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Microscopic theory of intervalley scattering in InP

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In analogy to previous work on GaAs, we apply the "rigid-pseudo-ion" model to intervalley-scattering (IVS) processes in InP. We give the IVS times from the Γ valley to the side valleys around L and X as a function of energy at 0 and 300 K as well as the return times from the L and X points to the Γ valley from 0 to 400 K. Our results suggest that the strength of the electron-phonon interaction in InP is similar to that in GaAs. Therefore the IVS times in InP can be obtained from those of GaAs by a simple extrapolation allowing for the different position of the satellite valleys. Nevertheless, our calculated IVS times are much slower than those found from hot-photoluminescence and photoemission experiments.

I. INTRODUCTION

The transport properties of electrons in InP under very high electric fields are determined by the transfer of carriers from the central valley at Γ (with a high mobility) to the satellite valleys at L or X (with lower mobilities),[1,2] which is called intervalley scattering (IVS). We have recently developed[3] a microscopic theory for IVS and applied it to GaAs,[4,5] where reasonable agreement with optical experiments[6–8] has been found.[9] Our calculations, which have no free parameters for electron-phonon coupling, are also compatible with Monte Carlo simulations based on the analysis of transport data.[10–13] Since the fastest bipolar transistors currently available[2] make use of high-velocity nonequilibrium transport in $In_{0.53}Ga_{0.47}As$/InP heterostructures, we feel that an estimation of the IVS times in InP warrants a report at this time. A microscopic theory for IVS in semiconductor alloys is currently under development.[14] This theory for alloys, based on second-order perturbation theory (with the difference of the pseudopotentials being the perturbing potential) and the coherent potential approximation, has to use a very different framework to include the effects of disorder.

II. THEORY

In a binary compound semiconductor, IVS processes are caused by the scattering of electrons with phonons through the short-range deformation-potential interaction.[3] Other electron-phonon interaction mechanisms like polar (Fröhlich) or piezoelectric scattering are due to long-range forces and therefore cannot couple electronic states in different equivalent or nonequivalent conduction-band valleys. IVS by impurities[15] is considered weaker than phonon-assisted IVS (if the doping level is not too high) and is not investigated here.

The theory for the short-range deformation potential interaction was initially developed by Cohen and Tsang[16] to explain the superconductivity observed in IV-VI compounds like GeTe and SnTe and later applied to hot-electron transport[17] and the temperature dependence of band gaps[18,19] and broadenings[19] of critical points observed in modulation spectroscopy. It is based on a local empirical pseudopotential (EPM) band structure[20] for the electrons, empirical shell models for the phonons[21] and the rigid-ion model for the electron-phonon interaction.[16,3] Various groups[3,17,22,23] have used this formalism (or slight variations thereof) to calculate intervalley deformation *potentials* (IDP's) for InP and agree on values of about 2.6±0.3 eV/Å for $D_{\Gamma L}$, see Table I. The value for $D_{\Gamma X}$ was found to be 1.6 eV/Å (Ref. 3) or 2.9 eV/Å (Ref. 23). Nonlocality effects were found not to be important.[23,24]

Recent modifications to the rigid-pseudo-ion method have been suggested by Fischetti and Higman.[24] They arrive at much higher IDP's than published by previous workers. There is some arbitrariness in the choice of the potential used to describe the electron-ion interaction, since the bare ionic potential (which is well known) must be screened, and details of the screening (i.e., the dielectric function) are uncertain. This has been discussed in detail elsewhere.[25,3,24] Although the matter is far from being settled, we feel that an application of the method to calculate IVS times for InP is justified at this time by its large success for GaAs (Ref. 9) and in explaining temperature-dependent ellipsometry data for a number of materials. The pseudopotential used for InP was chosen very carefully as described below and Thomas-Fermi screening for a free-electron gas was used to yield the potential in the long-wavelength limit, see Refs. 3 and 24.

