Prozess als kritische Technologie für das Erreichen der erforderlichen globalen Planarisierung der Waferoberfläche entwickelt. Die hohe Komplexität des CMP-Prozesses erschwert die Lokalisierung (d. h. das Feststellen von Defektbereich, Typ und Ursache) und Kontrolle der Prozess- und Maschinenparameter, die für die Defektentstehung während eines Prozesses verantwortlich sind. Dies führt zu untragbaren Maschinenstillstandszeiten, die durch zeitaufwändige Defektlokalisierungsverfahren verursacht werden. Die Ableitungen von Korrekturmaßnahmen und die Feststellung von Korrelationen zwischen ermittelten Defekten und Prozessparametern basieren größtenteils auf der langjährigen CMP-Prozesserfahrung der Prozessingenieure.

Der Stand der Technik für die Analyse der erforschten Defekte ist die Durchführung von Korrelationen dieser Defekte mit den Änderungen und Verschiebungen der Prozess- und Maschinenparameter offline, d.h. nachdem die Defekte bereits aufgetreten sind. Verschiedene bereits entwickelte Prozesskontrollmethoden zur Vermeidung von unerwünschten Defektentstehungen und Maschinenstillstandszeiten wurden untersucht. Zuerst wurden die für den CMP-Prozess entwickelten Prozesskontrollmethoden geprüft. Danach wurden die Untersuchungen erweitert, um die Prozesskontrollmethoden für andere Prozessmaschinen in der Halbleiterfertigung, wie Plasma-Etch-Prozessmaschine, CVD-Prozessmaschine und Photolithographie-Prozessmaschine, zu bewerten. Die Untersuchungen zeigten, dass die entwickelten Prozesskontrollmethoden die Entstehung von Defekten während des Prozesses nicht ermitteln konnten. Für die Maschinen des Plasma-Etch-Prozesses und des CVD-Prozesses war es jedoch möglich, Defekte mit zusätzlicher Integration von Impedanzsensoren zu ermitteln. Dennoch zeigte keine der Prozesskontrollmethoden eine Anpassungsfähigkeit an die sich ständig ändernden Prozess- und Maschinenparameter im Produktionsumfeld. Die zeitliche Darstellung der Eigenschaften der Prozess- und Maschinenparameter wurde nicht durch Prozesskontroll-Algorithmen implementiert und keine lieferte Informationen zur Chemie des CMP-Prozesses.

Im Rahmen dieser Arbeit wurde, zum Verständnis der CMP Grundlagen, die auf physikalischen Modellen in Verbindung mit experimentellen Daten basieren, die theoretische Analyse und Problemdomänenanalyse des CMP-Prozesses durchgeführt. Diese Daten wurden durch die Waferfertigungsanlage (WSAG, Burghausen, Deutschland) bereitgestellt. Die theoretische Analyse zeigte, dass der eingeschwungene Zustand der CMP Prozessmaschine ein dynamisches Gleichgewicht ist aus mechanischen Aktionen an der Polierauflage und der Waferoberfläche, chemischen Aktionen des Poliermittels, das eine atomare oder molekulare Schicht von der Waferoberfläche abträgt, und den

Poliermittelpartikeln in Verbindung mit den Polierauflageunebenheiten, die für den abschließenden Materialabtrag von der Waferoberfläche verantwortlich sind. Jede Änderung oder Verschiebung dieses dynamischen Gleichgewichts führt zur Entstehung von Defekten, welche in Beziehung zu den Geometriewerten stehen, die durch ex-situ Messungen bereitgestellt werden. Die Qualität der Waferoberfläche (spezifiziert durch geometrische und Prozesskontroll-Indizes) ist ein Hinweis auf das zu erwartende Resultat und die Zuverlässigkeit des CMP-Prozesses. Jeder Wafer, der mittels des CMP-Prozesses hergestellt wurde, wird gemäß der geometrischen Spezifikationen (nach DIN 50441/1, DIN 50441/4 und SEMI M1 2002) vermessen und überprüft. Abweichungen der spezifizierten geometrischen und Prozesskontroll-Indizes führen zu unerwünschten Defekten. Diese Defekte können mehrere mögliche Prozess- und Maschinenparameter als Ursache haben. Die Bestimmung der genauen Quelle der Defektentstehung ist sehr schwierig, da das Verhalten aller Prozess- und Maschinenparameter während des gesamten CMP-Prozesses beobachtet werden muss, und die Kenntnis des genauen Einflusses aller dieser Parameter Bedingung ist. Es erweist sich als sehr kompliziert, den unbekannten Einfluss der bekannten Parameter zu bestimmen.

