vibration. In addition, one should, for self-consistency, use a Madelung constant for the lattice which takes the spatial extent of the charge distributions into account.[15]

The spatial extent of ionic charges is significant also in cases involving impurities or defects, for example, in the calculation of crystal fields at impurity sites[16] and in the calculation of the optical absorption of impurities or color centers.[17] Such calculations are, however, less straightforward than the one described here.

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Matrix Element for Nonequivalent Intervalley Scattering in *n*-Ge

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A matrix element for nonequivalent intervalley scattering by a longitudinal acoustic phonon in *n*-Ge is calculated using a pseudopotential. The result is compared with a value reported by deVeer and Meyer for the corresponding deformation potential constant D_i^*. The calculated value is greater by 50%.

I. INTRODUCTION

THE possible relevance of nonequivalent intervalley lattice scattering (NI scattering) of conduction electrons to infrared absorption in many-valley semiconductors was indicated by Rosenberg and Lax.[1] Their theoretical treatment of photon absorption by free carriers in *n*-Ge did not include this type of scattering, but they noted that the data of Fan, Spitzer, and Collins[2] departed from the calculated cross sections at photon energies for which NI scattering becomes possible. The conduction-band minima for the valleys concerned lie in the ⟨111⟩, ⟨100⟩ directions and are separated in energy by an estimated 0.18 eV.[3] The theoretical treatment of infrared absorption was extended to include NI scattering, along the line of Harrison's[4] treatment of optical intervalley scattering in the deformation potential model, by Risken and Meyer.[5] The corresponding deformation potential constant D_i^* is employed as an unknown parameter to express the contribution to the absorption constant from the NI transitions. An estimate of this quantity, by an infrared absorption experiment, was obtained by deVeer and Meyer.[6] Their method employs a least-squares fit of their data to the theoretical absorption curves of Risken and Meyer.

Interest in the determination of D_i^* is stimulated, as well, by concern over the importance of NI scattering in the theoretical description of current saturation in *n*-Ge in high fields. Meyer and Jørgensen,[7] by means of an argument based upon the Reik–Risken[8] picture of the electron distribution under high electric field conditions in many-valley semiconductors, and upon a calculation by Conwell[9] of the relative energy loss of hot electrons to optical and acoustic phonons, question the theoretical understanding of current saturation in *n*-Ge. According to Meyer and Jørgensen, if acoustic energy losses are included in the energy dissipation of hot electrons in *n*-Ge, as from Conwell's calculation appears necessary for electron temperatures above 5000°K, the electron-drift velocity becomes strongly dependent upon the electric field, through the range 3–10 kV cm^{-1}, in contrast to experimental results.[10] They propose that NI scattering may be sufficiently strong for electrons heated by such high fields (permitting energetically the L-Δ transition), so that this means of energy dissipation by the electron distribution would keep the electron temperature below the level

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TABLE I. Coefficients of normalized symmetrized plane waves in the expansion of the normalized electron eigenfunction at Δ_1.

$(a/2\pi)^2$ $(\mathbf{k}'+\mathbf{g}')^2$	Δ_1
$\frac{9}{16}$	0.383
$2\frac{1}{16}$	−0.870
$5\frac{1}{16}$	−0.193
$5\frac{9}{16}$	−0.213
$7\frac{1}{16}$	−0.054
$8\frac{9}{16}$	0.0007
$9\frac{9}{16}$	−0.065
$10\frac{1}{16}$	−0.0165
$11\frac{9}{16}$	−0.0702
$13\frac{1}{16}$	−0.0009

at which acoustic phonon emission becomes a serious loss mechanism.

These two areas of interest have motivated the calculation of the electron–phonon coupling between the conduction-band valleys at L and Δ.

