THE ESHELBY FACTOR FOR CUBIC CRYSTALS WITH ARBITRARY ELASTIC ANISOTROPY

W. MAYSENHÖLDER [1]

Max-Planck-Institut für Metallforschung, Institut für Physik,
Heisenbergstrasse 1, D 7000 Stuttgart 80, Fed. Rep. Germany
and Universität Stuttgart, Institut für Theoretische und Angewandte Physik,
Pfaffenwaldring 57, D 7000 Stuttgart 80, Fed. Rep. Germany

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The Eshelby factor for cubic crystals has been calculated for arbitrary anisotropy. One of the two integrations needed could be performed analytically. An expansion up to 4th order in the anisotropy and exact results for special cases are also given.

The Eshelby factor plays an important role in the physics of point defects in crystals [1–3]. To recall its definition let us consider a crystal of volume V containing a point defect. The volume change of the crystal due to the defect depends on the boundary condition at the surface of the crystal: If the surface is force-free, the volume change be ΔV; if the crystal were embedded in an infinite medium with the same elastic properties, the volume change would be different, say ΔV_∞. The ratio

$$\gamma_E \equiv \Delta V/\Delta V_\infty \geqslant 1 \tag{1}$$

is called Eshelby factor [1,2] [+1]. Within the framework of linear elasticity theory one obtains for arbitrary crystal symmetry (see, e.g., ref. [3])

$$\Delta V = \mathrm{Tr}(\mathbf{SP}) , \tag{2}$$

$$\Delta V_\infty = -\mathbf{P} : \int_V \mathrm{d}^3 r [\boldsymbol{\nabla}\boldsymbol{\nabla}\cdot\mathbf{G}(r)] . \tag{3}$$

($\mathbf{P}$: double-force tensor of the point defect at $r = 0$, $\mathbf{S}$ and $\mathbf{G}$: tensor of compliances and tensor Green's function of the elastic medium.) The strain field leading to ΔV_∞ consists essentially of shear strains, i.e. ΔV_∞ is, roughly speaking, the dilation at the location of the point defect. By contrast, the volume change $\Delta V_I = \Delta V - \Delta V_\infty$ due to the free surface ("image forces") stems from dilations which are more or less homogeneously distributed over the whole crystal. ΔV is independent of the volume of the crystal, whereas ΔV_∞ and therefore γ_E will in general depend on size and shape of V [cf. (2),(3)].

In the following we confine ourselves to crystals with cubic symmetry [bulk modulus $K = (c_{11} + 2c_{12})/3$, shear moduli $G_1 = (c_{11} - c_{12})/2$ and $G_2 = c_{44}$] and spherical shape with the point defect in the centre of the sphere. Then ΔV_∞ and γ_E become independent of the crystal volume [3]:

$$\Delta V = \mathrm{Tr}\,\mathbf{P}/3K , \tag{2'}$$

$$\Delta V_\infty = \tfrac{1}{3}\mathrm{Tr}\,\mathbf{P}\langle\hat{k}\cdot\tilde{\mathbf{G}}(\hat{k})\cdot\hat{k}\rangle_{\hat{k}} , \tag{3'}$$

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[1] Address from September 1, 1983 onwards: Department of Physics, University of California, Berkeley, CA 94720, USA.
[+1] In ref. [3] γ_E^{-1} is termed Eshelby factor.

$$\gamma_E^{-1} = K \langle \hat{k} \cdot \widetilde{G}(\hat{k}) \cdot \hat{k} \rangle_{\hat{k}} \ . \tag{4}$$

($\widetilde{G}$: Fourier transform of G; $\hat{k}$: unit vector in reciprocal space; $\langle \ \rangle_{\hat{k}}$: directional average.) Although $\widetilde{G}$ is known analytically (e.g. ref. [4]), it appears not to be possible to get an analytical expression for γ_E except for special cases.

The result for isotropic media is well known [1]

$$\gamma_E = 1 + 4G/3K = 3(1 - \nu)/(1 + \nu) \tag{5}$$

($G = G_1 = G_2$; ν = Poisson's ratio) and can be used as a first approximation for anisotropic media if G is replaced by Voigt's average $\bar{G} = (2G_1 + 3G_2)/5$ [2,5]:

$$\gamma_{EV} \equiv 1 + \tfrac{4}{3}\bar{s}_1 \quad \bar{s} = \bar{G}/K \ . \tag{6}$$