In order to calculate IVS *times* the energetic positions of the satellite valleys have to be known rather precisely. These, however, are still controversial. In Ref. 26 we therefore performed an *ab initio* linear-muffin-tin-orbital band-structure calculation to obtain the valence-band structure with high accuracy and combined this information with carefully evaluated optical data from the literature to obtain the inter-conduction-band separation energies of $\Delta E_{\Gamma L}$=0.86±0.02 and $\Delta E_{\Gamma X}$=0.96±0.02 eV

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TABLE I. Intervalley deformation potentials (IDP's) for InP at high-symmetry points in units of eV/Å, calculated using the rigid-pseudo-ion method by various authors. The transverse phonons are doubly degenerate at the L point. The IDP's are for each one of these phonons (averaged).

		$D_{\Gamma L}$		$D_{\Gamma X_1}$	D_{LL}		$D_{X_1 X_1}$		$D_{L X_1}$		
	LA(L)	LO(L)	LA+LO	LA(X)	LA(X)	LO(X)	LA(X)	TA(L)	LA(L)	LO(L)	TO(L)
This work	1.3	2.4	2.7	1.6	0.3	0.9	3.6	0.7	1.0	3.3	1.2
Ref. 3	1.4	1.8	2.3	1.6	0.2	0.9	3.1	0.7	0.5	2.8	1.2
Ref. 23				2.9	0.6	0.7	4.8				
Ref. 17			2.9		1.1	2.4					
Ref. 22			2.6								
Ref. 24[a]			5.6	4.7	5.9		4.0		5.0		
Ref. 24[b]			4.7	6.1	5.1		3.7		4.3		

[a] Obtained with a local EPM model. The IDP's given for the X valleys refer to scattering to or from the conduction-band minima along Δ predicted by the local EPM model used in Ref. 24.

[b] Obtained with a nonlocal EPM model.

at 0 K. (See Ref. 26 for details.) In order to use the rigid-pseudo-ion method for InP we had to find new pseudopotential form factors that reproduce the conduction-band structure as above. These are also given in Ref. 26. In principle, the values of $\Delta E_{\Gamma L}$ and $\Delta E_{\Gamma X}$ are functions of temperature. They could change by about 10 meV between 0 and 300 K, see Ref. 27. For simplicity, however, we neglect this temperature dependence here. This point will be addressed at a later time.

We should note that recently Fischetti[28] and Fischetti and Higman[24] have also performed EPM band-structure calculations on InP. They agree with us on the position of the L minimum. In the local band structure of Ref. 28, however, a pronounced camel's-back structure along the Δ direction (similar to silicon) with the minimum 1.492 eV above Γ is predicted. In the nonlocal calculations of Ref. 24, on the other hand, they find the minimum at the X point 1.029 eV above Γ, essentially in agreement with our results.[26] We believe that in analogy to GaAs (where the conduction-band structure is well known, see Ref. 27) the indirect inter-conduction-band transitions observed in wavelength-modulated absorption by Onton, Chicotka, and Yacobi[29] can only be explained if one takes $\Delta E_{\Gamma X}=0.96$ eV. We also assume in this work that the minima are located at the X point, resulting in three X valleys. (A minimum along Δ with a camel's-back structure would cause six valleys as in silicon.)

In Ref. 30 we tested the electron-phonon properties predicted by our form factors[26] along with the ten-parameter overlap valence shell model of Ref. 21. We found that the temperature dependence of the E_0 gap is described better than with any other set of pseudopotential form factors from the literature. The broadenings of the E_1 critical point as a function of temperature, corresponding to scattering processes of holes with large-wave-vector phonons, can also be modeled with this set of form

