MICROSCOPIC THEORY OF INTERVALLEY SCATTERING IN GaAs: $\vec{k}$-DEPENDENCE OF INTERVALLEY DEFORMATION POTENTIALS

STEFAN ZOLLNER, SUDHA GOPALAN*, and MANUEL CARDONA

Max-Planck-Institut für Festkörperforschung,
Heisenbergstr. 1, D-7000 Stuttgart 80, FRG

*The University of Western Ontario, Department of Physics,
London, Ontario, CANADA N6A 3K7

1. INTRODUCTION

We have recently used the rigid-pseudoion method (RPIM) to calculate intervalley deformation potentials (IDPs) at high-symmetry points for III-V-semiconductors. [1] Our results agree with some recent experiments, [2] but for a full understanding of the measured scattering times it is necessary to calculate the IDPs as a function of the phonon wave vector and perform an integration over the Brillouin zone to include all energy-conserving intervalley transitions.

2. THE RIGID-PSEUDOION METHOD

In the framework of the rigid-pseudoion method, [3] the electron-phonon interaction Hamiltonian to first order in phonon displacement is given by the gradient of the crystal potential, which we calculate from an empirical local pseudopotential band structure. [4] The IDP is given by multiplying this gradient with the phonon polarization vector (obtained from a parametrized phonon shell model[5,6]) and summing over the basis.[1]

3. INTERVALLEY DEFORMATION POTENTIALS

We first discuss the IDPs for scattering between the Γ- and L-valleys in GaAs. An investigation of the selection rules connecting the Γ- and L-points in a zincblende crystal[1] shows that ΓL-scattering is allowed for the LA and LO phonons, but LO phonon scattering is forbidden in Ge (diamond symmetry) and therefore should be small in GaAs. The calculated IDPs, in Conwell's[7] notation, are $D(\Gamma, L, LA)$=3 eV/Å and $D(\Gamma, L, LO)$=0.4 eV/Å. The experimental result[2] is $D(\Gamma, L, LO)$=3.5 eV/Å and $D(\Gamma, L, LA)$=small.

The discrepancy between the experimental and theoretical result can be explained as follows: The calculated results are for energy non-conserving transitions connecting high symmetry points, whereas the experiment studies energy-conserving transitions from the Γ-valley to the L-valley. In order to investigate this difference we have calculated the $\vec{k}$-dependent IDPs $D(\vec{k}, L, j)$ for initial points $\vec{k}$ near Γ along the $\langle 100 \rangle$-direction, see Fig. 1(a). It can be seen that D decreases for the LA phonon and increases for the LO phonon. Above the energy threshold for ΓL-scattering (vertical line) the LO phonon gives the dominant intervalley scattering contribution. $D(\vec{k}, L, LA + LO)$=3.5 eV/Å is nearly independent of $\vec{k}$ and in very good agreement with the experiment. [2] The transverse phonons are either even or odd for this symmetry direction upon a reflection in a $(01\bar{1})$-plane. Both electronic states are even, therefore the odd phonons are not allowed to couple. The even phonons give a small contribution, shown in Fig. 1(a), and can be neglected in the experiments. [2] Similar calculations for initial $\vec{k}$-points along the $\langle 110 \rangle$- and $\langle 111 \rangle$-directions had the same result.

For scattering between the Γ-point and the X-point (X_1-symmetry, As at the origin), only the LO phonon is allowed in GaAs. We find $D(\Gamma, X_1, LO)$=2.9 eV/Å from our calculations, whereas Monte-Carlo simulations[8] usually assume a much larger IDP around 10 eV/Å. Again we study the $\vec{k}$-dependence of the IDP, but now for an initial point along the (111)-direction. $D(\vec{k}, X_1, LO)$ decreases slightly from 3 eV/Å down to 2 eV/Å, whereas $D(\vec{k}, X_1, LA)$ remains small. The interesting result of this calculation is the importance of the TA^+ and TO^+ phonons (same selection rules as before). Above the energy threshold of 480 meV (vertical line), they give the dominant contribution to intervalley scattering with IDPs of about $D(\vec{k}, X_1, TA^+)$=$D(\vec{k}, X_1, TO^+)$=2.5 eV/Å. Results for other symmetry directions give somewhat different numbers, but are qualitatively the same. As the TA^+ phonon has a very low energy, it may be responsible for the short ΓX-scattering times observed in GaAs. [8] Similar results for the $\vec{k}$-dependence of the IDPs have been obtained for GaP. [9]

4. SCATTERING TIMES

The calculation of the scattering time $\tau(\vec{k})$ for a given electron with wave vector $\vec{k}$ to a different valley is possible by summing over all phonon wave vectors $\vec{q}$ that lead to a final electron state with the correct energy. This summation is an integral over the Brillouin zone constrained by two delta functions, which can be calculated using the tetrahedron method. [10,11] The experimentally observed scattering times, however, are more difficult to calculate as $\tau(\vec{k})$ has to be weighted with the electron distribution function which is in general a not well known function of time, excitation density, etc. This makes a second integration over the Brillouin zone necessary.

