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Short-range deformation-potential interaction and its application to ultrafast processes in semiconductors

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Abstract. We have developed a semi-empirical model for the short-range deformation-potential (DP) interaction in bulk (elemental or compound) semiconductors (not semiconductor alloys), which governs the transfer of carriers between different equivalent or non-equivalent conduction band (CB) valleys. Our formalism treats the electron–phonon interaction in the rigid-ion approximation and uses parametrized models for describing electrons (empirical local pseudopotential method) and phonons (shell models). The parameters for electrons and phonons were taken from the literature and no additional parameter was introduced to model the electron–phonon coupling. This model, when applied to the scattering times of electrons between different CB valleys in GaAs, gives reasonable agreement with a number of recent ultrafast optical experiments and resolves apparent contradictions between them. The present model can also be used in Monte-Carlo simulations of electronic transport under high-field conditions. Our main conclusion is that the simple formula for intervalley scattering due to Conwell (based on parabolic CB valleys for the electrons, an Einstein model for the phonons, and a single coupling constant describing the interaction) can only qualitatively explain most experiments and leads to differing values of the strength of the DP interaction. The full electronic band structure and all six phonon modes have to be taken into account in order to obtain a consistent picture.

1. Introduction

The performance of electronic and optoelectronic devices (based on silicon or GaAs-type semiconductors) operating under hot-carrier conditions is usually modelled with Monte-Carlo simulations [1, 2]. It is obvious, however, that the quality of such simulations will depend critically on the physical models used [3]. It is helpful to perform experiments to test these models, such as electrical [4] or CW or ultrafast laser experiments [5], but information on processes governing hot-electron devices can also be obtained from areas in physics that have traditionally been considered to be outside the scope of hot-carrier conferences, like band-structure calculations [6], superconductivity [7–9], temperature [10, 11] and pressure [12] variations of optical gaps, indirect absorption [13], or modulation techniques [14] such as electroreflectance using synchrotron radiation [15] and spectroscopic ellipsometry [16].

The aim of this paper is to come closer to finding a quantitative theoretical description (based on information obtained with the techniques mentioned above) for the transfer of carriers between different conduction band (CB) valleys which leads to negative differential resistance and the Gunn effect [17]. This problem has been at the centre of hot-carrier physics for many years [18], but is still not solved satisfactorily. We will first describe the various methods that can be used to model electrons, phonons and their interactions in bulk semiconductor crystals and choose the one most appropriate for our goal. We then apply our method to discuss the scattering of electrons between different CB valleys in GaAs and compare it with three experiments that have appeared in the literature in recent years [19–21]. We stress that we do not report the results of Monte-Carlo simulations in this work. We rather investigate the physical models and calculate scattering times that are to be used as *input* to the Monte-Carlo programme.

2. How to model electrons, phonons and their interaction

By definition [1], the Monte-Carlo method, as applied to charge carrier transport in semiconductors, simulates the motion of electrons inside a crystal, subject to the action of external fields and of given scattering mechanisms (see

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table 2.5 in [2]). It is a numerical method to solve the Boltzmann equation [1] and therefore needs to evaluate the transition probability P for the scattering of a carrier from a state $|n\boldsymbol{k}\rangle$ with wavevector $\boldsymbol{k}$ in band n and energy $E_{n\boldsymbol{k}}$ to a different state $|n'\boldsymbol{k}'\rangle$, given by Fermi's 'Golden Rule', which enters the collision term:

$$P(n\boldsymbol{k}, n'\boldsymbol{k}') = \frac{1}{\tau_{n\boldsymbol{k},n'\boldsymbol{k}'}} = \frac{2\pi}{\hbar}|\langle n', \boldsymbol{k}'|H_{\mathrm{IA}}|n, \boldsymbol{k}\rangle|^2 \delta(E_{n',\boldsymbol{k}'} - E_{n,\boldsymbol{k}} \pm \Omega_{\mathrm{IA}}). \quad (1)$$

H_{IA} is the Hamiltonian of the scattering process, τ the scattering time and Ω_{IA} the energy of the elementary excitation (for example, a phonon) created or annihilated in the process.

Price [22] stated at the second hot-carrier conference in Denton that analytical formulae are generally able to give a better account of a physical phenomenon than can be provided by a numerical description. The goal of obtaining such analytical expressions clearly had to be abandoned (since the accuracy of simple distribution functions like a shifted Maxwellian is often poor) in favour of Monte-Carlo simulations or numerical solution of complicated systems of coupled nonlinear differential equations [23]. In the early stages of such simulations [1, 2, 24] there was an attempt to keep the description of the electronic and vibrational structure and of the various scattering processes simple and analytical. This approach, i.e. the numerical solution of an analytical Boltzmann equation, led to tremendous success and could supply all the physics in most situations, including the explanation of the Gunn effect through negative differential resistance, but sometimes failed to yield quantitative agreement with experiments [20].

