Phonon scattering in strained n-Ge

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Phonon scattering by an isolated donor electron in Ge under uniaxial stresses is calculated. It is shown that if the effective-mass approximation and Price's description of the valley-orbit splitting are adequate for a Sb donor, nonuniformity of strain plays an important role in explaining recent experiments on the stress dependence of the propagation of high-frequency monochromatic phonons and heat pulses in Sb-doped Ge.

I. INTRODUCTION

The thermal-phonon scattering and the ultrasonic attenuation in lightly doped n-Ge have been fairly well explained as regards their temperature and impurity-species dependence by theories[1–5] based on Hasegawa's theory on the donor-lattice interaction. Hasegawa's theory[6] is based on the effective-mass approximation for a donor state[7] and the Herring-Vogt theory[8] for the electron-lattice interaction in many-valley semiconductors, and it takes account of only the intravalley process.

Recently Dynes and Narayanamurti (hereafter DN) have investigated the effect of uniaxial stresses on the propagation of high-frequency monochromatic phonons and heat pulses in Sb-doped Ge.[9] Huet *et al.* have also measured the stress dependence of the propagation of heat pulses in Sb-doped Ge.[10] Their experimental data appear to have been qualitatively or quantitatively explained. However, the expressions of the phonon relaxation rate used by them are not adequate. (They used the donor wave functions at zero stress, which are not the eigenfunctions of the strained system.)

The purpose of this paper is to calculate the phonon scattering by the donor-phonon interaction in n-Ge under uniaxial stresses on the basis of Hasegawa's theory. It is shown that if the correctness of the effective-mass approximation and Price's description of the valley-orbit splitting[11] is assumed, nonuniformity of strain plays an important role in explaining experimental data.

II. THEORY

The donor ground state in Ge consists of a singlet (A_1) and triplet (T_2). The singlet is the lower, and the energy difference 4Δ between the A_1 and T_2 levels is called the valley-orbit splitting. The energies E_n and the corresponding wave functions Ψ_n of the donor ground state under [111] and [110] uniaxial stresses X are given in Refs. 2, 12, and 13. The matrix elements of the donor-phonon interaction between n and n' are given by

$$\langle n|\mathcal{H}_{e\text{-}p}|n'\rangle = \sum_{\vec{q}t}\left(\frac{\hbar\omega_{\vec{q}t}}{2Mv_t^2}\right)^{1/2} f(q)[\Xi_d\vec{e}_t\circ\hat{q}\,\delta_{nn'} + \tfrac{1}{3}\Xi_u\vec{e}_t\cdot\underline{D}^{nn'}\circ\hat{q})(a_{\vec{q}t}+a^\dagger_{\vec{q}t}), \quad (1)$$

$$f(q)=(1+\tfrac{1}{4}a^{*2}q^2)^{-2}, \quad (2)$$

where the symbols have the same meaning as they have in Ref. 14. The energies E_n and the tensors $\underline{D}^{nn'}$ for [111] and [110] uniaxial stresses are as follows:

(a) $\vec{X}\parallel[111]$,

$$E_0=-2\Delta[1+\tfrac{1}{2}x+(1-x+x^2)^{1/2}], \quad E_1=E_2=\epsilon, \quad E_3=-2\Delta[1+\tfrac{1}{2}x-(1-x+x^2)^{1/2}], \quad (3)$$

$$\begin{aligned}
&\underline{D}^{00}=D_0+(1-\tfrac{2}{3}\alpha_-^2)(D_1+D_3), \quad \underline{D}^{11}=D_0-D_3,\\
&\underline{D}^{22}=D_0+\tfrac{1}{3}(D_3-2D_1), \quad \underline{D}^{33}=D_0+(1-\tfrac{2}{3}\alpha_+^2)(D_1+D_3),\\
&\underline{D}^{01}=-(1/\sqrt{3})\alpha_-D_2, \quad \underline{D}^{02}=\tfrac{1}{3}\alpha_-(D_1-2D_3),\\
&\underline{D}^{03}=\tfrac{2}{3}\alpha_+\alpha_-(D_1+D_3), \quad \underline{D}^{12}=-(1/\sqrt{3})D_2,\\
&\underline{D}^{13}=(1/\sqrt{3})\alpha_+D_2, \quad \underline{D}^{23}=-\tfrac{1}{3}\alpha_+(D_1-2D_3),
\end{aligned} \quad (4)$$

$$\alpha_\pm=[1\pm(x-\tfrac{1}{2})/(1-x+x^2)^{1/2}]^{1/2}, \quad \alpha_+^2+\alpha_-^2=2, \quad x=4\epsilon/4\Delta, \quad \epsilon=\Xi_uX/9C_{44}; \quad (5)$$

