Intervalley deformation potentials and scattering rates in zinc blende semiconductors

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The intervalley electron-phonon deformation potentials between the lowest Γ-, *X*-, and *L*-conduction band valleys in zinc blende semiconductors are calculated using empirical pseudopotentials for the electrons and realistic shell models for the phonons. The intervalley scattering rates computed using these deformation potentials are in agreement with experiments.

Ultrafast semiconductor devices are subject to the application of high electric fields, where electrons in the lowest conduction band (CB) minimum (e.g., at Γ) can scatter to higher valleys, changing their mass and thus the performance of the device. This gives rise to phenomena like the Gunn effect. The same mechanism governs the absorption of light in indirect semiconductors and the initial relaxation of photoexcited carriers. For these reasons, intervalley (IV) scattering has been an area of large interest. Data involving IV scattering, gained from optical[1–3] or electrical[4] measurements, are difficult to interpret,[5,6] as many parameters (phonon and band energies, masses, nonparabolicity, etc.) enter the calculations. Therefore, the extraction of deformation potentials (DPs) is difficult, and the values in the literature scatter by an order of magnitude.[7]

We obtain here the IV DPs from a calculation of the IV electron-phonon matrix elements in zinc blende (ZB) semiconductors.[8,9] We describe the electron states using the empirical pseudopotential method (EPM) and the phonon states by realistic shell models. A more accurate description of the electron states does not yield better results as shown by an *ab initio* pseudopotential calculation of the Γ-*X* electron-phonon matrix elements in silicon.[10] We consider the scattering between the Γ-, *X*- and *L*-CB valleys in ZB semiconductors. We assume that these processes can approximately be understood by investigating the scattering between the high-symmetry points Γ, *X*, and *L*, i.e., that the dispersion of the matrix elements in the vicinity of these points is small. We give the selection rules imposed by symmetry and calculate the IV DPs. Finally, we evaluate the rates for the scattering of electrons between these valleys and compare them with experimental data.

Following the formalism of Ref. 9 we write the matrix element for the scattering of a carrier $|\mathbf{k}\rangle$ by absorption or emission of a phonon $|\mathbf{q}j\rangle$ in the absence of an external field as $\langle \mathbf{k} \pm \mathbf{q}|H_1|\mathbf{k}\rangle$, where H_1 is the first term in the Taylor expansion of the potential versus phonon displacements. As H_1 has the symmetry of the phonon involved, the transition is forbidden unless the representation belonging to the state $|\mathbf{k} \pm \mathbf{q}\rangle$ is contained in the product of the representations belonging to $|\mathbf{q}j\rangle$ and $|\mathbf{k}\rangle$.[11] In ZB semiconductors the symmetries for the two lowest CB states at *X* are X_1 and X_3, with the anion (group V atom) at the origin.[12] Usually X_1 is the lower state, with the exception of GaSb, where X_3 seems to have lower energy.[13] In InSb, the splitting between these states is only about 30 meV. The transverse phonons have X_5 symmetry and do not contribute to IV scattering between Γ and *X*. The longitudinal acoustic and optic phonons (LA and LO) have X_1 and X_3 symmetry. If the anion is heavier than the cation (as in the case of GaSb, AlAs, and AlSb), then the X_1 state (with the anion at rest) has higher energy (LO) than the X_3 state (LA). Neutron scattering experiments[14] have shown that this is also true for GaAs, where the two masses are similar. In the reverse case (GaP, InP, and InAs) the LA (LO) phonon has X_1 (X_3) symmetry.

The situation for Γ-*L* scattering is difficult as both the LA and LO phonons have L_1 symmetry and contribute to scattering processes at *L* (L_1), whereas transverse phonon scattering (L_3 symmetry) is forbidden. The relative magnitudes of the phonon amplitudes at the two atoms have to be known in order to estimate the importance of LA and LO scattering. These amplitudes have been measured for GaAs[14] and can be described with the overlap valence shell model (OVSM), which we use for our calculations (except for AlSb). Scattering between different equivalent *L* valleys (*X* valleys) is allowed for LO and LA phonons (the X_1 phonon).[11] All phonon modes are important for scattering from an L_1 state to an X_1 state, whereas only the transverse phonons can scatter to X_3.

