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EFFECT OF CARRIER CONCENTRATION ON THE SELF ENERGY OF SHORT WAVELENGTH PHONONS IN MANY VALLEY SEMICONDUCTORS

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In this work we study the effect of free carriers on the self energy of short wavelength phonons in heavily doped n-type many valley semiconductors. We find that the presence of free carriers produces a measurable shift to lower energies in the phonon frequency. The magnitude of the calculated shifts shifts is large enough to warrant experimental determination of this quantity. Comparison of our calculations with experimental measurements would yield useful parameters describing the electron–phonon interaction for large q-phonons.

RECENTLY, there has been considerable interest in the effect of free carriers on phonon self energy.[1–3] The experimental work was concentrated in determining the energy shift and lifetime broadenings produced by the free carriers on the Raman frequencies (long wavelengths optical phonons) of diamond type semiconductors. With the advance of high resolution neutron diffraction techniques, measurements of the same physical effects can be carried out on phonons of finite momentum. In this work we perform a theoretical calculation of the influence of free carriers on the self energy of short wavelength phonons in heavily doped n-type many valley semiconductors.

For n-type materials, the free electrons concentrate on the lowest valleys of the conduction band. These valleys occur along the {111} directions of k-space at the zone boundary (L_1 points) for Ge and along the {100} directions (Δ_1 points), near the zone boundary in Si.[4,5] Since the momentum transfer involved in scattering an electron from one conduction band valley to another equivalent one is of the order of the edge of the Brillouin zone, such scattering must be assisted by a short wavelength (of the order of the lattice constant) elementary excitation. We consider the scattering of electrons via phonons. The interaction Hamiltonian can be written as:

$$H_{\text{int}}^{\nu\nu'} = \int d^3r\, \psi^{+\nu}(\mathbf{r}, t)\, \Phi^{op}(\mathbf{r}, t)\, \psi^{\nu'}(\mathbf{r}, t) \quad (1)$$

where $\psi(\mathbf{r}, t)$ [$\psi^{+}(\mathbf{r}, t)$] is the destruction (creation) electron field operator, and the superscript ν determines the valley in k-space, and $\Phi^{op}(\mathbf{r}, t)$ is the electron phonon interaction given by

$$\Phi^{op}(\mathbf{r}, t) = -\sum_j \mathbf{u}_j(\mathbf{r}, t) \cdot \nabla U_j \quad (2)$$

where

$$u_j(\mathbf{R}, t) = \sum_{q\lambda} \left(\frac{\hbar}{2\rho V \omega_{q\lambda}}\right)^{1/2} (\mathbf{e}_{q\lambda}) b_{q\lambda} \exp\left[i(\mathbf{q}\cdot\mathbf{R} - \omega_{q\lambda} t)\right] \exp\left[i\psi_\lambda\right] + \text{c.c.} \quad (3)$$

where $\psi_\lambda = \pi$ for optical branches and zero for acoustic branches. Here, $\mathbf{q}$ and λ denote the momentum and polarization of the phonons, $\mathbf{e}_{q\lambda}$ is a unit vector in the direction of polarization of the phonons, ρ is the ion density, $\omega_{q\lambda}$ is the phonon frequency, and $b_{q\lambda}(b_{q\lambda}^{+})$ is the destruction (creation) operator of a phonon of momentum $\mathbf{q}$ and polarization λ. Although equation (3) is strictly valid only for one atom per primitive cell, the final results will not be affected in our case. However, the calculation can easily be extended to materials of the zincblende structure. If we expand the electron field operator

$$\psi^{\nu}(\mathbf{r}) = \sum_k a_k \Phi_k(\mathbf{r}) \quad (4)$$

where a_k is the creation operator of an electron of momentum k and $\Phi_k(r)$ are the normalized eigenfunctions of the non-interacting Hamiltonian, the interaction Hamiltonian becomes

$$H_{\text{int}}^{\nu\nu'} = i \sum_{\substack{k\nu k'\nu' \\ q\lambda j}} \left(\frac{\hbar}{2\rho V\omega_{q\lambda}}\right)^{1/2} \mathbf{e}_{q\lambda} \cdot (\vec{k}' + \mathbf{q})\, U(\vec{k}' + \mathbf{q}) \exp(-i\vec{k}' \cdot \mathbf{R}_j) a_k^{\dagger\nu} a_{k'\nu} b_{q\lambda} A_{k\nu k'\nu} + \text{c.c.} \quad (5)$$