In order to demonstrate the method, we calculate the return time for an electron at the L-point in GaAs to the Γ-valley. The dimensionless, temperature-independent electron-phonon spectral function (see Ref. 10 for a detailed description of the formalism), which contains all the

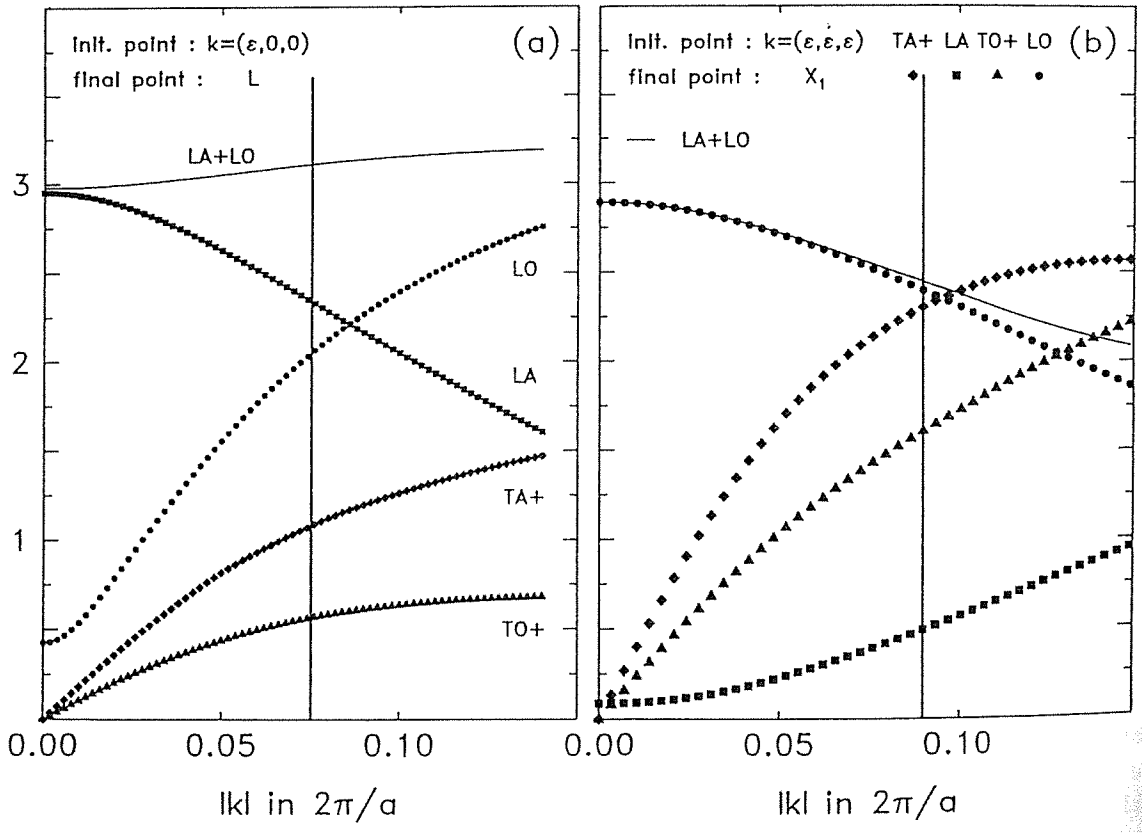

Fig. 1: $\vec{k}$-dependence of intervalley deformation potentials (in eV/Å) for ΓL- (a) and ΓX_1-scattering (b) in GaAs.

necessary information for the intervalley scattering time as a function of temperature, is shown in Fig. 2. An integration over the phonon occupation factor yields $L\Gamma$ return times of about 5 ps for 0 K and 1.8 ps for 300 K, in reasonable agreement with Monte-Carlos simulations for recent ultrafast laser experiments. [12,13]

5. SUMMARY

The $\vec{k}$-dependence of $\Gamma - X$ and $\Gamma - L$ intervalley deformation potentials was calculated with the rigid-pseudoion method. By integrating these IDPs with the tetrahedron method we find the return times of an electron from the L-point to the Γ-valley. The results are in reasonable agreement with recent experiments.