($\bar{s}$: stiffness.) γ_{EV} constitutes an upper limit to γ_E [5,6] and is taken as a starting point for more accurate approximations. In the following we shall express our results in terms of κ defined by

$$\gamma_E = \gamma_{EV}/(1 + \kappa) , \quad \kappa \geqslant 0 \ . \tag{7}$$

While γ_{EV} is independent of the anisotropy, the deviation κ is a function of both the stiffness $\bar{s}$ [defined in (6)] and the anisotropy a defined by

$$a = (G_1 - G_2)/(G_1 + G_2) \ . \tag{8}$$

Numerical values for γ_E can be obtained by two-dimensional numerical integration. This has been done for a number of materials (e.g. refs. [7,8]) and can be done for any cubic material using the computer program ANISCO [9]. However, it is possible to perform one of the integrations analytically. We get

$$\kappa = \frac{\bar{s}}{5} \int_0^1 [(T_1 - T_2)(1 - \epsilon^2)^{-1/2} + T_2]\,dx \ , \tag{9}$$

with

$$\epsilon = \frac{-(1 - x^2)^2 [\beta_1 + \beta_2 x^2]}{\beta_3 + (1 - x^2)[\beta_1(7x^2 + 1) + \beta_2(1 - x^2)x^2]} \ ,$$

$$T_1 = \frac{\beta_4 + (1 - x^2)[\beta_5(7x^2 + 1) + \beta_6(1 - x^2)x^2]}{\beta_3 + (1 - x^2)[\beta_1(7x^2 + 1) + \beta_2(1 - x^2)x^2]} \ , \quad T_2 = (\beta_5 + \beta_6 x^2)/(\beta_1 + \beta_2 x^2) \ ,$$

$$\beta_1 = a(1 - a)[\tfrac{1}{5}(5 - a) + \tfrac{1}{3}(1 + a)\bar{s}] , \quad \beta_2 = 2a^2[\tfrac{3}{5}(5 - a) + (1 - a)\bar{s}] , \quad \beta_3 = (1 - a)^2[\tfrac{1}{5}(5 - a) + \tfrac{4}{3}(1 + a)\bar{s}] ,$$

$$\beta_4 = -8a(1 - a)^2 , \quad \beta_5 = a(1 - a)(5 - 3a) , \quad \beta_6 = 2a^2(15 + a) .$$

This result may be useful for practical purposes because the remaining integration can be done with little numerical effort [+2], e.g. using Simpson's rule.

In three special cases κ can be evaluated in terms of elementary functions:

(i) $a = 1$: $\kappa = \tfrac{4}{3}\bar{s}$,   i.e. $\gamma_E = 1$. $\tag{10}$

(ii) $a = -1$: $\kappa = \dfrac{7\bar{s}}{9 + 5\bar{s}} + \dfrac{5}{18}(3 + 4\bar{s})\bar{s}\alpha^3 \ln \left| \dfrac{\alpha^3[5 - 9\alpha^2 - 3(1 - 2\alpha^2)^{1/2}]^4}{(2 + 3\alpha)^2(2 - 3\alpha)^5[2 - 6\alpha^2 + 3\alpha^4 - 2(1 - 2\alpha^2)^{3/2}]} \right|$,

$$\alpha^2 = 3/(9 + 5\bar{s}) \ . \tag{11}$$

[+2] For $a = -1$ the integrand has a discontinuous derivative at $x^2 = 1/2$ [$\epsilon^2 = 1$, integrand $= -\bar{s}/(3 + 5\bar{s})$].

(iii) $\bar{s} = \frac{3}{5}\frac{(5-a)}{(5a-1)}$,   i.e. $c_{12} + c_{44} = 0$ or $K = 2G_1/3 - G_2$:

$$\kappa = \frac{1}{20a}\left[15 + a - 3(7a + 5)\left(\frac{1-a}{4a}\right)^{1/2}\arcsin\left(\frac{4a}{3a+1}\right)^{1/2}\right]. \tag{12}$$

It may be noted that the slope $\partial\kappa/\partial a$ becomes infinite at $a = 1$, and expansion of κ around $a = 1$ is non-trivial be- because the Taylor expansion of the integrand does not converge for all values of x. Despite of its complicated appearance the second formula (11) describes an essentially linear behaviour in the region of physical interest (the relation $\kappa = \frac{3}{4}\bar{s}$ is accurate to better than 0.01 for $\bar{s} \leqslant 1$). The last case (12) can be obtained by straghtforward in- tegration of (3) because an analytical expression for G is available [4]. Unfortunately, there seem to be no crys- tals with $c_{12} + c_{44} = 0$ [*3].

Fig. 1 shows the variation of γ_E and κ by means of contour lines (lines of constant value) for the regime $\bar{s} \leqslant 1$, which presumably contains all real cubic materials. The approximation γ_{EV} would lead to horizontal contour lines in fig. 1a. In fig. 1b the infinite slope mentioned above causes − although scarcely visible − an infinite slope of the contour lines of κ at $a = 1$. The dahed line marks the relation $c_{12} + c_{44} = 0$, where (12) holds.

