

A CPA Calculation for Disorder-Induced Intervalley Scattering in AlGaAs

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Abstract

Disorder-induced scattering due to the random distribution of atomic species of the constituent semiconductors in alloys can lead to intervalley scattering transitions. A method based on a wavevector dependant formulation of the Coherent Potential Approximation is used to calculate the intervalley scattering potentials.

I Introduction

Recent experimental work of Kalt *et al.* [1] indicate that disorder scattering can have large wavevector components of the scattering potential, which may give rise to intervalley scattering. Grein *et al.* [2] also calculated the lifetime broadenings of electrons due to disorder-induced scattering from the Γ valley to the side valleys using an empirical pseudopotential formulation, and concluded that this is the dominant scattering process for electrons in the Γ valley minimum of AlGaAs with composition $x > 0.4$. In this study, we derive a general formulation for treating diagonal disorder-induced intervalley scattering transitions due to diagonal disorder based on the Coherent Potential Approximation (CPA). Previous formulations of the CPA for application to alloy bandstructures average out the self-energy over the entire Brillouin zone. In this work, the wavevector dependance of the relevant quantities are retained. The scattering potential $V_{sc}(\mathbf{q})$, which causes a scattering transition with wavevector \mathbf{q} , is found by calculating the imaginary part of the CPA self-energy at the \mathbf{q} point of interest.

II Coherent Potential Approximation

The coherent potential approximation method has been used previously to treat the electronic structure of alloys [3-5]. The exact Hamiltonian for an alloy is written as the sum of an ordered virtual crystal Hamiltonian, whose solution is known, and a random potential due to the random distribution of atoms:

$$H_{\text{alloy}} = H_0 + V_{\text{random}}, \quad (1)$$

$$V_{\text{random}} = \sum_{\mathbf{r}} (V_{\mathbf{r}} - V_0). \quad (2)$$

The random part of the crystal potential is replaced with an effective potential (self-energy) in the CPA approximation, which is described by an effective Hamiltonian

$$H_{\text{eff}} = H_0 + \Sigma(\mathbf{k}). \quad (3)$$

From the the iterative solution of the Dyson's equation relating the Green's functions for the exact alloy Hamiltonian and the effective Hamiltonian

$$G_{\text{alloy}} = G_{\text{eff}} + G_{\text{eff}}(V_{\text{random}} - \Sigma)G_{\text{alloy}} , \quad (4)$$

the atomic scattering matrix, T , can be defined as

$$T = \frac{V - \Sigma}{I - (V - \Sigma)G_{\text{eff}}} , \quad (5)$$

which transforms (4) into the form

$$G_{\text{alloy}} = G_{\text{eff}} + G_{\text{eff}}TG_{\text{eff}} . \quad (6)$$

Taking the configuration average of both sides,

$$\langle G_{\text{alloy}} \rangle = G_{\text{eff}} + G_{\text{eff}}\langle T \rangle G_{\text{eff}} , \quad (7)$$

results in a self-consistency relation for the self-energy $\Sigma(\mathbf{k})$. This leads to the condition that the configuration average of the atomic scattering matrix vanish at every point in the Brillouin zone:

$$x \frac{V_A(\mathbf{k}) - \Sigma(\mathbf{k})}{I - (V_A(\mathbf{k}) - \Sigma(\mathbf{k}))G_{\text{eff}}(\mathbf{k})} + (1 - x) \frac{V_B(\mathbf{k}) - \Sigma(\mathbf{k})}{I - (V_B(\mathbf{k}) - \Sigma(\mathbf{k}))G_{\text{eff}}(\mathbf{k})} = 0 \quad (8)$$

$V_A(\mathbf{k})$ and $V_B(\mathbf{k})$ are the anti-bonding potentials of the A and B semiconductors, calculated from the conduction band energy solutions, and are referenced with respect to the vacuum level. Chen *et al.* [3] use an approximation by which the effective Green's function, and the self-energy term are diagonalized. The effective Green's function is of the form of Bloch sums, which are valid for tight-binding, or bond-orbital basis functions and result in the cancellation of terms in the Brillouin zone integration. Then, the effective Green's function is of the form

$$G_{\text{eff}}(\mathbf{k}) = \sum_{\mathbf{k}'} \frac{1}{E_{\mathbf{k}} - E_{\mathbf{k}'} - \Sigma_{\mathbf{k}'}} \quad (9)$$