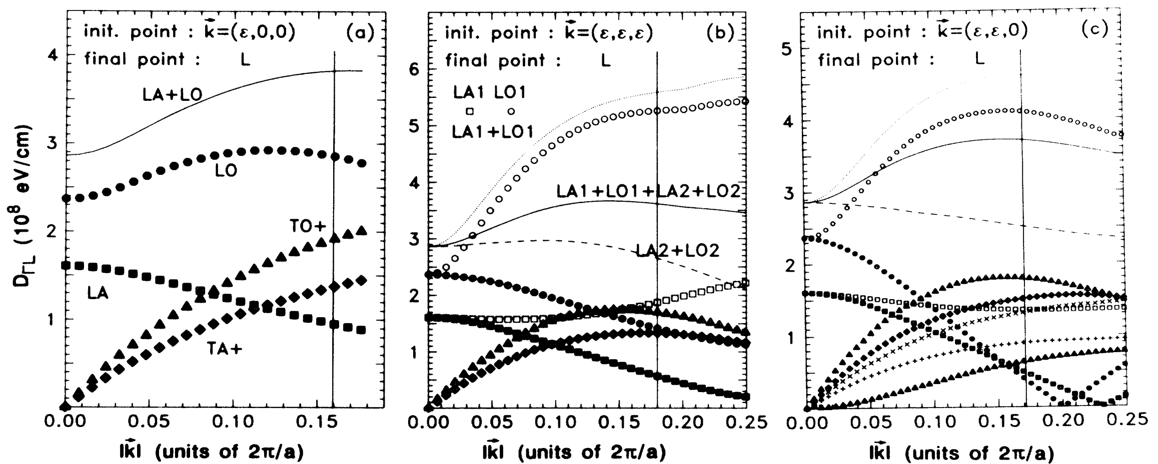

FIG. 1. Intervalley deformation potentials in InP for scattering from points in the Γ valley to the L point. (a) Initial point along [100], (b) along [111], (c) along [110]. The vertical line shows the onset of real (energy-conserving) intervalley transitions. The pseudopotentials were interpolated from Ref. 26 and used with a cutoff of 4.5 Ry, the phonon frequencies and eigenvectors were calculated with the ten-parameter valence overlap shell model with parameters from Ref. 21. The open and closed symbols distinguish between nonequivalent IVS processes to different L points (where the intervalley phonons have different lengths).

factors.[31,32] We therefore believe that the works of Refs. 3, 26, 30, and 31 form an adequate basis to calculate IVS times for InP.

III. RESULTS

A. k dependence of intervalley deformation potentials

As described previously,[3] the IDP's in Table I *cannot* be used to calculate IVS times with the Conwell formula,[33] since these IDP's give the electron-phonon matrix elements between electronic states at high-symmetry points. Because of energy conservation, however, real intervalley transitions take place somewhere in the bulk of the Brillouin zone. Since the satellite valleys are at higher energies in InP than in GaAs, the Conwell formula will give an even less adequate description for IVS times. We therefore investigated how the IDP's change with electron wave vector, see Figs. 1 and 2. It can be seen that there is indeed a considerable **k** dependence of the IDP's, similar to GaAs, as explained in Ref. 3. We stress that in addition to the longitudinal-acoustic (LA, ■, □) and longitudinal-optic (LO, •, ∘) phonons, there is some probability for scattering of an electron with a transverse-acoustic (TA, ♦) or transverse-optic (TO, ▲) phonon. Because of this complicated behavior, a numerical approach (including all possible scattering channels with a numerical integration over the Brillouin zone) is more appropriate than an analytical formula like that proposed by Conwell,[33] as described in Ref. 9.

B. Differences between GaAs and InP

We would like to stress some differences between InP and GaAs that can be observed when comparing Figs. 1 and 2 with Figs. 2 and 3 in Ref. 3. These differences are due to the dissimilar ionic masses in InP and the fact that InP is more polar than GaAs.