Indeed, one of the early papers [25] seems to suggest that a single parameter, a coupling constant, was all that was needed to model a particular interaction, and calls for experiments to measure these parameters for the relevant interactions. This misconception has led to a vast amount of experimental data, but also to great confusion and unnecessary contradictions in the literature (especially about the strength of the short-range DP interaction responsible for intervalley transfer, see [26]), and may still be prevalent. This trend has been reversed in more recent work [27, 28] where the full electronic band structure is included in the simulations.

Equation (1) shows that there are three ingredients to a Monte-Carlo calculation: electrons, elementary excitations (we will deal with phonons here) and their mutual interactions. Each of these ingredients can be described in three ways: (i) simply and analytically, explaining the basic physics of an effect and usually leading to qualitative agreement with experiments; (ii) with *ab initio* calculations that are very sophisticated, but sometimes not accurate enough (given a finite amount of CPU time) to be useful; (iii) by parametrized model calculations that are accurate and simple enough to be incorporated into Monte-Carlo simulations, but still provide the full picture of electrons, phonons and their interaction necessary for quantitative agreement with experiments.

2.1. Electrons

The electronic structure enters Monte-Carlo calculations in at least two places. (i) The electronic energies as a function of wavevector are contained in the δ-function of equation (1) and have to be known in order to integrate over all possible decay channels (final states $|n', \boldsymbol{k}'\rangle$) and to obtain the lifetime [22]

$$\frac{1}{\tau_{n\boldsymbol{k}}} = \sum_{n'} \int \mathrm{d}^3\boldsymbol{k}' P(n\boldsymbol{k}, n'\boldsymbol{k}'). \quad (2)$$

Experimental information about these energies can be obtained from photoemission measurements to fix the valence bands (VB) [29]. Optical modulation spectroscopy data for the gaps can be added to yield the CB energies at high-symmetry points [30], although some questions remain controversial, e.g., the position of the L-valleys in InP [30] or silicon. Little is known experimentally about the CBs at general points in the Brillouin zone, especially about the effective masses in the satellite valleys [30, 31]. (ii) The electron wavefunctions that enter the matrix element in equation (1) can only be obtained individually for a given n by means of band structure calculations. The total magnitude of all wavefunctions in the valence band, i.e. the valence charge, can sometimes be determined using x-rays, but certain restrictions apply [32].

The simplest theory to treat electrons in a semiconductor is the effective-mass model. It can be improved by taking into account ellipsoidal CB valleys (like in Si or Ge) [2], higher CB band minima [33, 34], nonparabolicity (for high carrier energies) [31] and warping [35] (in the VB). Such models lead to a basic understanding of the physics, but often not to a quantitative analysis of intervalley scattering (IVS).

Very sophisticated band structure calculations, on the other hand, using the *ab initio* pseudopotential [36] or linear muffin-tin orbitals (LMTO) calculations [30, 37], based on the local-density approximation (LDA), give VB energies usually in good agreement with photoemission data [30], but underestimate the band gaps by typically 1 eV or more (band gap problem). This difficulty can be overcome either with empirical corrections [37] or (by increasing the computational effort) with the so-called GW technique [6, 38], but the results are still not accurate, general and reliable enough to be useful for modelling hot-carrier experiments [6].

We believe that the most accurate and convenient description of electronic states, as required in the field of hot carriers, can be obtained with empirical models that are fitted to experimental data. Such methods include the full-zone $\boldsymbol{k}\cdot\boldsymbol{p}$ method [37, 39–41] and the local empirical pseudopotential method (EPM) due to Cohen and Bergstresser [42, 43]. Since both models were developed about 25 years ago and much more accurate experimental band structure data (in

particular, the important positions of the satellite valleys) have become available, it is usually necessary to obtain new sets of parameters for these models before any simulations can be performed, as shown recently for InP [30].

All the calculations presented here were performed with the EPM. The form factors were taken from [30, 44]. We normally used a cut-off of 4.5 Ryd, corresponding to a basis set of about 60 plane waves. In order to avoid discontinuities in the electron–phonon coupling constants (see below), we set the antisymmetric form factors $V_A(11)$ and $V_A(12)$ equal to each other.

