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High-Field Scattering Mechanisms in n-Germanium at 300 °K

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The hot-electron characteristic of n-germanium at room temperature is theoretically derived taking into account the effects of the ⟨100⟩ valleys and the nonparabolicity of the ⟨111⟩ valleys. It is shown that the experimental results may be explained by theory only when both these effects are included.

I. INTRODUCTION

The electron drift velocity in n-type germanium at high fields is experimentally found to be almost field independent.[1] But early hot-electron theories[2-5] considering only parabolic ⟨111⟩ valleys fail to give a field-independent velocity when the energy loss through both the acoustic and the optic phonons are taken into account. The velocity becomes field independent only if the energy loss through the acoustic phonons is neglected. However, even then the calculated values of the electron temperature are too high, and the value of the deformation-potential constant for optic scattering, required to fit the experimental values of the drift velocity, is lower than that obtained from the analysis of low-field results. It was shown by the present authors in an earlier paper[6] that if the effect of the ⟨100⟩ valleys are included in the usual simple theory, the velocity becomes field independent even when the energy loss through the acoustic phonons is taken into account. The electron temperature is also found to be reasonable, but the value of the optical-deformation-potential constant which gives fit between theory and experiment is almost unaltered. In this paper the alterations in these results caused by the incorporation of the nonparabolicity in the ⟨111⟩ valleys and the associated overlap corrections are discussed.

II. METHOD OF ANALYSIS

High-field-conductivity characteristics considering the nonparabolicity of the ⟨111⟩ valleys have been recently obtained by Dumke.[7] In this analysis, the effect of the nonclassical excitation of the acoustic phonons was also considered and the symmetric part of the distribution function was obtained by the Levinson method.[8] However, on detailed computation we find that the nonclassical excitation of the acoustic phonons has negligible effect. The distribution function obtained by Dumke[7] from his detailed analysis is also almost Maxwellian at room temperature. The small deviation at low energies is unlikely to affect the results significantly. The analysis may, therefore, be much simplified by assuming a Maxwellian distribution function with an electron temperature determined by the energy-balance condition. The equations giving the momentum relaxation time and the electron temperature for the nonparabolic ⟨111⟩ bands assuming a Maxwellian distribution function and classical excitation of acoustic phonons are given in the following:

$$1/\tau = 1/\tau_{\mathrm{ac}} + 1/\tau_{\mathrm{op}} = W\{(kT_L/\hbar\omega_0)(E/\hbar\omega_0)^{1/2} + B[N_0(E/\hbar\omega_0+1)^{1/2} + (N_0+1)(E/\hbar\omega_0-1)^{1/2}]\} \,, \tag{1}$$

$$-\vec{\mathrm{J}}_1\cdot\vec{\mathcal{E}} = \int E\left[\left(\frac{\partial f}{\partial t}\right)_{\mathrm{ac}} + \left(\frac{\partial f}{\partial t}\right)_{\mathrm{op}}\right] d\vec{\mathrm{k}} \,, \tag{2}$$

$$\int E\left(\frac{\partial f}{\partial t}\right)_{\mathrm{ac}} d\vec{\mathrm{k}} = -\frac{4\sqrt{2}\pi^6 s^2\hbar^9}{(\hbar\omega_0)^{3/2} m_T^2 m_L^{3/2}}\, W_e\left(1-\frac{T_L}{T_e}\right)\int_0^\infty f_0(E)\,\rho^4(E)\left(1+\frac{2E}{E_g}\right)^{-2} dE \,, \tag{3}$$

$$\int E\left(\frac{\partial f}{\partial t}\right)_{\mathrm{op}} d\vec{\mathrm{k}} = WB[(N_0+1)e^{-\hbar\omega_0/kT_e} - N_0]\left[\int_0^\infty E\left(\frac{E}{\hbar\omega_0}+1\right)^{1/2} R(E+\hbar\omega_0)L\rho(E)f_0(E)\,dE - e^{\hbar\omega_0/kT_e}\int_{\hbar\omega_0}^\infty E\left(\frac{E}{\hbar\omega_0}-1\right)^{1/2} R(E-\hbar\omega_0)L\rho(E)f_0(E)\,dE\right] . \tag{4}$$

$\vec{\mathrm{J}}_1$ is the current due to the carriers in the valley, T_L and T_e are the lattice and the electron temperatures, and the other symbols have the same significance as in Ref. 7.