In germanium, a diamond-type material with inversion symmetry, only the LA phonon can couple electronic states in the conduction band at L and Γ. In GaAs this symmetry is broken, but because of the similar masses of gallium and arsenic, $D_{\Gamma L}(\mathrm{LA})$ is still much bigger than $D_{\Gamma L}(\mathrm{LO})$. In InP, however, $D_{\Gamma L}(\mathrm{LO})$ is comparable to $D_{\Gamma L}(\mathrm{LA})$, but somewhat larger. Since indium is heavier than phosphorus, the optical phonons usually have larger electron-phonon matrix elements at a general point in the Brillouin zone than the acoustic phonons in InP. The reverse is true for GaAs. An exception to this rule is the X point, where $D_{\Gamma X}(\mathrm{LO})$ is zero, but $D_{\Gamma X}(\mathrm{LA})$ is nonzero for symmetry reasons.[34]

By the same token, the diamond space group contains some reflection planes which are absent in the zinc-blende space group. We have found that the selection rules implied by these symmetry operations are approximately obeyed in GaAs (see Table II in Ref. 3). As a consequence, the lower TA (+) and TO phonons (×) in GaAs are not important for intervalley scattering. In InP, however, all six phonon modes have to be considered, see Figs. 1(c) and 2(c).

C. Lifetimes at the L and X points

In order to find the lifetimes of electrons at the L or X points we calculate the intervalley spectral functions[3] (SF's), see Fig. 3. By weighting these SF's with the appropriate occupation numbers and integrating over all phonon energies Ω we find the IVS times as a function of temperature, see Fig. 4. The return times for InP at L are 900 fs at 0 K and 250 fs at 300 K. These times are increased by about 500 fs when the interaction with the TA phonons is switched off, see the dotted line in Fig. 4(a). We note that the return times from the L point in

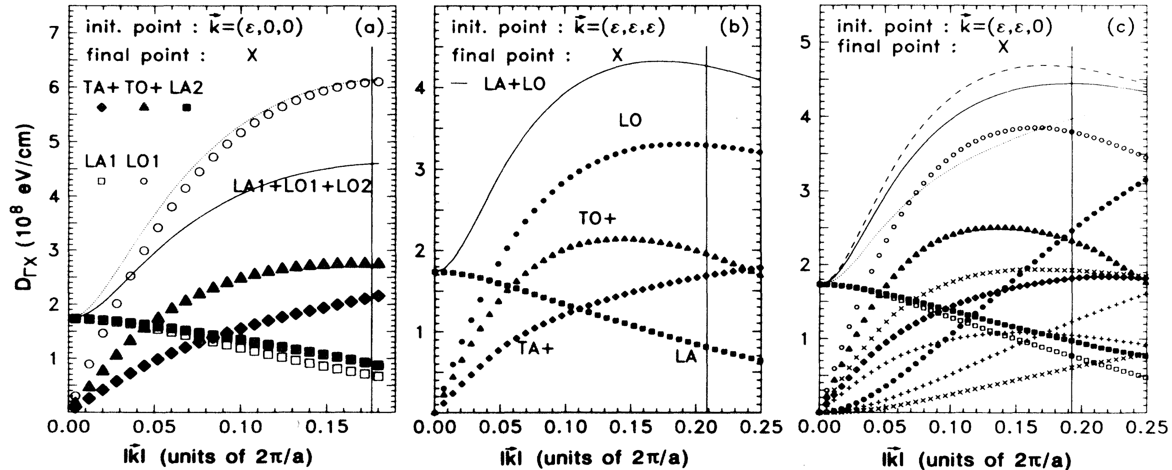

FIG. 2. As Fig. 1, but for scattering to the X point.

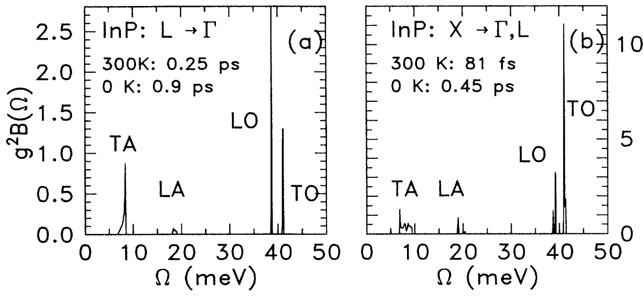

FIG. 3. Dimensionless intervalley spectral functions for electrons at (a) the L point and (b) the X point. It can be seen that most electrons at L will scatter to the Γ valley by emission or absorption of an LO or TO phonon, with some contribution of the TA phonons. The same is true for electrons at X scattering to the Γ or L valleys.