(b) $\vec{X}\parallel[110]$,

$$E_0=-2\Delta[1+\tfrac{1}{2}(4+x^2)^{1/2}], \quad E_1=-\epsilon, \quad E_2=\epsilon, \quad E_3=-2\Delta[1-\tfrac{1}{2}(4+x^2)^{1/2}], \quad (6)$$

$$\begin{aligned}
&\underline{D}^{00}=D_0+\tfrac{1}{2}(\alpha_+^2-\alpha_-^2)D_3, \quad \underline{D}^{11}=D_0+D_3, \quad \underline{D}^{22}=D_0-D_3,\\
&\underline{D}^{33}=D_0-\tfrac{1}{2}(\alpha_+^2-\alpha_-^2)D_3, \quad \underline{D}^{01}=(1/\sqrt{2})\alpha_+D_1,\\
&\underline{D}^{02}=-(1/\sqrt{2})\alpha_-D_2,\\
&\underline{D}^{03}=\alpha_+\alpha_-D_3, \quad \underline{D}^{12}=0, \quad \underline{D}^{13}=(1/\sqrt{2})\alpha_-D_1,\\
&\underline{D}^{23}=(1/\sqrt{2})\alpha_+D_2,
\end{aligned} \quad (7)$$

$$\alpha_\pm=[1\pm x/(4+x^2)^{1/2}]^{1/2}, \quad \alpha_+^2+\alpha_-^2=2, \quad x=4\epsilon/4\Delta, \quad \epsilon=\Xi_uX/6C_{44}, \quad (8)$$

where

$$D_0=\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix},\qquad D_1=\begin{pmatrix}0&0&1\\0&0&1\\1&1&0\end{pmatrix},$$
$$D_2=\begin{pmatrix}0&0&-1\\0&0&1\\-1&1&0\end{pmatrix},\qquad D_3=\begin{pmatrix}0&1&0\\1&0&0\\0&0&0\end{pmatrix}. \tag{9}$$

Here C_{44} is the elastic stiffness constant and $x>0$ and $x<0$ for compression and tension, respectively.

DN have observed the resonance absorption of high-frequency monochromatic phonons and the attenuation of heat pulses propagating along the $[1\bar{1}0]$ direction in Sb-doped Ge under compressive $[111]$ stress. The phonon relaxation rate by the resonance absorption and elastic scattering for this case can be obtained in the same way as in Refs. 3 and 15 and by using Table IV of Ref. 6.

A. Resonance absorption

(i) $\vec{q}\parallel[110]$, $\vec{e}_t\parallel[001]$:

$$\tau^{-1}=\tfrac{2}{3}\,\alpha_-^2 A(\omega)\Gamma_{10}/[(\Delta_{10}-\hbar\omega)^2+\Gamma_{10}^2]\,. \tag{10}$$

(ii) $\vec{q}\parallel[1\bar{1}0]$, $\vec{e}_t\parallel[1\bar{1}0]$:

$$\tau^{-1}=\tfrac{4}{9}\,\alpha_-^2 A(\omega)\left\{\frac{\Gamma_{20}}{(\Delta_{20}-\hbar\omega)^2+\Gamma_{20}^2}+\frac{\alpha_+^2\Gamma_{30}}{(\Delta_{30}-\hbar\omega)^2+\Gamma_{30}^2}\right\}, \tag{11}$$

where in both cases

$$A(\omega)=\frac{N_0\omega}{\rho v_s^2}(1-e^{-\hbar\omega/kT})(\tfrac{1}{3}\,\Xi_u)^2 f^2\!\left(\frac{\omega}{v_s}\right). \tag{12}$$

B. Elastic scattering

For case (i) above,

$$\tau^{-1}=\alpha_-^4 B(\omega)F(\omega)\,\frac{\Delta_{10}^2}{(\Delta_{10}^2-\hbar^2\omega^2)^2+4\Gamma_{10}^2\hbar^2\omega^2}\,. \tag{13}$$