The electric field has been assumed to be applied along the [100] direction, so that all the ⟨111⟩ valleys may be considered equivalent. The expression for the relaxation time for a particular carrier energy simplifies to that corresponding to parabolic bands as the effect of the nonparabolicity is canceled by that of the overlap correction. The average relaxation time is, however, affected by the nonparabolicity through the density of states.

The integral giving the energy loss due to acoustic-phonon scattering [Eq. (3)] has been obtained from the corresponding equation for parabolic bands[1,3] by including only the first-order correction in the density of states, $\rho(E)$.[7] The expression should be considered approximate, since the effect of the overlapping of the wave functions and that of the nonparabolicity in the angular average have been neglected. The approximation, however, causes little error as the total contribution of acoustic-phonon scattering to energy loss is less than 25% even at the highest field considered. The constant W_e is related to the deformation-potential constants for dilation and shear and is reported to lie between $(2)^2 W$ and $(2.5)^2 W$.

In Fig. 1, we give the velocity-field characteristics derived from the above equations using the parameter values of Ref. 7 [curve (b)]. In obtaining this curve, we have approximated the term $1 - T_L/T_e$ in Eq. (3) by unity, thus considering only the spontaneous emission of acoustic phonons, and have put $W_e = W$. Comparing this curve with the corresponding curve of Ref. 7 [marked (a) in Fig. 1], we find that our simplified analysis gives results agreeing with those of Ref. 7 to within 5%.

The electron mobility in the ⟨100⟩ valleys has been estimated to lie within 700 and 900 $\mathrm{cm}^2\,\mathrm{V}^{-1}\,\mathrm{sec}^{-1}$.[9–11] The change in electron temperature in these valleys would, therefore, be negligible up to the highest field (~ 6 $\mathrm{kV\,cm}^{-1}$) considered in this paper. The electrons in the ⟨100⟩ valleys may hence be assumed to have a field-independent mobility.

In order to include the effect of the ⟨100⟩ valleys we have to add terms in (1) and (2) arising from the nonequivalent intervalley scattering. The equations incorporating these terms are given in the following:

$$1/\tau = 1/\tau_{\mathrm{ac}} + 1/\tau_{\mathrm{op}} + 1/\tau_{\mathrm{int}} \,, \tag{5}$$

$$-\vec{\mathrm{J}}_1\circ\vec{\mathcal{E}} = \int E\left[\left(\frac{\partial f}{\partial t}\right)_{\mathrm{ac}} + \left(\frac{\partial f}{\partial t}\right)_{\mathrm{op}} + \left(\frac{\partial f}{\partial t}\right)_{\mathrm{int}}\right] d\vec{\mathrm{k}} \,, \tag{6}$$

where

$$\frac{1}{\tau_{\mathrm{int}}} = \sum_{\langle 100\rangle\,\mathrm{valleys}} \frac{D_{12}^2(m_T m_L^{1/2})_2}{\sqrt{2\pi}\, d\hbar^3\,\omega_{12}}\,[N_{12}(E-\Delta+\hbar\omega_{12})^{1/2} + (N_{12}+1)(E-\Delta-\hbar\omega_{12})^{1/2}] \tag{7}$$

and

$$\int E\left(\frac{\partial f}{\partial t}\right)_{\mathrm{int}} d\vec{\mathrm{k}} = -\sum_{\langle 100\rangle\,\mathrm{valleys}} \frac{D_{12}^2(m_T m_L^{1/2})_2}{\sqrt{2\pi}\, d\hbar^3\,\omega_{12}} \times\left\{\frac{n_1}{I_{n1}}\,[(N_{12}+1)c_e^- + N_{12}c_e^+] - \frac{n_2}{I_{n2}}\left[(N_{12}+1)\exp\left(\frac{\Delta-\hbar\omega_{12}}{kT_L}\right)c_L^+ + N_{12}\exp\left(\frac{\Delta+\hbar\omega_{12}}{kT_L}\right)c_L^-\right]\right\} . \tag{8}$$