We *define* the DP constant $D(\mathbf{q}j,\mathbf{k})$ for IV scattering through emission or absorption of a phonon with wave vector $\mathbf{q}$ and mode *j* as[15]

$$|\langle \mathbf{k} \pm \mathbf{q}|H_1|\mathbf{k}\rangle| = \hbar(2ME_{\mathbf{q}j})^{-1/2} D(\mathbf{q}j,\mathbf{k}) \sqrt{N_{\mathbf{q}j} + \tfrac{1}{2} \pm \tfrac{1}{2}}, \tag{1}$$

where *M* is the mass in the primitive cell, $E_{\mathbf{q}j}$ the phonon energy, and $N_{\mathbf{q}j}$ the Bose–Einstein occupation factor. The plus (minus) sign under the square root stands for phonon emission (absorption). We have used the OVSM program for the phonon states.[16–18] The electron states are calculated with the EPM,[12,19–21] using 59 plane waves. Then we can write the DP constant as

$$D(\mathbf{q}j,\mathbf{k}) = \hbar^{-1}(2ME_{\mathbf{q}j})^{1/2} \sum_a |\mathbf{A}(\mathbf{k},\mathbf{q},a)\epsilon(\mathbf{q}j,a)M_a^{1/2}|, \tag{2}$$

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TABLE I. Calculated intervalley deformation potentials (in eV/Å).

	$D_{\Gamma L}$		$D_{\Gamma X_1}$		$D_{\Gamma X_3}$		D_{LL}		$D_{X_1X_3}$		D_{LX_1}			
	LA	LO	LA	LO	LA	LO	LA	LO	LA	LO	TA	LA	LO	TO
AlAs[a,b]	2.3	2.2	0	4.4	2.7	0	0.2	2.2	0	6.6	1.1	1.7	0.6	2.4
AlSb[c,d]	2.3	3.4	0	4.9	1.3	0	0.5	0.6	0	9.5	1.1	0.8	2.4	3.7
GaAs[a,b]	4.1	0.6	0	4.1	4.7	0	0.1	1.7	0	7.0	1.2	0.5	2.5	2.6
GaSb[c,b]	2.8	2.7	0	4.5	2.5	0	0.6	1.2	0	6.0	1.0	1.4	1.5	2.2
InSb[f,g]	4.3	1.1	0	4.9	3.3	0	0.6	0.3	0	6.8	1.2	0.2	2.9	2.5
InP[c,g]	1.6	3.0	2.3	0	0	3.7	0.4	1.2	4.4	0	1.0	0.7	4.0	1.7
InAs[c,g]	2.5	1.4	3.2	0	0	2.8	1.4	0.7	3.6	0	0.9	0.8	2.7	1.6
GaP[c,b]	1.2	1.0	1.5	0	0	1.2	0.3	0.8	4.3	0	0.5	1.0	2.2	1.0

[a] Reference 21.
[b] Reference 17.
[c] Reference 12.
[d] Reference 23.
[e] Reference 19.
[f] Reference 20.
[g] Reference 18.

where $\mathbf{A}(\mathbf{k},\mathbf{q},a)$ is given in Ref. 22 and $\epsilon(\mathbf{q},\mathbf{j},a)$ is the phonon eigenvector of atom of type a with mass M_a.

Table I contains the calculated DPs for scattering between Γ, X, and L. Note that the selection rules are obeyed. For most materials the calculated LA contribution to Γ-L scattering is larger than the LO contribution, in contrast with experiments.[3] These D's do not depend critically on the EPM form factors, but some phonon models permute the roles of LA and LO phonons, even in the case of InP where the two masses are quite different. This is not surprising as the prediction of phonon eigenvectors by empirical models remains an open question. Our $D_{\Gamma L}$s are in the range of values in the literature.[7] The values for $D_{\Gamma X}$ are smaller by a factor of 2–3 than those needed to model velocity field curves (10 eV/Å). This could be explained by the fact that the carriers can scatter to two valleys at the X point that are very close in energy to each other,[13] thus increasing the scattering rate. Also processes not involving phonons, like impurity or electron-hole scattering, or scattering from L to X (which is very strong) could be important.