2.2. Phonons

Most Monte-Carlo calculations (for bulk systems) have used the very simple Debye and Einstein models for the vibrational structure of the crystal, i.e. acoustic phonons are approximated by three modes with (possibly different) sound velocities, whereas the optical phonons are assumed to have a constant energy [1]. As shown previously, this approach is not sufficient to explain the width of the re-entrant peak in hot-electron luminescence data [45]. In general, all six phonon modes and their dispersion in reciprocal space may have to be taken into account in hot-carrier experiments.

We stress that a phonon is characterized by an energy and an eigenvector (determining the motion of the two atoms relative to each other). The energies can be found very accurately with neutron scattering [46, 47], but knowledge of the eigenvectors requires a careful analysis of the scattering intensities [48]. The interference due to the motion of the two atoms may either destroy or enhance the strength of an interaction; therefore the information about the eigenvectors is essential to obtain scattering times.

Modern supercell frozen-phonon calculations using norm-conserving pseudopotentials [49] or the full-potential LMTO technique [9] yield the phonon energies at high-symmetry points with great accuracy. A recent modification of the technique [50] improves its efficiency at general points in the Brillouin zone. These calculations usually also yield the correct phonon eigenvectors [49].

In our calculations, we have used empirical phonon models fitted to neutron data [51]. Computer programs found in the literature [52] readily yield both energies and eigenvectors, in much less time than the frozen-phonon technique. Whereas agreement with neutron data is good for the energies, six different models find six (considerably) different eigenvectors [49]. We chose the ten-parameter shell model [51] for all of our calculations, since this model gives best agreement with the experimental eigenvectors of [48].

2.3. Deformation-potential electron–phonon interactions

Virtually all Monte-Carlo calculations describe electron–phonon interactions with very simple models for electrons and phonons. They also assume that the strength of the interaction shows no dispersion in reciprocal space and therefore use constant coupling constants, usually obtained from fits to experimental data. This allows the matrix element in equation (1) to be reduced to analytical form [1, 2, 24] in most cases and makes implementation in the computer code very simple. In the case of IVS, τ is given by Conwell's formula [24]

$$\frac{1}{\tau} = \frac{N_V D^2 m_V^{3/2}}{\sqrt{2}\pi\hbar^2\rho\Omega}\left[(N+1)\sqrt{E-\Delta E-\Omega} + N\sqrt{E-\Delta E+\Omega}\right] \tag{3}$$

where N_V is the number of (final) valleys with mass m_V, ΔE the intervalley separation energy (to be set to zero for scattering to a valley with lower energy), Ω the energy of the intervalley phonon, N its occupation number, ρ the density of the crystal and E the energy of the electron (measured from the CB edge) whose scattering time is computed. The strength of the interaction is determined by a single coupling constant D [2], the intervalley deformation potential (DP) [26]. We have shown recently, however, that the intervalley DPs do show dispersion [53], which makes equation (3) a poor approximation. Furthermore, equation (3) implies that the interaction can be attributed to a single phonon mode (the 'intervalley phonon'), which was proved wrong in [53, 54].

The frozen-phonon technique allows the evaluation of DPs. Recent calculations for the interaction of electrons and holes with zone-centre phonons are in very good agreement with experiments, and sometimes even more reliable, see [55–57] and the review [26]. Unfortunately, the interaction with zone-boundary phonons (which is of interest for this work) has only been evaluated for silicon [58, 59] and been applied to study the electron–phonon interactions in superconductors [8].

Experimentally, some DPs (for interaction with zone-centre phonons) can be obtained rather easily (and accurately) at high-symmetry points by measuring shifts or splittings of optical transitions under hydrostatic pressure or uniaxial strain [26]. Hydrostatic (i.e. corresponding to completely symmetric deformations) DPs evaluated from such shifts are usually called relative DPs, since they are differences of the *absolute* DPs of the final and initial states observed in the transition. The absolute hydrostatic DPs themselves are much harder to find [26]. Little is known about the dispersion of relative *and* absolute DPs. Intervalley DPs (describing the short-range interaction of electrons with zone-edge phonons) cannot be determined directly, but only after a careful analysis of hot-carrier experiments [26].