By discretizing the Brillouin zone into N points, we obtain an $N \times N$ system of coupled nonlinear equations for $\Sigma_{\mathbf{k}}$ to be solved self-consistently. Through a local \mathbf{k} approximation, we first calculate the density of states only at the \mathbf{k} -point of interest, through which the nonlinear system of equations can be decoupled. Rewriting the effective Green's function as

$$G_{\text{eff}}(\mathbf{k}) = -\frac{1}{\Sigma_{\mathbf{k}}} + \sum_{\mathbf{k}'}' \frac{1}{E_{\mathbf{k}} - E_{\mathbf{k}'} - \Sigma_{\mathbf{k}'}} \quad (10)$$

the summation term is neglected initially. We have checked that this approximation is valid, and find that the first term is about five times larger than the summation term. The resultant self energies $\Sigma_{\mathbf{k}}$, from the solution of (8) are fed back into the Green's function expression of (9) and the iteration is performed until self-consistency is reached. The self-energies do not change appreciably after the first iteration.

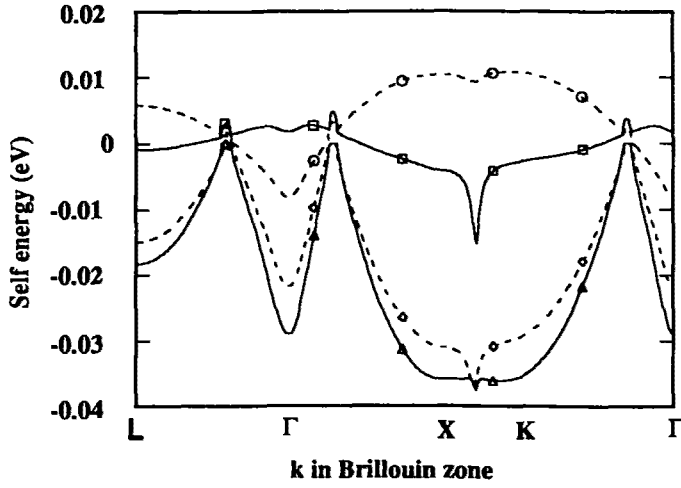


Figure 1. CPA Self-Energy in the Brillouin zone for $x = 0.2$ and 0.6 in AlGaAs. Circles and diamonds are the real and imaginary components of the self-energy for $x = 0.2$, and the squares and triangles are the real and imaginary self-energies for $x = 0.6$.

Using the sp^3s^* semi-empirical tight-binding method to calculate the eigenenergies, the scalar equations resulting from the above approximations are solved using a Newton-Raphson iteration for $\Sigma(\mathbf{k})$ at the discretized points in the irreducible 1/48-th wedge of the Brillouin zone. The results for the real and imaginary components of the self-energy are shown in Fig. 1 for two different compositions of AlGaAs. It is seen that the real part of the self-energy, which is a band-renormalization term in the virtual crystal approximation, results in a correction to the band energies whose magnitude is less than 10 meV throughout the Brillouin zone. The imaginary part is equal to the scattering potential, and shows a structure related to the symmetry points Γ , L and X . Between the X and K points, we have a dip in the self-energy, which is actually a result of the semi-empirical tight binding approximation to the bandstructure. In an sp^3s^* basis, the energy bandstructure between the X and K points has a degeneracy point, while in an Empirical Pseudopotential calculation of the band structure of AlGaAs, such a degeneracy point is not seen. The composition dependence of the imaginary part of the self-energy for the wavevector components L and X is shown in Fig. 2. There is a marked deviation from a $\sqrt{x(1-x)}$ type of behaviour, which is expected from a binomially distributed random atomic energy. Thus, the bowing parameter is not a simple scalar quantity.

III Applications

We apply our disorder-scattering potential results to the simulation of a femtosecond time-resolved pump probe experiment of intervalley scattering in $Al_{0.6}Ga_{0.4}As$ by Wang *et al.*[6]. The intervalley scattering transition is an L -wavevector transition, whose scattering potential is seen to be 18 meV from Figs. 1 and 2. We include this scattering process in an Ensemble Monte Carlo simulation of intervalley scattering in AlGaAs. The data points in Fig. 3 are the X -valley population in arbitrary units. A 400 femtosecond FWHM, 2.12 eV laser pulse excites carriers into the L and X valleys (the laser pulse is centered at $t = 1000$ femtoseconds in the