InP are much shorter than those in GaAs (6.6 ps at 0 K and 2.2 ps at 300 K, see Ref. 3) since the L valley has a much higher energy in InP (860 meV above Γ) than in GaAs (300 meV above Γ).

An electron at the X point can scatter into the Γ valley or one of the four L valleys. The total lifetime at X is 450 fs at 0 K and 81 fs at 300 K, see the solid line in Fig. 4. The dashed line in Fig. 4(b) shows the IVS time from X to the L valleys only (700 fs at 0 K and 128 fs at 300 K). This shows that most of the electrons (about 64%) at X will scatter into the L valleys rather than return directly to the Γ valley. It may be surprising to note that these calculated lifetimes at X are not substantially different from the values quoted for GaAs (400 fs at 0 K and 130 fs at 300 K, see Ref. 3). The reason is that the energy difference between X and L, the most important factor in determining the lifetimes at X, is only slightly larger in GaAs (0.18 eV) than in InP (0.11 eV).

To our knowledge, there have been no experimental reports about these lifetimes in the literature. Since the satellite valleys are located at very high energies, an ultrafast laser with a large photon energy (2.5 eV or above) would have to be used for optical experiments.

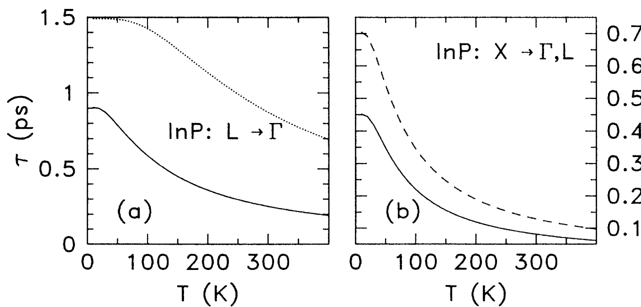

FIG. 4. (a) Lifetimes of electrons at the L point for scattering to the Γ valley as a function of temperature. The dotted line shows the IVS time when the interaction with the TA phonon is switched off. (b) Lifetimes of electrons at the X point for scattering to the Γ or L valleys. The dashed line shows the IVS time for scattering to the L valleys only.

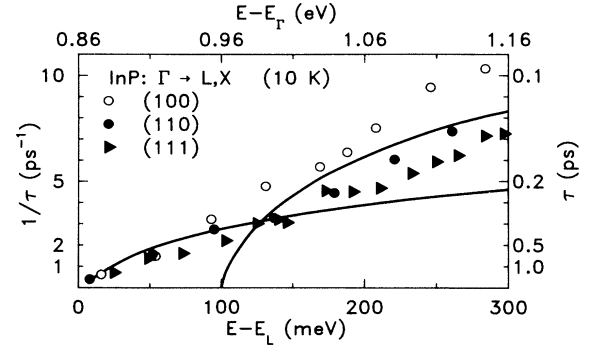

FIG. 5. Intervalley scattering times from the Γ valley to the satellite valleys at L and X at 10 K as a function of carrier energy. The symbols show the direction of the initial electron wave vector. The lines (drawn to guide the eye, not for quantitative analysis) separate the contributions of scattering to L and X.

D. Scattering times from the Γ valley to the satellite valleys

We have calculated the intervalley spectral functions (SF's) for about 30 (initial) electronic states in the Γ valley with energies ranging from 0 to 300 meV above the L point (860–1160 meV above the Γ point) along three different symmetry lines in the Brillouin zone. The integration volume was chosen carefully such as to include intervalley, but no *intravalley* scattering processes. From these SF's, the IVS times at 0 and 300 K were calculated, see Figs. 5 and 6. The solid lines are drawn to guide the eye and split the contributions of scattering to L and X. For simplicity, the small phonon energies ($\Omega \lesssim 40$ meV) were neglected in the calculation. Therefore, emission and absorption of phonons occur at the same energy.[35]