It is worth noting an experimental fact known as Paul's rule [60] obtained from gap shifts under hydrostatic pressure: The shifts of band gaps (due to the long-range part of the deformation-potential interaction) between the same sets of points in the Brillouin zone are about the same for all semiconductors. (In Paul's rule the shifts are referred to a fixed pressure, but the rule applies nearly as well to shifts per unit change in volume, i.e. strain.) If one assumes that this rule holds also for the

short-range part of the interaction we come up with the following universal rule: *The intervalley DPs coupling the same sets of points in the Brillouin zone (for example $D_{\Gamma L}$) have similar values for Si, Ge and all III–V semiconductors with zincblende structure.* Experimental evidence for this rule has been obtained with temperature-dependent ellipsometric measurements of the broadenings of the E_1 gaps in Si, Ge, α-Sn, AlAs, GaP, GaAs, GaSb, InP, InAs and InSb [16]. These data support the fact that the short-range deformation potential constants for the valence bands along Γ–L of Ge, α-Sn, GaAs, GaSb, InP, InAs and InSb vary by no more than $\sqrt{2}$. The temperature shifts of the E_1 gaps in these materials also follow along the same lines [61]. The rule could not be proved for Si (completely different conduction band structure), GaP (very small spin–orbit splitting Δ_1), AlAs and AlSb (material problems).

In this work, we have used the rigid-pseudoion model to calculate intervalley DPs, where the Hamiltonian of the interaction is given by the scalar product of the gradient of the crystal potential (which we approximate by the pseudopotential used in the band structure calculations) and the phonon eigenvector. Evaluating the coupling constants only requires a summation over the plane wave basis set, since the gradient operator reduces to a simple multiplication in reciprocal space. See [53] for details of the procedure and references to earlier work, including the important contributions by Cohen and Tsang [62] and Herbert [63].

Using this technique, we have evaluated intervalley DPs for the most common processes in AlAs, AlSb, GaAs, GaSb, GaP, InP, InAs and InSb [53, 64, 65]. (Because of an inconsistency in the notation, the values in table I of [64] have to be divided by $\sqrt{2}$.) These results are in good agreement with the universal rule stated above. They are also in accord with independent results obtained by other groups with slightly different methods [63, 66–68]. In contrast to most previous work (with the exception of the early work by Herbert [63]) we not only calculate the intervalley DPs at high-symmetry points (Γ, X and L), but also study their dispersion for GaAs [53], InP [65], and GaP [69]. We show that there is considerable dispersion and therefore one has to perform the integration in reciprocal space (see equation (2)) with a numerical method [53].

3. Results

We will compare the results of our calculations with three experiments that have been performed in recent years [19–21] to determine the strength of the short-range deformation potential interaction and measure IVS times.

3.1. Time-resolved luminescence

Shah *et al* performed luminescence measurements on bulk GaAs samples at 300 K using up-conversion detection with a time resolution of about 300 fs [19]. They found a slow rise (nearly 10 ps) of the bandgap luminescence intensity with a laser energy of 2.04 eV (above the energy threshold for scattering into the L-valleys), but a much faster rise (less than 3 ps, limited by carrier-cooling in the central valley) at 1.66 eV (below the threshold). A careful Monte-Carlo analysis of their spectra [19] (including photoexcitation from all three valence bands, electron–electron, intravalley and intervalley carrier–phonon interaction as well as hot-phonon effects) reaches quantitative agreement with the transient spectra, if a lifetime in the L-valley (Γ–L return time) of 2.5 ps is assumed, see the symbol ○ in figure 1(*a*).

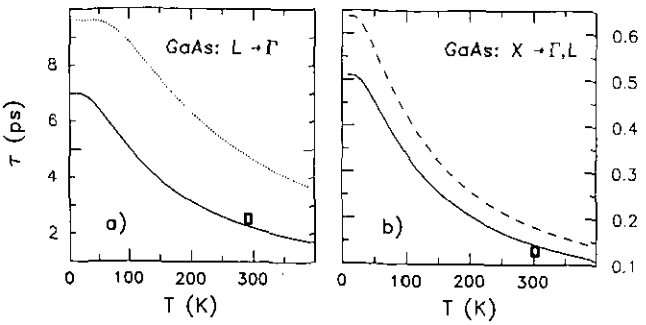

Figure 1. Lifetimes (return times) of electrons at (*a*) the L_6 and (*b*) the X_6 conduction band minima as a function of lattice temperature T in the zero carrier-density limit, calculated with the rigid-pseudoion method, including all six phonon modes and the full dispersion of the electrons, phonons and electron–phonon matrix elements. The dotted curve in (*a*) shows the lifetime at L_6 when the interaction with the TA phonons is switched off. The broken curve in (*b*) gives the scattering time from X_6 to the L-valleys only, accounting for about 80% of all scattering processes at X_6. The symbols show the experimental result determined by Shah *et al* [19] (*a*) and the lifetime at X calculated from usual Monte-Carlo parameters [33] with equation (3) (*b*).

We compare this experiment with our calculations in figure 1(*a*), where the lifetime in the L-valley as a function of temperature is shown by the full curve. We obtain a lifetime of 2.2 ± 0.5 ps at 300 K, in good agreement with the data of [19], and 6.6 ps at 10 K, when all six phonon modes and the dispersion of the electron–phonon matrix element [53] are taken into account. The lifetimes would be much longer if the transverse acoustic (TA) phonon were neglected (dotted curve).

