

Effect of Point Defects on the Decay of the LO Mode

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The longitudinal optical mode at the zone center has often the highest frequency in the phonon spectrum, so that its phonons cannot be scattered elastically into other modes. Their decay rate Γ is enhanced by defects above the intrinsic anharmonic rate Γ_{an} only by the combined action of anharmonic processes and defects such as point defects. This can occur by a second order process. The phonon is scattered first into a neighboring mode of wave vector q , and this intermediate state is followed by anharmonic decay. The intermediate state has an energy deficit

$$\hbar\Delta\omega = \frac{\hbar\omega}{k^2}(q^2 - q_0^2)$$

where k is a measure of the curvature of the dispersion relation in the immediate vicinity of the extremum, and q_0 is the wave number of the decaying LO mode, and it is the photon wave vector change for Raman scattering. Since the intrinsic anharmonic decay rate Γ_{an} is almost independent of q , Γ_{an} can be factored out of the second order decay rate, so that the increase in line width becomes

$$\Delta\Gamma = \Gamma_{an} \frac{\pi}{32n} \frac{k^4}{q_z^3 q_0} g .$$

Here q_z is the radius of the Debye sphere for n atoms per unit cell, and g is the point defect scattering parameter, which for simple mass defect scattering is $g=c(\Delta M/M)^2$ for a concentration c .

A different result is obtained by convolution of the point defect scattering over the line width $\Delta\omega=\Gamma_{an}$, replacing the density of states N_d by $(4\pi/3) \Delta q^3 / \Gamma_{an}$ where Δq corresponds to $\Delta\omega$. This is the procedure used numerically by Zhang et al.¹ and by Widulle et al.² for isotopes in Ge and Si. Put into algebraic form, this yields

$$\Delta\Gamma = \frac{\pi}{6n} g \frac{k^3}{q_z^3} \omega_0^{1/2} \Gamma_{an}^{1/2}$$

these two expressions give comparable values for isotope line broadening at low temperatures, as observed^{1,2}, but differ in dependence on temperature and on q_0 . Existing data on Raman line broadening will be discussed.

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¹ Zhang, J.M., M. Gehler, A. Göbel, T. Ruf, M. Cardona, E.E. Haller, and K. Itoh, Phys. Rev. **B57**, 1348 (1998).

² Widulle, F., T. Ruf, A. Göbel, I. Silier, E. Schönherr, M. Cardona, J. Camacho, A. Cantarero, W. Kriegseis, and V.I. Ozogin, Physica **B263/4**, 381 (1999).