Phonon Spectroscopy of Low-Energy Vibrations of Interstitial Oxygen in Germanium

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In oxygen doped germanium we find by phonon spectroscopy with superconducting tunnelling junctions [1] (Fig.1) a series of states from 0.18 meV up to 4.08 meV above the ground state (Fig.3). The sequence can be approximated by a free rotation of the interstitial oxygen atom (Fig.2) corresponding to \( E = (\hbar l)^2/(2m\tau_0^2) \). \( \hbar l = 0, \pm 1, \pm 2, \ldots \) is the angular momentum for the rotation around the [111]-axis, \( m \) the reduced mass of the system and \( \tau_0 \) the average distance of the oxygen to the [111]-axis.

The 0.18 meV distance between \( l = 0 \) and \( l = \pm 1 \) is below the detector threshold; it is seen only as corresponding doublets in the transitions to the excited states. This interpretation of the doublets is confirmed by an activation energy obtained from the temperature dependence of the relative intensity within a doublet. Similarly, transitions from the \( l = \pm 2 \) level have been identified from the temperature dependence.

In a sample with low oxygen concentration we find that the transitions from the ground state to the \( l = \pm 3 \) levels are weaker by a factor of 50 than the transitions from the \( l = \pm 1 \) levels to the \( l = \pm 3 \) levels.

![Fig.1: Phonon transmission signal of O\textsubscript{i} in Ge versus the phonon energy. Detector threshold at 1.2 meV.](image1)

![Fig.2: Interstitial site of oxygen in the Ge lattice [2, 3].](image2)
Fig. 3: Energy level scheme and stress dependence of the interstitial oxygen in Ge determined by phonon spectroscopy. Phonon transitions from the states labeled $l = 0, \pm 1, \pm 2$ could be measured.

In this series the states at 1.37 meV and 1.65 meV are interpreted as states belonging to $l = \pm 3$ split by the additional six potential barriers from the neighbouring Ge-atoms hindering the rotation [4]. All states show small stress dependence due to the orientational degeneracy, whereas in the sixfold symmetry the $l = \pm 1$ level additionally splits for stresses along [100] and [110]. The stress dependence of trigonal centres in cubic crystals is determined by 4 coefficients [5]. We have estimated $A_1 = A_2 = -0.058 \pm 0.02$ meV/GPa, $B = 0.55 \pm 0.05$ meV/GPa, $C = 0 \pm 0.02$ meV/GPa. We can summarize our results as follows:

Whereas the band of lowest lying mechanical states of interstitial oxygen in Si can be approximated by a two-dimensional oscillator perturbed by a central potential [6, 7], the corresponding states in Ge can be well understood by a hindered rotator with a large central potential opposing a bending oscillation and with a sixfold modulation of the rotation due to the influence of the 6 neighbours to the Ge-O-Ge molecule.

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