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

K. Lassmann, M. Gienger, and M. Glaser

1. Physikalisches Institut, Universität Stuttgart,
W-7000 Stuttgart 80, Fed. Rep. of Germany

In oxygen doped germanium we find by phonon spectroscopy with supercon-
ducting 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 approxi-
mated by a free rotation of the interstitial oxygen atom (Fig.2) corresponding
to $E = (\hbar l)^2/(2mr_0^2)$. $\hbar l = 0, \pm 1, \pm 2, \ldots$ is the angular momentum for the
rotation around the [111]-axis, m the reduced mass of the system and r_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 thresh-
old; 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
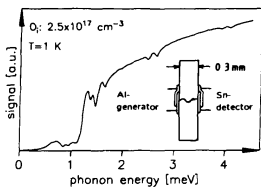transitions from the $l = \pm 1$ levels to the $l = \pm 3$ levels.

Fig.1: Phonon transmission signal of O_i in Ge
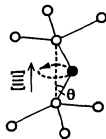versus the phonon energy. Detector threshold at
1.2 meV.

Fig.2: Interstitial site
of oxygen in the Ge
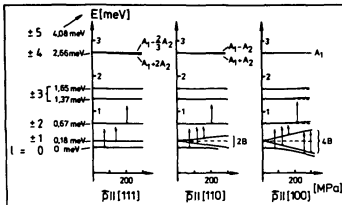lattice [2, 3].
$\theta_{Ge-O-Ge} \approx 25°$

Fig.3: Energy level scheme and stress dependence of the interstitial oxygen in Ge determined by phonon spectroscopy. Phonon transitions from the states labeled $l = 0, \pm 1, \pm 2$ can 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.

[1] W. Eisenmenger, Physical Acoustics XII, 79 (1976)
[2] B. Pajot and P. Clauws, Proc. of the 18th Int. Conf. on Phys. of Semic., Stockholm 1986, World Scientific, Singapore, Vol.2, 911 (1997)
[3] L. I. Khirunenko et al., Sov. Phys. Semicond. 24(6), 663 (1990
[4] H. J. Hrostowski and B. J. Alder, J. Chem. Phys. 33(4), 980 (1960)
[5] H. J. Hughes and W. A. Runciman, Proc. Phys. Soc. 90, 827 (1967)
[6] D. R. Bosomworth et al., Proc. Roy. Soc. Lond. A 317, 133 (1970)
[7] H. Yamada-Kaneta et al., Phys. Rev. B 42(15), 9650 (1990)