Figure 1(*b*) shows the lifetimes at the X-point (full curve). The broken curve shows the scattering time from X to the L-valleys only, which accounts for about 80% of all scattering processes at X, independent of temperature. Our lifetime of 130 ± 20 fs at 300 K is in good agreement with the strength of IVS normally assumed in Monte-Carlo simulations, see the symbol ○ in figure 1(*b*) and [33].

3.2. Hot-electron photoluminescence spectroscopy

Ulbrich *et al* observed luminescence from hot electrons in the conduction band recombining with neutral acceptors in GaAs at 2 K and determined from these measurements the scattering times into the satellite valleys as a function of carrier energy [20]. The IVS times calculated from the

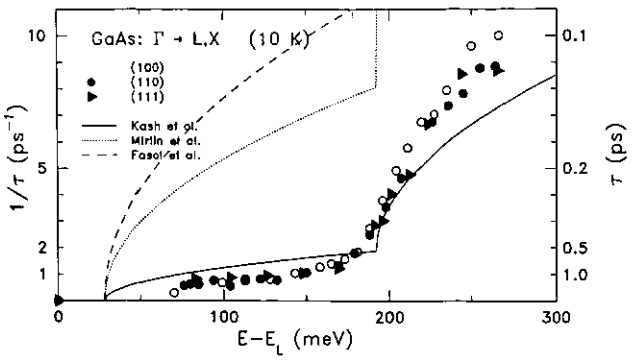

Figure 2. Intervalley scattering rates for electrons (with wavevectors in different high-symmetry directions) in GaAs ($\Gamma \rightarrow$ L, X) at 10 K in the zero carrier-density limit, obtained from the rigid-pseudoion method (symbols), in comparison with the results of three hot-electron luminescence experiments [20, 54, 70] (curves).

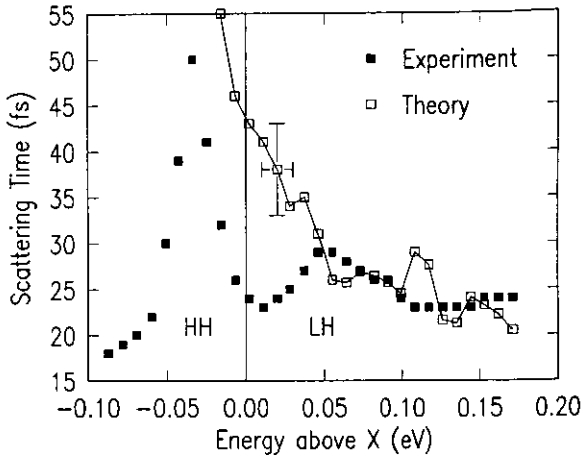

Figure 3. Transmittance recovery times obtained in a femtosecond pump-probe experiment [21] with carrier densities up to $10^{18}\,cm^{-3}$ (full squares). The experiment shows two features due to excitation of carriers from the heavy-hole (HH) and light-hole (LH) bands. Calculated intervalley scattering times (full curve) as a function of excess electron energy in the Γ-valley (relative to the X-valley minimum, excitation from the heavy hole assumed) have the correct order of magnitude at sufficiently high energies.

parameters they determined are given in figure 2 (full curve). We should note, however, that these results are controversial and in disagreement with [70] (broken curve) and [54] (dotted curve). Our results, obtained for electrons with wavevectors in the (100), (110) and (111) directions, are shown by the symbols in figure 2 in comparison with the experimental data. It can be seen that the agreement with the data of Ulbrich *et al* is very good. See [45] for details.

We should note the following. When the experiments of [19, 20] are evaluated with Conwell's formula, equation (3), they yield intervalley DPS different by a factor of two. This is due to the inadequacy of equation (3) and the strong contribution of TA phonons at room temperature (but not at low temperatures, where all phonons have the same occupation number, i.e. zero) at a finite wavevector, as discussed in [11]. The contribution of the TA phonon is forbidden by symmetry [64], but this condition only holds at high-symmetry points and not at general points in the Brillouin zone where IVS processes take place. This is a consequence of the dispersion curves in [53]. Our improved formalism agrees with both experiments.

