
PH. SCHMID

Laboratoire de Physique Appliquée, EPFL-Lausanne - Lausanne

Summary. — In layered semiconductors, short-range interaction with optical phonons is the dominant electron scattering mechanism. Within the limit of weak coupling and moderate anisotropy, the interaction is treated as a perturbation linear in the atomic displacements. The lowest-order correction to the energies of the electron states is calculated, and the exact relaxation time solution of the Boltzmann equation is presented.

1. – Introduction.

Electron scattering by optical phonons usually is a weak second-order effect in covalent semiconductors with high structural symmetry: in such crystals, the stretching of a particular bond requires the simultaneous contraction of an adjacent, equivalent bond. Thus, the scattering potential arising from counterphase motions of covalently bonded atoms averages to zero (1). In other terms, the symmetry of each atomic site conditions the strength of the coupling: if site symmetry is high enough, the deformations set up by an optical mode are such that the average of the distances from one atom to all its equivalent neighbours remains unchanged. Therefore, no net scattering potential develops to first order in the displacements.

On the contrary, linear effects are significant in covalent crystals with low site symmetry. Large site dissymmetries are found in molecular crystals, and in layered semiconductors. In these cases, large gradients of the atomic potentials exist, so that short-range interaction with optical phonons is found

ELECTRON-LATTICE INTERACTION IN LAYERED SEMICONDUCTORS

to dominate the electron-lattice scattering. FIVAZ (2) pointed out that the interaction can then be treated to first order in the displacements. However his theory was developed for extremely anisotropic layered structures only, and thus deals largely with dimensionality effects. The present paper describes the electron–optical-phonon interaction for layered semiconductors of moderate anisotropy, where band electrons are weakly coupled to the lattice. The need for a three-dimensional description of the electron–optical-phonon interaction in some layered semiconductors originates from measurements on GaSe, which exhibits a rather low anisotropy (3). A detailed analysis of experimental results will be presented in forthcoming papers.

Within the deformation potential formalism, we consider transition matrix elements which are linear in the atomic displacements, i.e. linear in the normal phonon co-ordinate. We determine the lowest-order corrections to the energies of the noninteracting electron states in the weak-coupling limit and evaluate the exact relaxation time solution which exists for the Boltzmann equation in this particular case.

2. – The physical model.

2'1. We consider a semiconductor with nondegenerate bands and a large energy gap, so that interband transitions can be neglected. We further assume that the bands are broad, that is, the bandwidth is much larger than \( kT \) and than the phonon energy \( \hbar \omega \). The constant-energy surfaces are taken as ellipsoids around \( k = 0 \). (The calculations are actually carried out with spherical energy surfaces which can always be obtained by a suitable linear transformation of \( k \)-space.) The Brillouin zone is replaced by a constant-energy surface enclosing the same volume.

2'2. In the absence of degeneracy, the occupied states lie close to the band extremum. Since real transitions involve small values of the wave vectors only, we use the Kohn-Luttinger basis

\[
\langle r | k \rangle = u_0(r) \exp[i k \cdot r]
\]

for the electron wave functions.

2'3. For simplicity we consider one optical-phonon branch \( (\omega, q) \) only. For the long-wavelength phonons of interest here, the vibrating crystal can