Temperature Dependence of Acoustic-Phonon Attenuation by Bound Donor Electrons in Germanium

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In the present work it has been shown that the discrepancy between Kwok's theory and the observed temperature dependence of acoustic-phonon attenuation in P-doped Ge beyond its maximum can be partially explained if one modifies Kwok's theory to include the transitions to singlet and triplet states from higher-energy states which may be relevant at higher temperatures. This work confirms that Kwok's theory overestimates phonon attenuation in the higher-temperature region.

I. INTRODUCTION

THE attenuation of transverse acoustic phonons has been experimentally determined by Pomerantz[1] at the microwave frequency 9 Gc/sec by isolated donor electrons in slightly doped n-type Ge (impurity concentration $=3\times10^{15}$ cm^{-3}) in the temperature range 5–40°K. Theoretical justification of the temperature dependence of the attenuation coefficient of phonons in n-Ge was first of all provided by Keyes[2] and by Griffin and Carruthers.[3] They took into consideration only the elastic scattering of phonons off electrons in the singlet ground state. Their result was too small to account for the observed acoustic-phonon attenuation. Their theory was further extended by Kwok who not only considered the elastic scattering off the triplet state (next higher-energy state) but also the inelastic phonon scattering processes as well as thermally assisted phonon absorption processes. Kwok[4] showed that one can account both for the magnitude and the temperature dependences of the phonon attenuation of P- and As-doped Ge if one considers the inelastic scattering of phonons plus the thermally assisted phonon attenuation processes, whose contribution is almost equal to the former. However, there is a systematic deviation between theory and experiment at higher temperatures especially in P-doped Ge beyond the attenuation maximum at about 20°K. The deviation at 40°K is as high as 60% of the experimental result. The agreement between theory and experiment is quite good in the temperature range 5–20°K. The deviation at higher temperatures suggests that one can improve the theoretical results if one considers the transitions from the singlet and triplet states to higher excited states. The aim of the present paper is to investigate whether one can explain the above discrepancy between Kwok's theory and the experiment by taking into account the transitions to higher-energy states, which may be relevant at higher temperatures. With this aim in view Kwok's expressions for phonon attenuation are suitably modified to take into account the above transitions. It may be noted that Kwok's theory considers transitions only between the singlet ground state and the next higher-energy triplet state.

II. THEORY

A typical inelastic phonon scattering process, which involves the singlet ground state and the next higher-energy triplet state, can be symbolically represented by the process

$$\hbar\omega_{q\lambda}+(\text{triplet})\leftrightarrow(\text{int.})\leftrightarrow\hbar\omega_{q'\lambda'}+(\text{singlet}). \quad (1)$$

The acoustic phonon $(\mathbf{q},\lambda)$ of energy $\hbar\omega_{q\lambda}$ is inelastically scattered into a high-energy phonon ($\hbar\omega_{q'\lambda'}\simeq4\Delta=E_1$), while the electron jumps down from the triplet to the singlet state. Here $4\Delta=E_1$ is the energy separation between the triplet state and the singlet state. Thermally assisted phonon absorption processes can be represented by

$$\hbar\omega_{q\lambda}+\hbar\omega_{q'\lambda'}+(\text{singlet})\leftrightarrow(\text{int.})\leftrightarrow(\text{triplet}), \quad (2)$$

where $\omega_{q'\lambda'}$ is the thermal phonon.

If α_b is the phonon attenuation due to the process (1) and α_c due to the process (2), the total attenuation α is given by $\alpha=\alpha_b+\alpha_c$. Kwok has shown that $\alpha_b\simeq\alpha_c$ so that $\alpha\simeq2\alpha_b$.

For acoustic frequencies $\hbar\omega_{q\lambda}\ll K_BT$ and for $\hbar\omega_{q\lambda}\ll4\Delta$ Kwok's expressions for the processes (1) and (2) can be simplified. If one neglects the angular averages of the phonon velocities, the total attenuation α, which takes into account the transitions involving ground state and other higher-energy states, can be

[1] M. Pomerantz, Proc. IEEE **53**, 1438 (1965).
[2] R. W. Keyes, Phys. Rev. **122**, 1171 (1961).
[3] A. Griffin and P. Carruthers, Phys. Rev. **131**, 1976 (1963).
[4] P. C. Kwok, Phys. Rev. **149**, 666 (1966).