Sämtliche Ergebnisse führen zu dem Schluss, dass die Wechselwirkungsdynamik von Prozess- und Maschinenparametern während des CMP-Prozesses ein System erfordert, das das Verhalten aller Prozess- und Maschinenparameter während des gesamten CMP-Prozesses beobachtet. Das System muss lernen, das CMP-Prozess-Verhalten vorherzusagen, zu lokalisieren, darzustellen und außerdem mögliche Korrekturmaßnahmen zu liefern, um das Auftreten von Defekten während des CMP-Prozesses zu vermeiden.

Hauptbestandteil dieser Arbeit ist die Entwicklung und Implementierung eines agentenbasierten Diagnosesystems zur Defektanalyse während des CMP-Prozesses für die untersuchte CMP-Prozessmaschine. Das System sollte die Defektentstehung in einem sehr frühen Stadium des Waferfertigungsprozesses erkennen. Weitere Aufgaben des Systems sind das Reduzieren der Defektdichte, die Verbesserung der Zuverlässigkeit und Genauigkeit des Prozesses durch in-situ Beobachtung des CMP-Prozesses, das Bereitstellen von Vorschlägen zu entsprechenden Korrekturmaßnahmen für den Prozessingenieur, die Risikominderung für das Auftreten von Defekten, die Anpassung an sich ändernde CMP-Prozess-Charakteristika und Umgebung und die explizite Beobachtung der zeitlich veränderlichen Eigenschaften der Prozess- und Maschinenparameter.

Hierfür wurde zunächst ein mathematisches Modell entwickelt, um den CMP-Prozess zu beschreiben. Dieses Modell war Grundlage für die Beschreibung des Prozess- und Maschinenparameterverhaltens und der Verhaltensmustereigenschaften des CMP-Prozesses. Des Weiteren diente es zum Aufbau eines Korrelationsmodells zwischen Defektklassen und Verhaltensmustern im Produktionsumfeld. Um aufgetretene bekannte oder unbekannte Defekte zu klassifizieren und auszuwerten, wurde ein Defektauswertungssystem entworfen. Diese Komponente verwendet generische Algorithmen, um Defekte und die zugehörigen CMP Verhaltensmuster zu klassifizieren. Im folgenden Schritt wurde das komplette Design des Diagnosesystems mit enthaltener Wissensbasis und Inferenzmaschine, die die Beobachtungen bewertet, entwickelt. Das Design des Diagnosesystems beinhaltet die zeitliche Darstellung der Prozess- und Maschinenparameter mittels temporalem Schließen und auch die Anpassungsfähigkeit der beobachteten Prozess- und Maschinenparameter an den sich ständig ändernden CMP-Prozess und Produktionseigenschaften. Das Design des Agenten, der das Defektauswertungssystem und das Diagnosesystem steuert und koordiniert, wurde als nächstes entworfen. Ein Framework wurde entwickelt, um eine Kommunikation zwischen dem Defektauswertungssystem, dem Diagnosesystem und dem Agenten herzustellen. Der Agent soll die Kommunikation mit dem CMP-Prozessautomatisierungs-Controller herstellen, um das Diagnosesystem mit dem CMP-Prozessvektor zu vereinfachen. Das Design erleichtert dem agentenbasierten Diagnosesystem die Integration in den vollständigen Prozessregelkreis der Produktionsumgebung.