For case (ii) above,

$$\tau^{-1}=\tfrac{2}{3}\alpha_-^4 B(\omega)F(\omega)\left(\frac{\Delta_{20}^2}{(\Delta_{20}^2-\hbar^2\omega^2)^2+4\Gamma_{20}^2\hbar^2\omega^2}+\frac{2\alpha_+^4\Delta_{30}^2}{(\Delta_{30}^2-\hbar^2\omega^2)^2+4\Gamma_{30}^2\hbar^2\omega^2}\right), \tag{14}$$

where in both cases

$$B(\omega)=\frac{16N_0\omega^4}{135\pi\rho^2 v_s^2}(\tfrac{1}{3}\,\Xi_u)^4 f^2\!\left(\frac{\omega}{v_s}\right), \tag{15}$$

and

$$\Gamma_1=\Gamma_2=\frac{2}{45\pi\rho}(\tfrac{1}{3}\,\Xi_u)^2\left[\alpha_-^2\left(\frac{\Delta_{10}}{\hbar}\right)^3 F\!\left(\frac{\Delta_{10}}{\hbar}\right)\times(1-e^{-\Delta_{10}/kT})^{-1}+\alpha_+^2\left(\frac{\Delta_{13}}{\hbar}\right)^3 F\!\left(\frac{\Delta_{13}}{\hbar}\right)(1-e^{-\Delta_{13}/kT})^{-1}\right], \tag{16}$$

$$\Gamma_3=\frac{4\alpha_+^2}{45\pi\rho}(\tfrac{1}{3}\,\Xi_u)^2\left[\alpha_-^2\left(\frac{\Delta_{30}}{\hbar}\right)^3 F\!\left(\frac{\Delta_{30}}{\hbar}\right)(1-e^{-\Delta_{30}/kT})^{-1}+\left(\frac{\Delta_{13}}{\hbar}\right)^3 F\!\left(\frac{\Delta_{13}}{\hbar}\right)(e^{\Delta_{13}/kT}-1)^{-1}\right., \tag{17}$$

$$\Delta_{ij}=E_i-E_j\,,\quad \Gamma_{ij}=\Gamma_i+\Gamma_j\,,\quad \omega\equiv\omega_{\vec{q}t}\,,$$
$$F(Y)=\bar{v}_1^{-5}f^2(Y/\bar{v}_1)+\tfrac{3}{2}\,v_2^{-5}f^2(Y/\bar{v}_2)\,,$$

where Γ_i is the level width of the ith level, N_0 is the number of electrons per unit volume in the lowest level 0, and v_s is the appropriate velocity of sound. Inelastic scattering and the scattering by the electrons in upper levels 1, 2, and 3 are weak in the present case, and the expressions of the relaxation rates for them are not given here.

The important factors $\alpha_\pm^2$ are shown as a function of X (parallel to $[111]$) in Fig. 1, where we used $4\Delta=032$ meV, $\Xi_u=16$ eV, and $C_{44}=0.684\times10^{12}$ dyn cm^{-2}. The uniaxial stress changes the coefficients which represent the contribution of each valley to the donor wave function. The contributions of some valleys increase and those of the others decrease with stress. For compressive stress, α_- (α_+) denotes the decreasing (increasing) com-

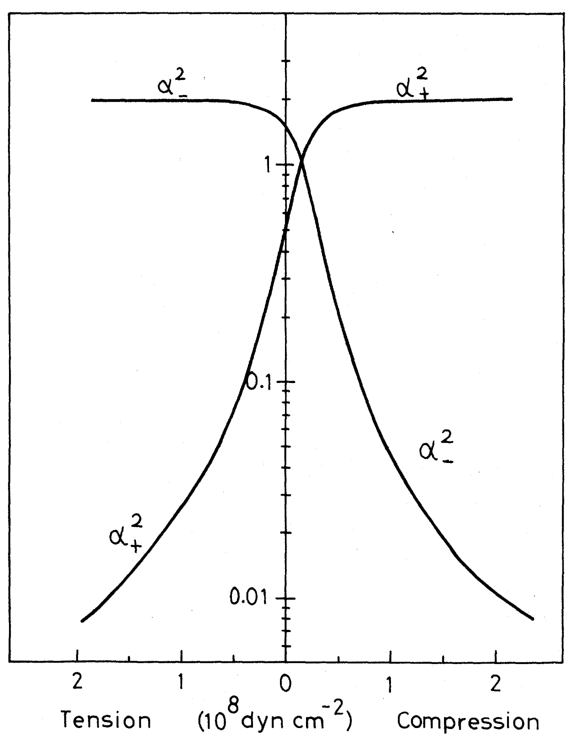

FIG. 1. Stress dependence of $\alpha_\pm^2$. $\vec{X}\parallel[111]$.