II. THE PSEUDOPOTENTIAL MATRIX ELEMENT

In contrast to the deformation-potential interaction, which is questionable for transitions in which the lattice must supply large changes in electronic wave vector, the pseudopotential technique is applicable to transitions involving the large wave-vector displacements between points of high symmetry in the reciprocal lattice. Such matrix elements have been calculated by Shuey[11] for several electronic transitions in germanium, which, however, do not include the transition of interest here. The matrix element for the electron–phonon interaction in the pseudopotential representation, using a rigid-ion approximation is given by[12]

$$M(L_1,\Delta_1)=(\hbar n_q/2NVM\omega_{\mathrm{NI}})^{1/2}\sum_{\mathbf{g},\mathbf{g}'}(\hat{q}\cdot\mathbf{K}) \times C_{\mathbf{k}\mathbf{g}}C_{\mathbf{k}'\mathbf{g}'}{}^{*}U(K)\cos(\tfrac{1}{2}\mathbf{K}\cdot\boldsymbol{\tau}), \quad (1)$$

where L_1 and Δ_1 symbolize the initial and final conduction-electron states, respectively: L_1 is at the point $\mathbf{k}=2\pi a^{-1}(0.5,0.5,0.5)$, and Δ_1 is taken to be at $\mathbf{k}'=2\pi a^{-1}(0.75,0,0)$. The phonon of wave vector $\mathbf{q}=2\pi a^{-1}(-0.25, 0.5, 0.5)$, connecting the two states, is arbitrarily taken to be longitudinal acoustic (LA). The energy of the NI phonon is $\hbar\omega_{\mathrm{NI}}$, and the vector $\mathbf{K}$ is given by $\mathbf{K}=\mathbf{k}'-\mathbf{k}+\mathbf{g}'-\mathbf{g}=-\mathbf{q}+\mathbf{g}'-\mathbf{g}$, where g', g are reciprocal lattice vectors for the face-centered cubic lattice. The quantities $C_{\mathbf{k}',\mathbf{g}'}$ and $C_{\mathbf{k},\mathbf{g}}$ are the coefficients of the normalized plane wave expansions of the final and initial electronic states, respectively, e.g.,

$$\psi_{\mathbf{k}}(\mathbf{r})=\sum_{\mathbf{g}}C_{\mathbf{k},\mathbf{g}}\frac{1}{(N\Omega_0)^{1/2}}\exp i(\mathbf{k}+\mathbf{g})\cdot\mathbf{r}. \quad (2)$$

Each set, $\{C_k\}$, forms an eigenvector of the one-electron Hamiltonian operator H,

$$H=(P^2/2m)+V_{\mathrm{eff}}, \quad (3)$$

represented in a basis of plane waves of wave vector equivalent to $\mathbf{k}$. In particular, these eigenvectors belong to the eigenvalues of H corresponding to the conduction-band minima at L_1 and Δ_1. The form factor, $U(K)$, is the Fourier transform of the rigid ion potentials contributing to V_{eff}.

Both $U(K)$ and $\{C_k\}$ (the eigenvector corresponding to L_1) were obtained from Ref. 11. For U, Shuey's pseudopotential form factor U_A was used. The $\{C_{k'}\}$, belonging to Δ_1, was obtained by solving the eigenvector problem for a 51×51 matrix representation of H. The eigenvalue corresponding to Δ_1 was found by factoring the secular determinant.[13] With the average value of V_{eff} taken to be zero, the eigenvalue for Δ_1 is found to be 10.37 eV, which is 0.04 eV greater than the value quoted for L_1 in Ref. 11. The eigenvector at Δ_1 is given in Table I. From (1), the value of M is found by truncating the sums at about 50 waves in each index. Table II lists this matrix element, along with two others given in Ref. 11.

TABLE II. Matrix elements for transitions shown in units of $\left(\frac{\hbar n}{2NVM\omega_{\mathrm{NI}}}\right)^{1/2}\left(\frac{2\pi}{a}\right)$ eV.

Transition	M
$\Delta_1+LA\rightarrow L_1$	2.6
$\Gamma_{2'}+LA\rightarrow L_1$	2.0[a]
$\Gamma_{25'}+LA\rightarrow L_{3'}$	5.9[a]

[a] Reference 11.

The result given in Table II may be compared approximately with D_i^* (Ref. 6) since all of the L-Δ matrix elements which contribute to D_i^* are equal by symmetry. There are 24 such contributions. Thus D_i^* is given by

$$D_i^*=(24|q|^2M^2)^{1/2}=10.6\times10^8\ \mathrm{eV\ cm^{-1}}.$$

The value found by deVeer and Meyer is

$$D_i^*=(5\pm2)\times10^8\ \mathrm{eV\ cm^{-1}}.$$

The computations were performed on an IBM 1620.[14]

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