expressed in a simplified form as

$$\alpha=\frac{96}{3^4(225)}\frac{F^2(q)E_u^4 f_0(T)n_{ex}}{\pi K_B\rho^2C^8\hbar^4}\frac{1}{T}\Big[\frac{3E_1^3F^2(E_1/hC)}{(e^{E_1/K_BT}-1)}+\frac{4E_2^3F^2(E_2/hC)}{(e^{E_2/K_BT}-1)}+\frac{4E_3^3F^2(E_3/hC)}{(e^{E_3/K_BT}-1)}+\frac{8E_4^3F^2(E_4/hC)}{(e^{E_4/K_BT}-1)}+\frac{8E_5^3F^2(E_5/hC)}{(e^{E_5/K_BT}-1)}\Big], \quad (3)$$

where $f_0(T)$ is the thermal equilibrium population of electrons in the singlet ground state, $F^2(q)$ is the form factor or cutoff function and equals $(1+\frac{1}{4}a_0^2q^2)^{-2}$, $a_0=a\chi_d/(m^*/m)=3\times10^{-7}$ cm is the Bohr radius of the impurity atom, m is the free mass of the electron, m^* is the effective mass of the electron. χ_d is the static dielectric constant, ρ is the density of the sample and equals 5.35 g/cm^3, n_{ex} is the concentration of the impurity and equals 3×10^{15} cm^{-3}, C is the phonon velocity and equals 3.5×10^5 cm sec, K_B is the Boltzman constant, and E_u is the shear deformation potential and equals 19 eV. At resonance $\hbar\omega=E$ or $hCq=E$ so that $q=E/hC$ and $F^2(E/hC)=[1+\frac{1}{4}a_0^2(E^2/h^2C^2)]^{-2}$.

For a given concentration n_{ex}, one can lump all the constants into one constant H:

$$H=\frac{96}{3^4(225)}\frac{F^2(q)}{\pi K_B}\frac{E_u^4n_{ex}}{\rho^2C^8\hbar^4}. \quad (4)$$

The probabilities of various states are governed by the following relations:

$$\frac{f_0(T)}{f_1(T)}=e^{E_1/K_BT},\quad \frac{f_0(T)}{f_2(T)}=e^{E_2/K_BT},\ \cdots,\quad \frac{f_0(T)}{f_5(T)}=e^{E_5/K_BT},$$

$$f_0(T)+3f_1(T)+4f_2(T)+4f_3(T)+8f_4(T)+8f_5(T)=1, \quad (5)$$

where f_1, f_2, f_3, etc., are the occupation probabilities of triplet and higher-energy states, respectively. The factors 3, 4, and 8 are the degeneracies of the corresponding levels. E_1, E_2, E_3, etc., are the energy separations of triplet state and higher-energy states, respectively, from the ground state.

Similarly if we consider transitions from the triplet state to higher-energy levels, α will be given by

$$\alpha=H\frac{f_1(T)}{T}\Big[\frac{12E_1'^3F^2(E_1'/hC)}{(e^{E_1'/K_BT}-1)}+\frac{12E_2'^3F^2(E_2'/hC)}{(e^{E_2'/K_BT}-1)}+\frac{24E_3'^3F^2(E_3'/hC)}{(e^{E_3'/K_BT}-1)}+\frac{24E_4'^3F^2(E_4'/hC)}{(e^{E_4'/K_BT}-1)}\Big]. \quad (6)$$

TABLE I. Energy separations E/K_B of the different states in As-doped Ge.[a]

Energy separations from the singlet state in the temperature unit	Energy separations from the triplet state in the temperature unit
49	60
108	85
133	95
143	103
150	

[a] Reference 5.

The first term has been multiplied by 12, because triplet state is threefold degenerate and the next higher-energy state is fourfold degenerate and similarly other numerical multiplications can be explained. Here E_1', E_2', etc., refer to energy separation between the triplet state and higher-energy states.

The total attenuation α is given by the sum of the two contributions given by Eqs. (3) and (6).

III. RESULTS AND DISCUSSION

Tables I and II give the values of the energy separation E/K_B for various energy levels from the singlet and triplet states in the case of As- and P-doped Ge.[5] The occupation probabilities of various energy levels $f(T)$ for the impurity modes lying between the conduction band and valence band have been calculated at different temperatures. The results of the calculation are shown in Fig. 1. For the sake of comparison the results of As-doped Ge and P-doped Ge are shown in the same graph and it may be seen that $f(T)$ for higher-energy states becomes more appreciable at comparatively lower temperatures in the case of P-doped Ge and hence one should expect greater deviations in the case of P-doped Ge when one does not consider transitions from the higher-energy states to the triplet as well as the ground state.