The values of the IV DPs in Table I are accurate to within 20% for the Ga and In compounds, as estimated by repeating the calculation for several slightly different interpolations[22] of the pseudopotential form factors and different phonon models. The uncertainty is larger for AlSb and AlAs, as no neutron scattering data are available for these materials and crude phonon models had to be used.[17,23]

The DP constants are essential in calculating the scattering times between nonequivalent valleys. We assume that the carriers are optically excited with an energy E_0 (all energies measured with respect to the lowest CB edge) in a direct band-gap sample, then scatter to higher valleys at L or X and back to Γ. We also study the case of an indirect sample, where the carriers scatter from Γ to L or X and then recombine via indirect transitions. The scattering probability to a higher valley V (with mass m_V and energy ΔE above the CB edge) is given by Fermi's "golden rule." An integration of the matrix element over all possible final states (neglecting the k dependence of the DP and the phonon energy near the band minimum) gives the well known scattering rate[24]

$$\tau^{-1} = \frac{D^2 m_V^{3/2} N_V}{\sqrt{2}\pi\hbar^2 M E_{qj}} \left[N_{qj} \mathrm{Re}\sqrt{E_i - \Delta E + E_{qj}} + (N_{qj}+1)\mathrm{Re}\sqrt{E_i - \Delta E - E_{qj}} \right], \quad (3)$$

where E_i is the energy of the carrier before the scattering and N_V the number of equivalent valleys (1 for Γ, 3 for X, and 4 for L). As the phase space available for the IV phonons is large, nonequilibrium phonons can be neglected.[6] For scattering to a lower valley, we have to replace ΔE by 0, if we measure all energies from the CB edge.

To study the evolution of the carrier distribution of the electrons with time an appropriate rate equation involving these scattering times has to be solved.[2] We discuss two limiting cases, which we call the slow and fast scattering limits. In the *fast scattering limit*, the IV scattering time is shorter than the times for carrier-carrier and LO-phonon scattering. We assume that this limit describes the scattering from the Γ valley as the density of states at the other valleys is much higher. Thus we can obtain τ from Eq. (3) after setting E_i equal to the laser excess energy E_0. For scattering back to Γ, we use the *slow scattering limit*, where the carriers first relax and reach an equilibrium with the lattice (at the L or X point). The expression for scattering from X or L back to Γ (for $\Delta E > E_{qj}$) in a direct sample is found after averaging over a Maxwellian carrier distribution to be

$$\tau_{\mathrm{slow}}^{-1} = \frac{D^2 m_\Gamma^{3/2}\sqrt{2kT}}{\pi^{3/2}\hbar^2 M E_{qj}} \left[N_{qj} B\left(\frac{\Delta E + E_{qj}}{kT}\right) + (N_{qj}+1) B\left(\frac{\Delta E - E_{qj}}{kT}\right) \right], \quad (4)$$

with $B(2x) = x\exp(x)K_1(x)$, where k is the Boltzmann constant and K_1 the first-order modified Bessel function of the second kind. In Eqs. (3) and (4), an appropriate mass has to be chosen, which takes the nonparabolicity into account.[15] The return time of the carriers gets larger as the energy ΔE decreases, because the density of states in the Γ valley becomes smaller. Therefore, GaSb with $\Delta E_{\Gamma L} \simeq 80$

TABLE II. Theoretical (LA, LO) and experimental scattering times between Γ and L or X (optical excitation with an energy E_0 above the CB edge, sample temperature T). The experimental values are from Refs. 3 and 6, material parameters from Ref. 7.

	E_0 (meV)	$\Delta E_{\Gamma L}$ (meV)	$\Delta E_{\Gamma X}$ (meV)	T (K)	$\tau_{\Gamma L}$ (ps) LA	LO	exp	$\tau_{L\Gamma}$ (ps) LA	LO	exp	$\tau_{\Gamma X}$ (ps) LO	exp
GaAs	550	285	480	300	0.16	10		2	120	0.95	0.11	
GaAs	480	300	460	2	0.44	25	0.48	4.2	230		...	...
GaAs	580	300	460	2	0.34	19		4.2	230		0.15	0.16
GaSb	95	61	330	300	0.63	1.3		6.8	25		...	...

meV would be an interesting material to study. In GaSb/AlSb quantum wells $\Delta E_{\Gamma L}$ is even smaller, and the return times can reach 100 ps or more. Table II lists the calculated scattering times (LA and LO contributions) between Γ and L or X, together with experimental values from Refs. 3 and 6.

In summary, we have calculated the intervalley deformation potentials at high symmetry points. The results are in the range of values extracted from electrical and optical data. The IV scattering times calculated from the deformation potentials agree with recent experiments.

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[1]J. Shah, B. Deveaud, T. C. Damen, W. T. Tsang, A. C. Gossard, and P. Lugli, Phys. Rev. Lett. **59**, 2222 (1987); T. L. Koch, L. C. Chiu, Ch. Harder, and A. Yariv, Appl. Phys. Lett. **41**, 6 (1982); K. Kash, P. A. Wolff, and W. A. Bonner, *ibid.* **42**, 173 (1983); D. N. Mirlin, V. F. Sapega, I. Ya. Karlik, and R. Katilius, Solid State Commun. **61**, 799 (1987); J. Vaitkus, A. Matulionis, L. Subacius, and K. Jarasiunas, in 18th/19th International Conference on the Physics of Semiconductors, Warsaw, 1988 (in press).