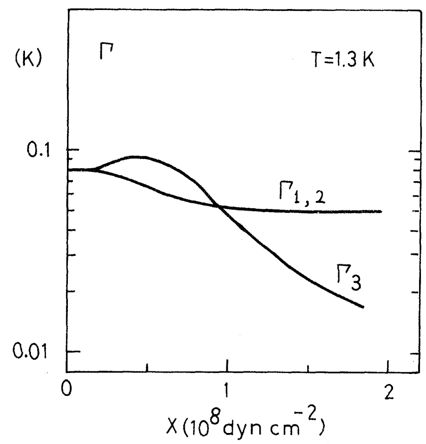

FIG. 2. Stress dependence of Γ_i at $T = 1.3$ K.

ponent of the coefficients. It can be seen from Eqs. (4) and (5) and Fig. 1 that the electron-phonon interaction between the lowest and upper levels is strongly reduced and becomes zero in the large-stress limit under compressive [111] stress as long as we consider the intravalley process. (The intervalley process is not important in the present case.)

III. RESULTS AND DISCUSSION

The following are obtained from Eqs. (10)–(17), Fig. 1, and numerical calculations:

(a) The fast transverse (FT) mode induces the transition $0 \to 1$, as has been pointed out by DN, but the longitudinal (L) mode does the transition $0 \to 2$ as well as $0 \to 3$. It should be remarked that the levels 1 and 2 (E state in DN's notation) are degenerate, but they are specified by different wave functions. The selection rule for L mode allows the transition $0 \to 2$ as well as $0 \to 3$, and then the resonance absorption is expected to be observed at two different values of X. (The ratio of the scattering strength by $0 \to 3$ to $0 \to 2$ is about 4 : 1 and the energy difference $\Delta_{23} \cong 2.8$ K.) However, the experiment has shown only one resonance.

(b) Figure 2 shows the stress dependence of Γ_i ($i = 1, 2, 3$) at $T = 1.3$ K. In this calculation $a^* = 40$ Å has been used. Γ_i are determined by the electron-phonon interaction between upper levels for large stresses, and Γ_0 becomes very small.

(c) High-frequency monochromatic phonons with given frequencies (~ 1.2 meV and ~ 1.7 meV for Sn and $Pb_{0.5}Tl_{0.5}$ phonon generators, respectively) are strongly scattered only in the very narrow stress region near resonance. α_- may give rise to the shift in the baseline on either side of resonance observed by DN.

(d) The stress dependence of the heat-pulse propagation for the FT and L modes, which have been calculated by using Eqs. (13) and (14), taking account of the other scattering processes mentioned below Eq. (17) and isotopic scattering, and following Fjeldly *et al.* and are shown by the broken and dotted lines, respectively, in Fig. 3, are in disagreement with the experiments. The experimental curve for the L mode is similar to that for the FT mode and is not shown. In these calculations we used $N_0 = 6 \times 10^{15}$ cm^{-3}, $T_h = 3.7$ K, and $T_s = 1.3$ K, where T_h and T_s are the heat-pulse temperature and the ambient temperature of the sample, respectively.

It is found that theory cannot well explain the experimental data. The calculations mentioned above have been carried out under two assumptions, that is, the correctness of the effective mass approximation with Price's description of the valley-orbit splitting and the uniformity of strain. Next we shall consider the effect of inhomogeneous strain and limit ourselves to the case of heat pulses of the FT mode. For a homogenious strain the contribution of the resonance absorption to the attenuation of heat pulses is not important because of the broad frequency distribution of phonons, while for an inhomogenious one it may become important owing to a distribution of Δ_{10} over a certain energy range. Since, however, we do not have any accurate information about the actual strain distribution, discussions given below should be considered as qualitative ones.