Figure 2 shows the plot of α versus T for P-doped Ge. It may be seen that, using present approach, where one considers the transitions from the higher-energy states

TABLE II. Energy separations E/K_B of the different states in P-doped Ge.[a]

Energy separations from the singlet state in the temperature unit	Energy separations from the triplet state in the temperature unit
33	62
95	86
119	97
130	105
138	

[a] Reference 5.

[5] J. H. Reuszer and P. Fisher, Phys. Rev. **135**, A1125 (1964).

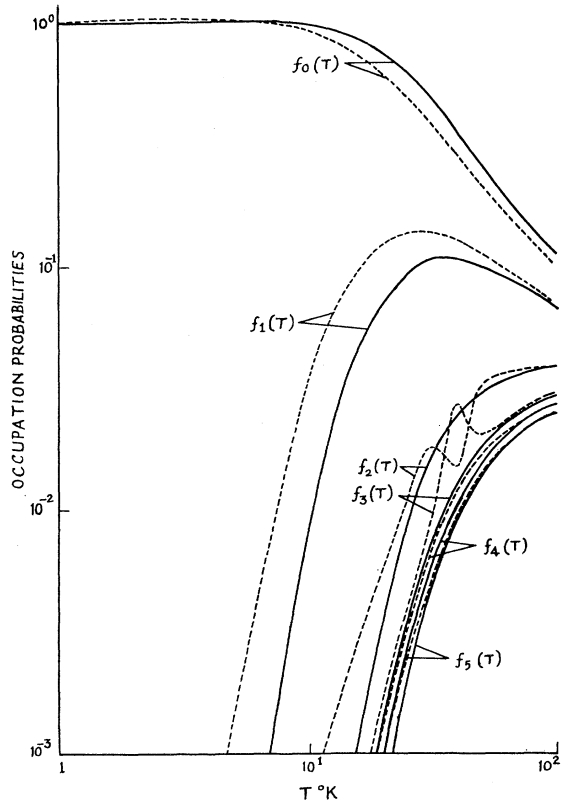

FIG. 1. Plot of the occupation probabilities versus temperature. Dashed line is for P-doped Ge and solid line for As-doped Ge.

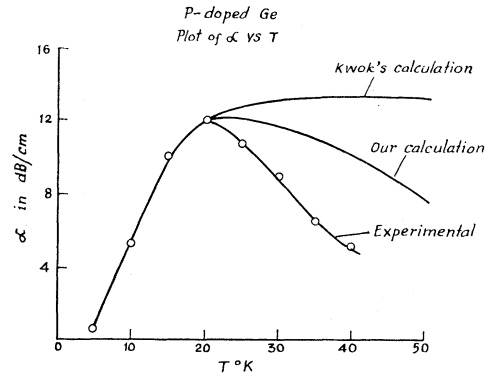

FIG. 2. Plot of attenuation coefficient versus temperature for P-doped Ge for concentration $n_{ex}=3\times10^{15}$ cm^{-3}. Solid line with circles is the experimental curve. Bare solid lines are Kwok's and our calculations.

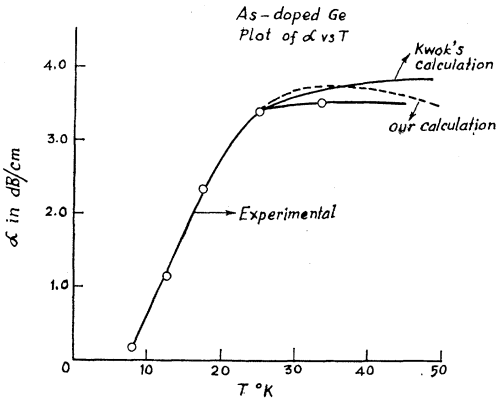

FIG. 3. Plot of attenuation coefficient versus temperature for As-doped Ge for concentration $n_{ex}=3\times10^{15}$ cm^{-3}. Bare solid line is the calculation on the basis of Kwok's theory. Dashed line is our calculation. Solid line with circles is the experimental curve.

to the triplet state as well as the singlet ground state, one obtains at high temperatures an agreement between theory and experiment better than Kwok's theory, which neglects such transitions. However, the discrepancy at about 40°K is only reduced by about 50% and the discrepancy goes on increasing as the temperature is increased beyond 20°K at which a maximum occurs in attenuation. This also shows that even if one takes into account the transitions to higher-energy states, Kwok's theory overestimates phonon attenuation at higher temperatures. Similarly, Fig. 3 shows the plot of α versus T for As-doped Ge. Here again the present approach gives better results although attenuation measurements are confined only to the region where the maximum occurs and not beyond that.

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