3.3. Femtosecond pump-probe measurements

Bigot *et al* used 6 fs optical pulses to study the carrier relaxation in GaAs at 300 K at very early times and energies high above the X-minima [21]. We digitized their data and subtracted the band gap E_0 (1.422 eV at 300 K), the energy of the photoexcited heavy holes ($m_e/m_{hh} = 0.126$) and the ΓX separation (0.476 eV, all data from [71]) from the laser photon energy to obtain the excess electron energy relative to the position of the X-valley; see the full squares in figure 3. (In the experiment, electron–hole pairs were created from all three VBS. We only consider excitation from the heavy hole band; therefore the strucure labelled LH will not be explained here.) The transmittance recovery times shown in the figure (obtained in a pump-probe configuration with carrier densities up to $10^{18}\,cm^{-3}$) reflect a number of phenomena (including carrier–carrier scattering and phonon-induced intravalley relaxation), so a comparison of these data [21] with our calculated IVS times [45] can lead to only a partial understanding of the processes occurring on these time scales. The return of carriers from the satellite valley to the Γ-valley, on the other hand, does not have to be taken into account, since it is generally assumed that these carriers have a lifetime of more than 100 fs (see figure 1), much longer than the time scales observed in the experiment.

Our main purpose here is to demonstrate that our calculated IVS times (see the full curve in figure 3, the error bar showing the uncertainty in our calculation) *have the correct order of magnitude, and probably no new physical concepts are necessary to explain these data.* Indeed, the agreement with the experiment [21] above the energy of the X-minimum is much better than could be expected.

The experiment creates electrons in the Γ-valley. These carriers will, if they have sufficient energy, scatter to the X-valley. The minimum energy required (in an absorption process) is the energy of the X-valley minus that of the intervalley phonon (10–30 meV). The absorption of an LO phonon ($N = 0.48$) is much less likely at 300 K than absorption of a TA phonon ($N = 2.2$), which has a similar coupling strength, see figure 5(*b*) in [45]. Typical scattering times to the X-valley range from 150 fs down to 20 fs or less; see figure 4 in [45]. Carriers that do not have sufficient energy can only scatter to the L-valleys ($\tau = 150$ fs or more). This behaviour is met well by the data, at least for electron energies not less than 30 meV below the X-valley. The very short scattering times at low energies, however, have not been explained so far [21].

4. Conclusion

We have suggested a number of numerical procedures for treating electrons, phonons and their interactions in bulk semiconductors. We have applied the rigid-ion empirical-pseudopotential model to describe the short-range deformation-potential interaction and calculated intervalley scattering times for GaAs, including the lifetimes (return times) of electrons at the conduction band minima at L and X as well the out-scattering times from the Γ-valley to the satellite valleys. These calculations include all six phonon branches and the dependence of the electron–phonon coupling constants on $\boldsymbol{k}$. Several time-resolved spectroscopic experiments are analysed on the basis of these results. It is shown that scattering by TA phonons, forbidden between states at high-symmetry points, is essential to interpret the experimental data at room temperature. The reasonable agreement between our calculations and these experiments leads us to believe that intervalley scattering is finally a phenomenon that is satisfactorily well understood.