For simplicity, the following assumption and approximation are made:

(i) The distribution of Δ_{10}, $P(\Delta_{10})$, is a Gaussian form given by

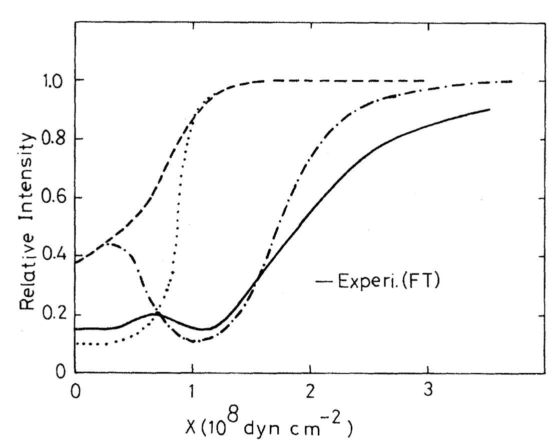

FIG. 3. Relative intensity of heat pulse as a function of X. Broken and dot-dashed lines denote the calculated curves for the FT mode for homogeneous and inhomogeneous strains, and the dotted line denotes the calculated curve for the L mode.

$$P(\Delta_{10}) = \frac{1}{\sqrt{2\pi}\,\delta}\int_{4\Delta}^{\infty} \exp[-(\Delta_{10}-\bar{\Delta})^2/2\delta^2]\, d\Delta_{10}\,, \tag{18}$$

$$\bar{\Delta} = \Delta_{10}(X)\,, \quad \delta = \Delta_{10}(C_+ X) - \Delta_{10}(C_- X)\,.$$

where $C_\pm$ are numerical factors denoting the degree of nonuniformity.

(ii) Off-resonance terms are evaluated at $\bar{\Delta}$ to avoid to perform a double integral.

The resonance absorption is given by

$$\tau^{-1} = \tfrac{2}{3}A(\omega)\int_{4\Delta}^{\infty} \alpha_-^2 \frac{1}{\sqrt{2\pi}\,\delta}\frac{\Gamma_{10}}{(\Delta_{10}-\hbar\omega)^2+\Gamma_{10}^2} \times \exp\left(-\frac{(\Delta_{10}-\bar{\Delta})^2}{2\delta^2}\right) d\Delta_{10}$$

$$\cong \frac{\sqrt{2\pi}}{3}A(\omega)\left[\frac{\alpha_-^2}{\delta}\exp\left(-\frac{(\hbar\omega-\bar{\Delta})^2}{2\delta^2}\right)\right]_{\Delta_{10}=\hbar\omega} \quad \text{for } \hbar\omega \geqslant 4\Delta\,, \tag{19}$$

The same calculations as in item (d) except for inclusion of Eq. (19) have been performed. The result for $C_\pm = 1 \pm 0.1$ is shown by the dot-dashed line in Fig. 3. The shape of the calculated curve and the position of minimum, if any, of intensity for a given T_h depends on $C_\pm$ and, of course, also on the form of $P(\Delta_{10})$.

So far we have neglected the stress dependence of the effective Bohr radius a^* which may be taken to be $a^*(X) = (1 - 0.032X)\, a^*(0)$ Å (X in units of 10^8 dyn cm^{-2}) for the FT mode from Fig. 2 in Ref. 12. Inclusion of this gives rise to a slight increase of scattering for $X \gtrsim 1.5 \times 10^8$ dyn cm^{-2}.

It has been noted that the expressions used by DN and Huet *et al.* could not explain their data. Since in the experiments of Huet *et al.* and DN, respectively,[16] T_h is 6.5 and 3.7 K, their expressions predict that the minimum of intensity occurs at a higher stress in the former than in the latter. (See also Ref. 15.) However, the experiments show the opposite. The present theory also cannot explain this, provided that the degree of nonuniformity of strain in two experiments is same. These then seem to show importance of inhomogeneous strain. This has also been pointed out in DN's paper. (However, the possibility that the donor system plays a role should not be ruled out, as the donor concentrations in their samples are different.) As for item (a), the discrepancy might be explained by inhomogeneous strain, the linewidth of the generated phonons, and the difference in intensity (4 : 1) of the two transitions.

So far we have performed calculations within a framework of the effective-mass approximation. The central-cell corrections will have more pronounced effects on the wave function of the donor ground state than on its energy. However, when we go beyond the effective-mass approximation, the situation becomes very complicated. We do not discuss this because of the lack of detailed information on the modifications of the wave function by these corrections.

The nearly degenerate ground state of the Sb donor is easily modified by internal strain or unintentional external stress, the donor-donor interaction, and so on even at zero external stress. This has some effect on the phonon scattering in a small-stress region. In any case, at present, nonuniform stress seems to be a powerful candidate for the primary cause of the discrepancy between theory and experiment. In order to settle this problem it is necessary to carry out further experiments on this system and also other donors P and As in Ge.

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