Alekseev and co-workers[36] measured the lifetimes in the Γ valley of InP using hot photoluminescence spectroscopy at 2 K. For electrons with an excess energy of 980 meV (or 120 meV above the L point) they found a lifetime of 50 fs, about six times faster than the results of our calculations.[37] We would like to point out, however, that this group also finds short IVS times for

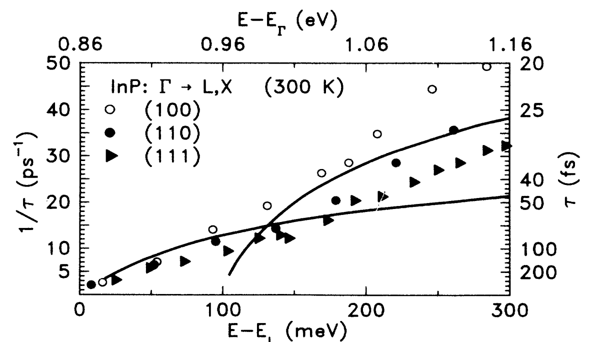

FIG. 6. As Fig. 5, but at 300 K.

GaAs,[38] when compared to our calculations[34] or other experiments.[7]

Peretti, Drouhin, and Paget[39] used a photoemission approach to hot-electron transport and determined the ΓX_1-transfer time for electrons under a high electric field with 1 eV energy to be 20 fs at 120 K. Our calculation (which does not consider any effects a high electric field may possibly have) comes up with 130±40 fs at 120 K, which is six times slower than found in the experiment. We have doubts, however, whether the interpretation of these measurements is unique, since the authors[39] find a conduction-band structure different from the one we obtained in Ref. 26.

E. An empirical rule for electron-phonon interactions

An empirical rule due to Paul[40] states that the pressure-induced shifts of band gaps (due to the long-range part of the electron-phonon interaction) between the same set of points in the Brillouin zone are about the same for all semiconductors. This is also true for the absolute shifts of electronic states with pressure, i.e., the absolute deformation potentials.[41] The similarity in the IVS properties between GaAs and InP and a comparison with six other materials[34] suggests that a similar rule should also hold for the *short-range* deformation potential interaction, which can be stated as follows: *The intervalley deformation potentials coupling the same set of points in the Brillouin zone (for example, $D_{\Gamma L}$) have similar values for Si, Ge, and all III-V semiconductors with zinc-blende structure.* From this we can conclude that IVS times are also about the same, when the energy differences and effective masses are similar.[42]

IV. CONCLUSION

We have applied the rigid-pseudo-ion method to intervalley scattering processes in InP. The calculated return times of electrons at L were found to be 900 fs at 0 K and 250 fs at 300 K, much shorter than in GaAs. At X they were obtained as 450 fs at 0 K and 81 fs at 300 K, about the same as in GaAs. The onset of IVS from the Γ valley to the satellite valleys occurs at 860 meV above Γ. The scattering times are about 250 fs at 0 K (50 fs at 300 K) at an energy of 150 meV above the L point (1 eV above Γ).

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[41]The deformation potential of a gap is given by the product of the pressure shift and the bulk modulus of the material. Paul's empirical rule gives a better description for the pressure shifts than for the deformation potentials, whence our IDP's should increase slightly with increasing bulk modulus. In our data, however, we see little or no correlation between the IDP and the bulk modulus. We observed that the IDP's were smallest for GaP (the stiffest material under investigation) and largest for InSb, which has a comparatively small bulk modulus.

[42]The results of Fischetti and Higman (Ref. 24) show a larger variation of IDP's across the Periodic Table. This may be due to their particular choice of pseudopotential form factors and the different band structure. They claim that there is a small increase of the IDP's when moving from silicon to heavier materials like InAs. We see a similar behavior (both in our calculations and in the chemical trends observed in temperature-dependent spectroellipsometry data), but still feel that the universal rule stated here is an adequate approximation.