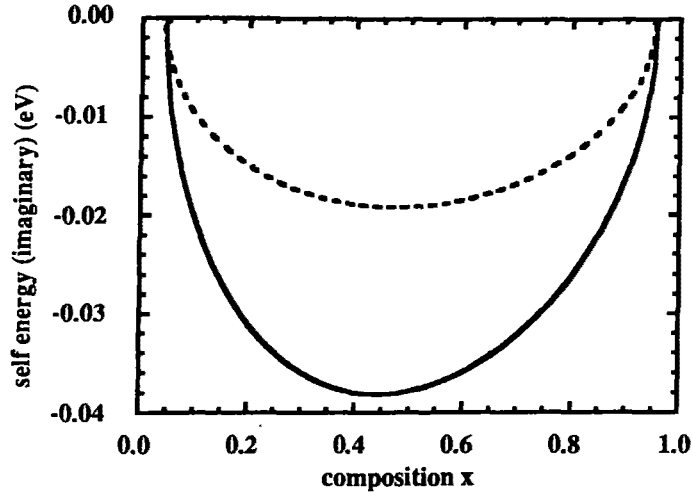


Figure 2. Imaginary part of the CPA self energy at the L point (dashed line) and the X point (solid line).

figure). Photo-excited carriers undergo inter- and intra-valley phonon- and disorder-induced scattering events to pile up at the bottom of the X valley. The population of the X valley is monitored by a 500 femtosecond FWHM convolving pulse which causes an infrared transition to the X_7 valley. Previously, we had reported a parameter fit of the non-polar optical deformation potential constant to be $D_{LX} = 1.5 \pm 0.5 \times 10^8$ eV/cm [7]. The results of the simulation for a value of $D_{LX} = 1.5 \times 10^8$ eV/cm per binary alloy mode are shown in Fig. 3 for three different disorder-induced intervalley scattering potentials. It can be seen that the effect of including disorder-induced scattering processes for L-X intervalley scattering is small.

IV Conclusion

Disorder-induced intervalley scattering is investigated using a Coherent Potential Approximation to model the random potential in the alloy AlGaAs. The imaginary part of the self-energy correction is responsible for scattering so we can use this self-energy to derive scattering potentials. In particular, a \mathbf{k} -dependant formulation for the self-energy gives us the disorder potential components directly responsible for the large wavevector scattering transitions which can result in intervalley transfer. The disorder-induced intervalley scattering potential for Γ -X transitions (an X-wavevector) for the experimental case of [1] is found to be 38 meV at composition $x = 0.4$, somewhat smaller than the value reported (53 meV). However, this value seems overestimated from the derivation in [1]. Intervalley scattering between the L and X valleys has only a weak disorder-induced scattering potential. For AlGaAs with composition $x = 0.6$, disorder-induced scattering processes for L-X intervalley scattering are small compared with phonon-induced processes.

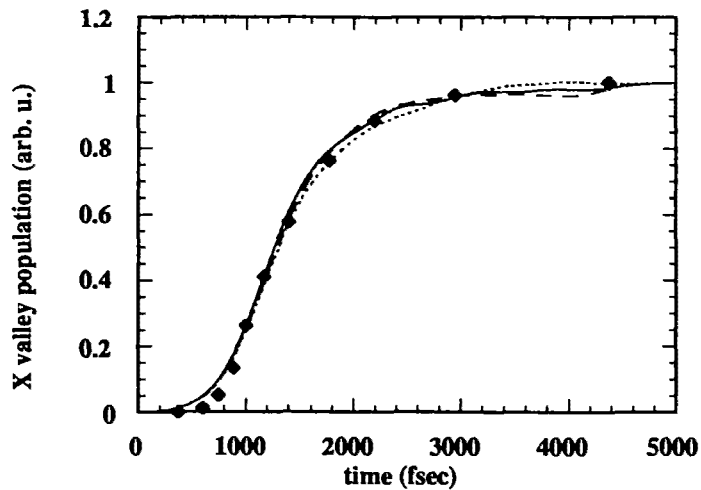


Figure 3. Effect of disorder-induced L-X intervalley scattering. The dotted line, solid line and the dashed line are for scattering potentials $V_{sc}(L) = 0, 18 \text{ meV}$ and 25 meV respectively. The diamonds are the data points of Wang *et al.* [6].

References

- [1] H. Kalt, W.W. Rühle, K. Reimann, M. Rinker, and E. Bauser, *Phys. Rev. B* **43**, 12364 (1991).
- [2] C. H. Grein, S. Zollner, and M. Cardona, *Phys. Rev. B* **44**, 12761 (1991).
- [3] A. B. Chen, and A. Sher, *Phys. Rev. B* **17**, 4726 (1978).
- [4] Y. T. Shen, and C. W. Myles, *J. Phys. Chem. Solids* **48**, 1173 (1987).
- [5] M. Bugajski, A. M. Kontkiewicz, and H. Mariette, *Phys. Rev. B* **28**, 7105 (1983).
- [6] W. B. Wang, K. Shum, R. R. Alfano, D. Szymd, and A. J. Nozik, *Phys. Rev. Lett.* **68**, 662 (1991).
- [7] S. E. Güñçer, and D. K. Ferry, *Phys. Rev. B* **46**, 15309 (1992).