where

$$A_{k\nu,k'\nu} = \int d^3r\, e^{i\mathbf{q}\cdot\mathbf{r}} \phi_{k\nu}(\mathbf{r}) \phi_{k'\nu}(\mathbf{r}) \quad (6)$$

$$= \begin{cases} c^{\nu,\nu} & \text{when } k'^{\nu} = k^{\nu} + q \text{ and } k^{\nu} \text{ belong to equivalent valleys,} \\ 0 & \text{otherwise,} \end{cases}$$

and $U(\mathbf{q} + \vec{k}')$ is the Fourier transform of $U(\mathbf{r})$.

Notice that the definition of $A_{k,k'}$ makes use of the fact that all the other valleys in the conduction band lie much higher in energy compared to $\omega_{q\lambda}$. We define a new function:

$$M^{\nu}(\mathbf{q}, \omega) = \sum_{j\vec{k}'} \mathbf{e}_{q\lambda} \cdot (\vec{k}' + \mathbf{q})\, U(\vec{k}' + \mathbf{q}) \exp(-i\vec{k}' \cdot \mathbf{R}_j) \quad (7)$$

therefore the Hamiltonian becomes:

$$H_{\text{int}}^{\nu\nu'} = \sum_{\substack{q \\ kk'}} \left(\frac{\hbar}{2\rho V\omega_{q\lambda}}\right)^{1/2} M^{\nu}(\mathbf{q}, \lambda) A_{k\nu k'\nu} a_{k\nu}^{\dagger} a_{k'\nu} b_{q\lambda} + \text{c.c.} \quad (8)$$

For further calculations we assume the produce $M(\mathbf{q}, \lambda)A_{k,k'}$ to be a constant inside a particular valley, which is a reasonable assumption since q (or k^{ν}) $\gg k_F$ (where k_F is the Fermi wave number). The function $M(\mathbf{q}, \lambda)$ is well known in the long wavelength limit and is given by

$$M^{\nu}(\mathbf{q}, \lambda) = \Xi_d (\mathbf{e}_{q\lambda} \cdot \mathbf{q}) + \Xi_u (\mathbf{e}^{\nu} \cdot \mathbf{q})(\mathbf{e}_{q\lambda} \cdot \mathbf{e}^{\nu}) \quad (9)$$

for acoustic phonons,[6] where $\mathbf{e}^{\nu}$ is a unit vector in the direction of $\mathbf{k}^{\nu}$; and $\Xi_{d,\mu}$ the deformation potential constants; and by

$$M^{\nu}(\mathbf{q}, \lambda) = D_0 (\mathbf{e}_{q\lambda} \cdot \mathbf{e}^{\nu}) \quad (10)$$

for optical phonons.[7]

The first order correction to the phonon energy is given by[8]

$$\pi(\mathbf{q}, \omega) = 2i \sum_{\nu} \frac{\hbar}{2\rho\omega_{q\lambda}} |M(\mathbf{q}, \lambda)|^2 |A_{k\nu,k\nu+q}|^2 \int_{\substack{\nu\text{th} \\ \text{valley}}} \frac{d^4k}{(2\pi)^4} G_{\omega}^{0}(\mathbf{k}) G_{\omega+\omega_{q\lambda}}^{0}(\mathbf{k} + \mathbf{q}) \quad (11)$$

here we have neglected vertex correction since $q\, V_F > \omega_{q\lambda}$[3] where V_F is the electron Fermi velocity. The electron–electron interaction inside each valley is also neglected because of its small size for large q;[9] although we restrict our calculation to very low temperatures we neglect the possibility of a superconducting transition. In this case the electron Green's function is given by:

$$G_{\omega}^{-1}(p) = \omega - \epsilon(p) + i\delta \operatorname{sgn} \omega \quad (12)$$

$$\epsilon(p) = \frac{p^2}{2m^*} - \epsilon_F \quad (13)$$

and

$$\operatorname{sgn} \omega = \begin{cases} 1 & \omega > 0 \\ -1 & \omega < 0 \end{cases}$$

m^* is a conduction band effective mass and ϵ_F the Fermi energy. Hence, we find for $\pi(q, \omega)$:

$$\text{Re}\, \pi(\mathbf{q}, \omega) = -\frac{m^* p_F}{2\pi^2\hbar^2\rho\omega} \left(1 + \frac{1 - x^2}{2x} \ln \frac{1 + x}{1 - x}\right) \sum_{\nu} |M^{\nu}(\mathbf{q}, \lambda)|^2 |A_{k\nu,k\nu+q}|^2 \quad (14)$$

with $x \simeq q/2k_F$, and

$$\text{Im}\, \pi(\mathbf{q}, \omega) = \frac{mp_F}{2\pi q V_F \hbar^2 \rho} \sum_{\nu} |M^{\nu}(\mathbf{q}, \lambda)|^2 |A_{k\nu,k\nu+q}|^2 \quad (15)$$

Equations (14) and (15) give the real and imaginary part of the self energy of a phonon connecting two equivalent conduction band valleys as a function of carrier concentration. These results look similar to the phonon self energy for metals derived by Migdal.[10] In Migdal's, the sum in equation (15) is replaced by a constant. These formulas are quite general and apply to any semiconductor of the given family and to any phonon connecting any equivalent pair of conduction band valleys. In order to obtain numerical estimates of this effect, we have to restrict ourselves to some particular case. Let us consider an X-point [$(2\pi/a)(100)$] transverse optical phonon in Ge; we assume $M(\mathbf{q}, \lambda)$ to be practically the same as for long wavelength phonons and take D_0 to be approximately 10^9 eV/cm.[11] The value of $|A_{k\nu,k\nu+q}|^2$ was found to be 0.82.[5,12] We obtain a decrease in the phonon energy of 6 per cent for a doping of 10^{20} carriers/cm^3. This effect would be easily detectable experimentally, such measurements would produce values of the corresponding matrix

elements and throw light on the nature of the electron phonon interaction. Such information could prove extremely useful in the understanding of several important effects like transport properties.

In conclusion, we have calculated the effect of free carriers on the self energy of short wavelength phonons for *n*-type materials of the Ge family as a function of carrier concentration. We found a decrease in the real part of the phonon self energy due to the electron phonon interaction which is large enough to be detected experimentally at high carrier concentrations. Effects of similar nature have already been observed experimentally for long wavelength optical phonons.[1,2] Our development of the theory to short wavelength phonons lay the foundations for future measurements which should yield parameters of great usefulness.

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REFERENCES

1. CERDEIRA F. and CARDONA M., *Phys. Rev.* **B5**, 1440 (1972).
2. BESERMAN R., JOVANNE M. and BALKANSKI M., *Proc. 11th Int. Conf. on the Physics of Semiconductors, Warsaw, Poland* (1972).
3. IPATOVA I.P., SUBASHIEV A.A. and MARADUDIN A.A., *Proc. Int. Conf. on Light Scattering in Solids, Paris* p. 86, (1971).
4. LONG D., *Energy Bands in Semiconductors,* Chap. 5, Interscience, New York (1968).
5. CARDONA M. and POLLAK F.H., *Phys. Rev.* **142**, 530 (1966).
6. HERRING C. and VOGT E., *Phys. Rev.* **101**, 944 (1956).
7. HARRISON W.A., *Phys. Rev.* **104**, 1281 (1956).
8. KEATING P.N., *Phys. Rev.* **175**, 1171 (1968).
9. WALTER P. and COHEN M.L., *Phys. Rev.* **B5**, 3101 (1972); LINDHARD S., *K. Danske Vidensk. Selskab, Mat. Fys. Medd.* **28**, 8 (1954).
10. MIGDAL A.B., *Soviet Phys. JETP* **34**, 996 (1958).
11. REIK H.G., *Aarhus Summer School Lectures, 1963,* Benjamin, New York (1964).
12. HIGGINBOTHAM C.W., Thesis, Brown University, 1970, (unpublished).

In dieser Arbeit untersuchen wir den Einfluss von freien Ladungsträgern auf die Selbstenergie von kurzwelligen Phononen in stark dotierten *n*-artigen Vieltalhalbleitern. Wir finden, dass die Anwesenheit der freien Ladungsträger eine messbare Verschiebung der Phononenfrequenz zu niedrigeren Frequenzen verursacht. Die berechneten Verschiebungen sind gross genug für eine experimentelle Bestimmung. Durch einen Vergleich von Theorie und Experiment könnte man nützliche Parameter der Elektron–Phonon–Wechselwirkung für grosse q bestimmen.