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References

[1] Jacoboni C and Reggiani L 1983 *Rev. Mod. Phys.* **55** 645
[2] Reggiani L 1985 *Hot-Electron Transport in Semiconductors* ed L Reggiani (Berlin: Springer) p 60
[3] Jacoboni C 1979 *Physics of Nonlinear Transport in Semiconductors* ed D K Ferry *et al* (New York: Plenum) p xiii
[4] Brennan K and Hess K 1984 *Solid-State Electron* **27** 347
Stanton C J, Baranger H U and Wilkins J W 1986 *Appl. Phys. Lett.* **49** 176
[5] Shah J 1989 *Solid-State Electron* **32** 1051
[6] Hott R 1991 *Phys. Rev.* B **44** 1057
[7] Cohen M L 1964 *Phys. Rev.* **134** A511
[8] Chang K J, Dacorogna M M, Cohen M L, Mignot J M, Chouteau G and Martinez G 1985 *Phys. Rev. Lett.* **54** 2375
[9] Rodriguez C O, Liechtenstein A I, Mazin I I, Jepsen O, Andersen O K and Methfessel M 1990 *Phys. Rev.* B **42** 2692
[10] Cohen M L 1962 *Phys. Rev.* **128** 131
[11] Zollner S, Gopalan S and Cardona M 1991 *Solid State Commun.* **77** 485
[12] Satpathy S, Chandrasekhar M and Chandrasekhar H R 1990 *Proc. 20th Int. Conf. on the Physics of Semiconductors* ed E M Anastassakis and J D Joannopoulos (Singapore: World Scientific) vol 2, p 1521
[13] Goñi A R, Cantarero A, Syassen K and Cardona M 1990 *Phys. Rev.* B **41** 10111
[14] Cardona M 1969 *Modulation Spectroscopy* (New York: Academic)
[15] Aspnes D E 1976 *Phys. Rev.* B **14** 5331
[16] Zollner S, Gopalan S, Garriga M, Humlíček J, Viña L and Cardona M 1990 *Appl. Phys. Lett.* **57** 2838
[17] Gunn J B 1964 *IBM J. Res. Dev.* **8** 141; 1963 *Solid State Commun.* **1** 88
Kroemer H 1964 *Proc. IEEE* **52** 1736
Sze S M 1981 *Physics of Semiconductor Devices* (New York: Wiley) p 637
[18] Hilsum C 1978 *Solid-State Electron.* **21** 5
[19] Shah J, Deveaud B, Damen T C, Tsang W T, Gossard A C and Lugli P 1987 *Phys. Rev. Lett.* **59** 2222
Oberli D Y, Shah J and Damen T C 1989 *Phys. Rev.* B **40** 1323
[20] Ulbrich R G, Kash J A and Tsang J C 1989 *Phys. Rev. Lett.* **62** 949
Alekseev M A and Mirlin D N 1990 *Phys. Rev. Lett.* **65** 274
Kash J A, Tsang J C and Ulbrich R G 1990 *Phys. Rev. Lett.* **65** 275
Kash J A, Ulbrich R G and Tsang J C 1989 *Solid-State Electron.* **32** 1277
[21] Bigot J-Y, Portella M T, Schoenlein R W, Cunningham J E and Shank C V 1990 *Phys. Rev. Lett.* **65** 3429
[22] Price P J 1978 *Solid-State Electron.* **78** 9
[23] Liu M, Xing D Y and Ting C S 1989 *J. Phys.: Condens. Matter* **1** 407
Xing D Y, Liu M and Ting C S 1988 *Phys. Rev.* B **37** 10283
[24] Conwell E M 1967 *High Field Transport in Semiconductors* (New York: Academic)
[25] Ferry D K 1978 *Solid-State Electron.* **21** 319
[26] Cardona M and Zollner S 1990 *Properties of GaAs* EMIS Datareview Series No 2, 2nd edn (London: INSPEC) p 126
[27] Fischetti M V and Laux S E 1988 *Phys. Rev.* B **38** 9721
[28] Stanton C J, Bailey D W and Hess K 1990 *Phys. Rev. Lett.* **65** 231
Bailey D W, Stanton C J and Hess K 1990 *Phys. Rev.* B **42** 3423
[29] Goldmann A and Koch E-E 1989 *Numerical Data and Functional Relationships in Science and Technology* vol. 23a (Berlin: Springer)
[30] Zollner S, Schmid U, Christensen N E and Cardona M 1990 *Appl. Phys. Lett.* **57** 2339
[31] Ruf T and Cardona M 1990 *Phys. Rev.* B **41** 10747
[32] Cohen M L and Chelikowsky J R 1988 *Electronic Structure and Optical Properties of Semiconductors* (Berlin: Springer)
[33] Kann M J, Kriman A M and Ferry D K 1990 *Ultrafast Laser Probe Phenomena in Bulk and Microstructure Semiconductors III* ed R R Alfano (*Proc. SPIE* **1282** 98); *Phys. Rev.* B **41** 12659
[34] Chamoun S N, Joshi R, Arnold E N, Grondin R O, Meyer K E, Pessot M and Mourou G A 1989 *J. Appl. Phys.* **66** 236
[35] Wiley J D 1975 *Semiconductors and Semimetals* ed R K Willardson and A C Beer (New York: Academic) p 91
[36] Cohen M L 1986 *Science* **234** 549
[37] Cardona M, Christensen N E and Fasol G 1988 *Phys. Rev.* B **38** 1806
[38] Zhang S B, Tománek D, Cohen M L, Louie S G and Hybertsen M S 1989 *Phys. Rev.* B **40** 3162
[39] Kane E O 1957 *J. Phys. Chem. Solids* **1** 249
[40] Pollak F H, Higginbotham C W and Cardona M 1966 *J. Phys. Soc. Japan* **21** (suppl.) 20
[41] Rössler U 1984 *Solid State Commun.* **49** 943
[42] Cohen M L and Bergstresser T K 1966 *Phys. Rev.* **141** 789
[43] Mašović D R and Vukajlović F 1981 *Comput. Phys. Commun.* **24** 181