6. REFERENCES

[1]S. Zollner, Sudha Gopalan, and M. Cardona, Appl. Phys. Lett. 54, 614 (1989).

[2]J. A. Kash, R. G. Ulbrich, and J. C. Tsang, to appear in Solid State Electron.

[3]P. B. Allen and M. Cardona, Phys. Rev. B 27, 4760 (1983).

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

[5]K. Kunc and H. Bilz, Solid State Commun. 19, 1027 (1976).

[6]K. Kunc and O. H. Nielsen, Computer Physics Commun. 17, 413 (1979).

[7]E. M. Conwell, *High field transport in semiconductors*, (Academic, New York, 1967).

[8]K. F. Brennan, D. H. Park, K. Hess, and M. A. Littlejohn, J. Appl. Phys. 63, 5004 (1988).

[9]S. Zollner, J. Kircher, M. Cardona, and Sudha Gopalan, to appear in Solid State Electron.

[10]P. Lautenschlager, P. B. Allen, and M. Cardona, Phys. Rev. B 33, 5501 (1986).

[11]Sudha Gopalan, P. Lautenschlager, and M. Cardona, Phys. Rev. B 35, 5577 (1987).

[12]A. Katz and R. R. Alfano, Appl. Phys. Lett. 53, 1065 (1988).

[13]J. Shah, B. Deveaud, T. C. Damen, W. T. Tsang, A. C. Gossard, and P. Lugli, Phys. Rev. Lett. 59, 2222 (1987).

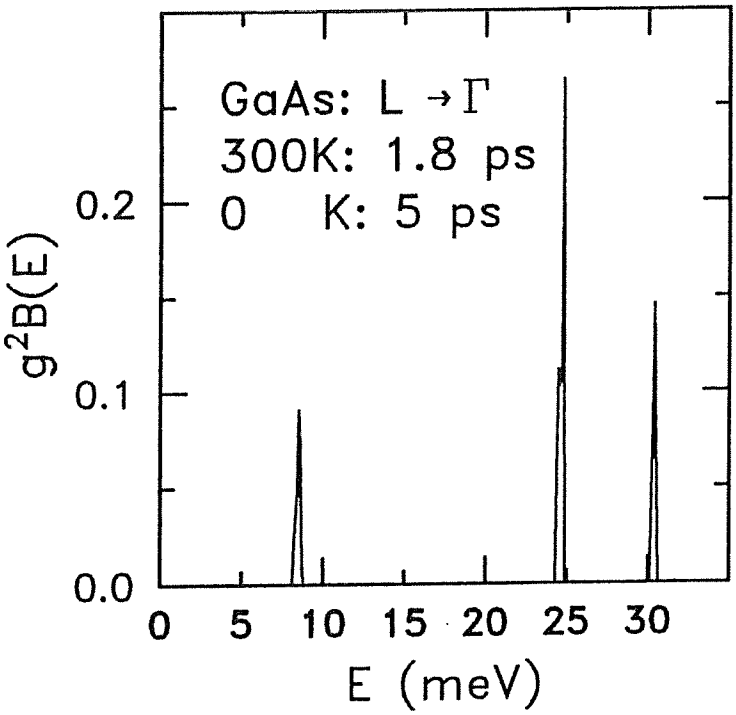

Fig. 2: Temperature-independent electron-phonon spectral function for the return of an electron from the L-point to the Γ-valley.

PHONONS 89

Heidelberg, 21–25 August 1989
Federal Republic of Germany

Proceedings of the
Third International Conference on
Phonon Physics
and the
Sixth International Conference on
Phonon Scattering
in Condensed Matter

Volume 2

Editors

S Hunklinger **W Ludwig** **G Weiss**

World Scientific
Singapore • New Jersey • London • Hong Kong

Published by

World Scientific Publishing Co. Pte. Ltd.,
P O Box 128, Farrer Road, Singapore 9128
USA office: 687 Hartwell Street, Teaneck, NJ 07666
UK office: 73 Lynton Mead, Totteridge, London N20 8DH

Library of Congress Cataloging-in-Publication data is available.

PHONONS '89

ISBN 981-02-0034-X

Printed in Singapore by JBW Printers & Binders Pte. Ltd.