[2]C. L. Collins and P. Y. Yu, Phys. Rev. B **27**, 2602 (1983); **30**, 4501 (1984).

[3]R. G. Ulbrich, J. A. Kash, and J. C. Tsang, in 18th/19th International Conference on the Physics of Semiconductors, Warsaw, 1988 (in press).

[4]P. A. Houston and A. G. R. Evans, Solid-State Electron. **20**, 197 (1977); T. H. Windhorn, T. J. Roth, L. M. Zinkiewicz, O. L. Gaddy, and G. E. Stillman, Appl. Phys. Lett. **40**, 513 (1982); M. Heiblum, E. Calleja, I. M. Anderson, W. P. Dumke, C. M. Knoedler, and L. Osterling, Phys. Rev. Lett. **56**, 2854 (1986).

[5]M. A. Littlejohn, J. R. Hauser, and T. H. Glisson, J. Appl. Phys. **48**, 4587 (1977); J. Požela and A. Reklaitis, Solid-State Electron. **23**, 927 (1980); K. Brennan and K. Hess, *ibid.* **27**, 347 (1984); H. J. Lee and J. C. Woolley, Can. J. Phys. **59**, 1844 (1981).

[6]P. Lugli, L. Reggiani, P. Kocevar, and M. Rieger, in 18th/19th International Conference on the Physics of Semiconductors, Warsaw, 1988 (in press).

[7]*Numerical Data and Functional Relationships in Science*, edited by O. Madelung (Springer, Berlin, 1982 and 1986), Vols. 17a and 22.

[8]W. Fawcett and D. C. Herbert, J. Phys. C **7**, 1641 (1974).

[9]For early work on IV-VI compounds, see M. L. Cohen and Y. W. Tsang, in *The Physics of Semimetals and Narrow-Gap Semiconductors*, edited by D. L. Carter and R. T. Bate (Pergamon, Oxford, 1971), p. 303.

[10]S. L. Richardson, M. M. Dacorogna, F. H. Pollak, M. L. Cohen, and O. J. Glembocki, in *18th/19th International Conference on the Physics of Semiconductors*, edited by O. Engström (World Scientific, Singapore, 1987), p. 1353.

[11]J. L. Birman, Phys. Rev. **127**, 1093 (1962); J. L. Birman, M. Lax, and R. Loudon, *ibid.* **145**, 620 (1966).

[12]M. L. Cohen and T. K. Bergstresser, Phys. Rev. **141**, 789 (1966).

[13]R. M. Wentzcovitch, M. Cardona, M. L. Cohen, and N. E. Christensen, Solid State Commun. **67**, 927 (1988).

[14]D. Strauch and B. Dorner, J. Phys. C **19**, 2853 (1986).

[15]In a three-band $k\cdot p$-model at Γ, the mass has to be multiplied with E_i/E_0, where E_0 is the lowest direct gap. See also C. Jacoboni and L. Reggiani, Rev. Mod. Phys. **55**, 645 (1983).

[16]K. Kunc and O. H. Nielsen, Computer Phys. Commun. **17**, 413 (1979).

[17]K. Kunc and H. Bilz, Solid State Commun. **19**, 1027 (1976). For AlAs we have used the shell parameters of GaAs with the AlAs lattice constant and masses.

[18]P. H. Borcherds and K. Kunc, J. Phys. C **11**, 4145 (1978). We have used model B of this reference for InAs.

[19]J. P. Walter and M. L. Cohen, Phys. Rev. **183**, 763 (1969).

[20]C. Varea de Alvarez, J. P. Walter, R. W. Boyd, and M. L. Cohen, J. Phys. Chem. Solids **34**, 337 (1973).

[21]A. Baldereschi, E. Hess, K. Maschke, H. Neumann, K.-R. Schulze, and K. Unger, J. Phys. C **10**, 4709 (1977).

[22]Sudha Gopalan, P. Lautenschlager, and M. Garriga, Phys. Rev. B **35**, 5577 (1987). The matrix A in this reference contains the pseudopotential and plane wave expansion coefficients.

[23]R. Banerjee and Y. P. Varshni, Can. J. Phys. **47**, 451 (1969).

[24]E. M. Conwell, *High Field Transport in Semiconductors* (Academic, New York, 1967).