[44] Caruthers E and Lin-Chung P J 1978 *Phys. Rev.* B **17** 2705
[45] Zollner S, Gopalan S and Cardona M 1990 *Ultrafast Laser Probe Phenomena in Bulk and Microstructure Semiconductors III* ed R R Alfano (*Proc. SPIE* **1282** 78)
[46] Bilz H and Kress W 1979 *Phonon Dispersion Relations in Insulators* (Berlin: Springer)
[47] Strauch D and Dorner B 1990 *J. Phys.: Condens. Matter* **2** 1457
[48] Strauch D and Dorner B 1986 *J. Phys. C: Solid State Phys.* **19** 2853
[49] Kunc K and Martin R M 1983 *Ab Initio Calculations of Phonon Spectra* ed J T Devreese, V E Van Doren and P E Van Camp (New York: Plenum) p 65
Gianozzi P, de Gironcoli S, Pavone P and Baroni S 1991 *Phys. Rev.* B **43** 7231
[50] King-Smith D and Needs R J 1990 *J. Phys.: Condens. Matter* **2** 3431
[51] Kunc K and Bilz H 1976 *Solid State Commun.* **19** 1017
[52] Kunc K and Nielsen O H 1979 *Comput. Phys. Commun.* **17** 413
[53] Zollner S, Gopalan S and Cardona M 1990 *J. Appl. Phys.* **68** 1682
[54] Mirlin D N, Sapega V F, Karlik I Ya and Katilius R 1987 *Solid State Commun.* **61** 799
Mirlin D N, Karlik I Ya and Sapega V F 1988 *Solid State Commun.* **65** 171
Mirlin D N, Karlik I Ja, Nikitin L P, Reshina I I and Sapega V F 1981 *Solid State Commun.* **37** 757
Alekseev M A, Karlik I Ya, Mirlin D N and Sapega V F 1989 *Sov. Phys.–Semicond.* **23** 479
Karlik I Ya, Mirlin D N and Sapega V F 1987 *Sov. Phys.–Semicond.* **21** 630
[55] Van de Walle C and Martin R M 1989 *Phys. Rev. Lett.* **62** 2028
Van de Walle C G 1989 *Phys. Rev.* B **39** 1871
[56] Schmid U, Christensen N E and Cardona M 1990 *Solid State Commun.* **75** 39
[57] Wang B S, Gu Z Q, Wang J Q and Li M F 1989 *Phys. Rev.* B **39** 12789
[58] Richardson S L, Dacorogna M M, Pollak F H, Cohen M L and Glembocki O J 1987 *Proc. 18th Int. Conf. on the Physics of Semiconductors* ed O Engström (Singapore World Scientific) vol 2, p 1353
[59] Klenner M, Rakel H, Falter C and Ludwig W 1990 *Phonons 89: Proc. 3rd Int. Conf. on Phonon Physics and the Sixth Int. Conf. on Phonon Scattering in Condensed Matter* ed S Hunklinger, W Ludwig and G Weiss (Singapore: World Scientific) vol 1, p 196
[60] Paul W 1958 *J. Phys. Chem. Solids* **8** 196
[61] Cardona M and Gopalan S 1989 *Progress on Electron Properties of Solids* ed R Girlanda (Deventer: Kluwer)
[62] Cohen M L and Tsang Y W 1971 *The Physics of Semimetals and Narrow-Gap Semicondutors* ed D L Carter and R T Bate (Oxford: Pergamon) p 31
[63] Herbert D C 1973 *J. Phys. C: Solid State Phys.* **6** 2788
Fawcett W and Herbert D C 1974 *J. Phys. C: Solid State Phys.* **7** 1641
[64] Zollner S, Gopalan S and Cardona M 1989 *Appl. Phys. Lett.* **54** 614
[65] Zollner S, Gopalan S and Cardona M *1991 Phys. Rev.* B **44** at press
[66] Glembocki O J and Pollak F H 1982 *Phys. Rev. Lett.* **48** 413; *Phys. Rev.* B **25** 7863
Pollack F H and Glembocki O J 1985 *Electronic Structure, Dynamics, and Quantum Structural Properties of Condensed Matter* ed J T Devreese and P Van Camp (New York: Plenum) p 451
[67] Krishnamurthy S, Sher A and Chen A-B 1988 *Appl. Phys. Lett.* **53** 1853
[68] Grinyaev S N, Karavaev G F and Tyuterev V G 1990 *Sov. Phys.–Semicond.* **23** 905
[69] Zollner S, Kircher J, Cardona M and Gopalan S 1989 *Solid-State Electron.* **32** 1585
[70] Fasol G, Hackenberg W, Hughes H P, Ploog K, Bauser E and Kano H 1990 *Phys. Rev.* B **41** 1461
Hackenberg W and Fasol G 1989 *Solid-State Electron.* **32** 1247
[71] Blakemore J S 1982 *J. Appl. Phys.* **53** R123