For weak anisotropy κ can be expanded in powers of the anisotropy a. Because of the choice of γ_{Ev} the term linear in a vanishes.

[*3] In search of analytical expressions for κ one is concerned with the reduction of hyperelliptic integrals of genus two. The sub- stitution $y = 1 - x^2$ in (9) transforms the radicand into a 6th order polynomial which factorizes into polynomials of degrees 3, 2, and 1. Hence all zeroes are known explicitly. If two zeroes are equal, the hyperelliptic integrals reduce to elliptic ones. In the region of physical interest this occurs only in the cases (i)−(iii). In (i) we have two triple zeroes, in (ii) and (iii) two double zeroes, and the elliptic integrals can be further reduced to elementary functions. A more general condition for the reducibility [10] is satisfied along the dotted line in fig. 1. On this line κ can be expressed by a linear combination of elliptic integrals.
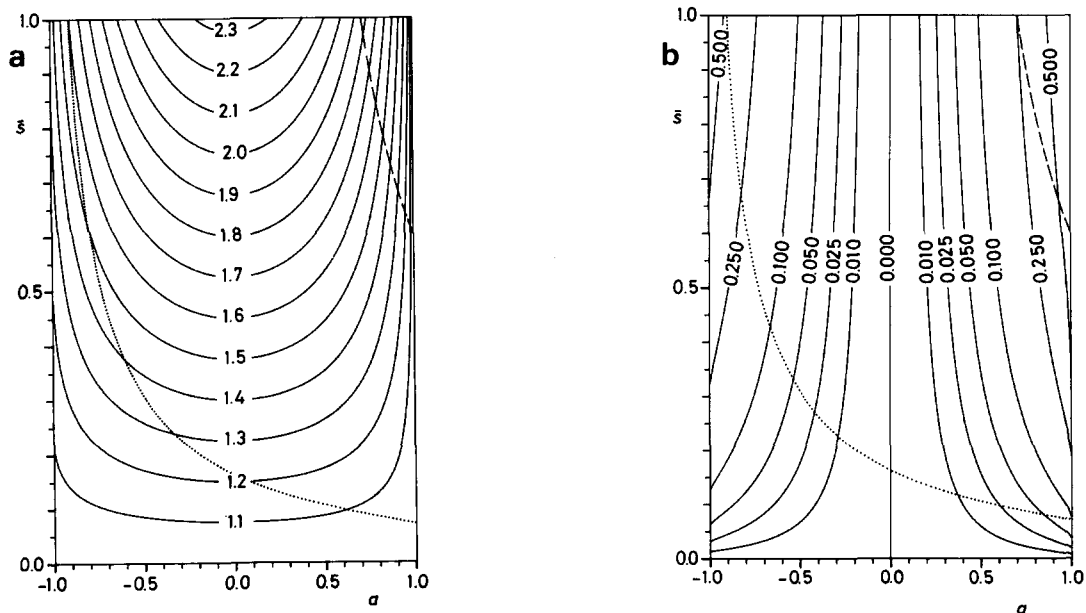

Fig. 1. Contour lines of the Eshelby factor γ_E (a) and of its deviation κ (b) from the isotropic approximation γ_{EV} as a function of the anisotropy a and the stiffness $\bar{s}$. The dashed line indicates $c_{12} + c_{44} = 0$. For the dotted line see footnote 3.

$$\kappa \approx \frac{64(15 + 32\bar{s})\bar{s}}{175(3 + 4\bar{s})^2} a^2 + \frac{128(2655 + 5748\bar{s} - 2240\bar{s}^2)\bar{s}}{125125(3 + 4\bar{s})^3} a^3$$

$$+ \frac{64[27(74905 + 435832\bar{s}) + 400\bar{s}^{-2}(70587 + 72256\bar{s})]\bar{s}}{10635625(3 + 4\bar{s})^4} a^4 \ . \tag{13}$$

Taking only the first term in (13) leads to a relative error in κ less than 16% for $|a| \leqslant 0.5$ and $\bar{s} \leqslant 1$. Inclusion of terms up to a^4 reduces the error to less than 3%. Since $\kappa \lesssim 0.1$ in this range, the accuracy of the Eshelby factor is better than 1.6% and 0.3%, respectively.

Similar approximations have been derived already by Dederichs and Pollman [5]. In fact, eq. (20) in ref. [5] corresponds to the first term of (13) divided by $(1 - \frac{1}{5}a)^2$. As a consequence, that approximation is worse for $a < 0$ and better for $a > 0$ than the first term of (13). The variational approximation of Dederichs and Pollmann (eq. (21) in ref. [5]) and the approximation (13) presented here possess comparable accuracy.

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