Nach Beendigung des Designs wurde das gesamte System in kleinen Schritten implementiert, was zunächst die Darstellung des CMP-Prozessraums in der Wissensbasis SOLVATIO® beinhaltet. Die Darstellung in der Wissensbasis geschah durch eine sehr gründliche Beobachtung des CMP-Prozesses, der betroffenen Prozess- und Maschinenparameter und der korrespondierenden Defekte während verschiedener Prozesszustände und Prozesszustandsübergänge. So wurde jede bekannte oder unbekannte Defektklasse, zugehörige Verhaltensmuster und Prozess- und Maschinenparameterverhalten in der Wissensbasis mit Logikoperatoren, Regeln, Bedingungen, Heuristik, Entscheidungsbäumen und temporalem Schließen beschrieben, um Symptomhierarchien und Diagnosehierarchien in der Wissensbasis zu implementieren. Die Symptomhierarchien, Diagnosehierarchien, Strategien und Pläne wurden von der Inferenzmaschine verwendet, um Konflikte zwischen zwei widersprüchlichen Diagnosen zu beheben. Die Inferenzmaschine dient zur in-situ Diagnose der Entstehung von Abweichungen des CMP-Prozess-Vektors während eines CMP-Prozess-Durchlaufs. Das Defektauswertungssystem wurde implementiert, um unbekannte Defekte und ihre Ursachen zu erkennen und um auftretende Defekte und die zugehörigen Verhaltensmuster in der Wissensbasis zu aktualisieren. Der Agent sammelte sämtliche Daten vom Prozessautomatisierungs-Controller, lieferte diese Daten dem Diagnosesystem, falls die Inferenzmaschine diesen nicht lösen konnte, startete er die Defektauswertung. Der Agent stellte die ausgewerteten Defektklassen dem CMP-Prozessexperten zur Überprüfung und Validierung zur Verfügung, welcher schließlich die Aktualisierung des Diagnosesystems veranlasste.

Nach dem ersten Einsatz des Diagnosesystems in der Produktionsumgebung musste die Wissensbasis über ein Jahr lang aufgebaut werden, um überhaupt Defektentstehungen in einem sehr frühen Stadium ermitteln zu können. Erst danach war das System in der Lage, Defektentstehungen genau lokalisieren und charakterisieren zu können, eine hohe Zuverlässigkeit und Wiederholbarkeit in der Defektbestimmung zu erzielen und seine Erkennungsgeschwindigkeit zu erhöhen. Nach diesem Lernprozess liefert das System genau die Ursache, beteiligte Verhaltensmuster, den zugehörigen Prozessschritt und die beteiligten Prozess- und Maschinenparameterverhalten der erkannten Defektentstehung als CMP-Prozesswissen. Seine Integration in die CMP-Prozessüberwachung des Produktionsumfeldes erleichtert die in-situ Bestimmung der Defektentstehung.

Hauptziel dieser Arbeit war die Optimierung und Verbesserung des CMP-Prozesses. In Zukunft wird die Beobachtung des Waferaufkitt-Prozesses Aufgabe sein. Viele Ursachen, die nicht während des CMP-Prozesses ermittelt wurden, entstehen während des Waferaufkitt-Prozesses. So kann ein Diagnosesystem, das den Waferaufkitt-Prozess beobachtet, dem Diagnosesystem des CMP-Prozesses Daten durch Kommunikation zweier Agenten zur Verfügung stellen. Der Waferaufkitt-Prozess ist ein sehr kritischer und empfindlicher Bereich hinsichtlich Partikelverschmutzung und Oberflächenbeschaffenheit. Das Software-Framework, das hier entwickelt und eingeführt wurde, könnte leicht für den

Waferaufkitt-Prozess eingesetzt werden, was aber eine sehr intensive Untersuchung des Waferaufkitt-Prozesses für die Darstellung in der Wissensbasis bedeuten würde.

Eine künftige Aufgabe ist die Entwicklung eines selbstlernenden Diagnosesystems, das das derzeit implementierte Defektdiagnosesystem ersetzt.

Weitere Forschung erfordert die Erweiterung der entwickelten Wissensbasis durch das Implementieren einer detaillierten Darstellung der Verhaltensmustereigenschaften des Poliertuchs und des Poliermittels.

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