D_{12}, $\hbar\omega_{12}$, and N_{12} represent the deformation-potential constant, the energy quantum, and the occupation number of the intervalley phonons; d is the density of the material, Δ is the energy separation between a ⟨111⟩ and a ⟨100⟩ valley, and n_i and I_{ni} are, respectively, the carrier concentration and the normalizing integral for the ith valley. The label i takes on values 1 and 2 for a ⟨111⟩ and a ⟨100⟩ valley, respectively. Also,

$$C_l^{\pm} = \int E(E - \Delta \pm \hbar\omega_{12})^{1/2} \rho(E) e^{-E/kT_l} dE,$$
$$l \equiv e, L \quad . \qquad (9)$$

The number of carriers transferred to the ⟨100⟩ valleys due to the nonequivalent intervalley scattering is determined from the equation of detailed balance in intervalley scattering

$$\frac{n_1}{I_{n1}} \left[(N_{12}+1) I_e^- + N_{12} I_e^+ \right] = \frac{n_2}{I_{n2}} \left[(N_{12}+1) \exp\left(\frac{\Delta - \hbar\omega_{12}}{kT_L} \right) I_L^+ + N_{12} \exp\left(\frac{\Delta + \hbar\omega_{12}}{kT_L} \right) I_L^- \right] \quad . \qquad (10)$$

This is subject to the normalization requirement

$$\sum n_i = n \quad . \qquad (11)$$

The summation extends over all the ⟨111⟩ and the ⟨100⟩ valleys. n is the total carrier concentration, and

$$I_l^{\pm} = \int (E - \Delta \pm \hbar\omega_{12})^{1/2} \rho(E) e^{-E/kT_l} dE,$$
$$l \equiv e, L \quad . \qquad (12)$$

The average drift velocity of the carriers may be calculated by evaluating the mobility of the ⟨111⟩ carriers with the help of Eqs. (5) and (6) and the number of the transferred carriers from Eq. (10). In carrying out the associated integrations the square roots of negative energies are to be set equal to zero. The results obtained are discussed in Sec. III.

III. RESULTS AND DISCUSSION

In our calculations we have used the same parameter values for the electrons in the ⟨111⟩ valleys as in Ref. 7. The value of W_e has been taken to be $(2.3)^2 W$,[1,3] and T_L/T_e in Eq. (3) has been retained.

The electron mobility for the ⟨100⟩ valleys has been taken to be 700 $cm^2 V^{-1} sec^{-1}$ and the longitudinal and the transverse masses for these valleys have been assumed to be, respectively, $0.90m_0$ and $0.19m_0$, which are the same as those of silicon.[12,13] Also, we have taken $\Delta = 0.18$ eV and $\hbar\omega_{12} = 0.0276$ eV. Results have been calculated for several combinations of the values of D_{12} and D_0 (the deformation potential constant for optic scattering), and the curves for two combinations of values are shown in Fig. 1.

On comparing our theoretical curves with the experimental curve,[14] we find that theory agrees closely with experiment if we take $D_0 = 0.6 \times 10^9$ eV cm^{-1} (corresponding to $B = 0.103$) and $D_{12} = 0.2 \times 10^8$ eV cm^{-1}. The value of D_0 is close to the value 0.66×10^9 eV cm^{-1} (corresponding to $B = 0.125$), required to explain the temperature variation of low-field mobility considering the nonparabolicity of the ⟨111⟩ valleys.[7] It may be mentioned that the required values of D_0 and D_{12} for similar fit between theory and experiment are, respectively, 0.4×10^9 and 0.5×10^8 eV cm^{-1} when the effects of nonparabolicity are neglected.[6] The nonparabolicity, in addition, reduces the electron temperature in the ⟨111⟩ valleys and the number of carrier transferred to the ⟨100⟩ valleys.

The hot-electron characteristics of n-type germanium may, therefore, be considered to be satisfactorily explained by theory when the effects of both the nonparabolicity of the ⟨111⟩ valleys and the carrier transfer to the ⟨100⟩ valleys are taken into account.

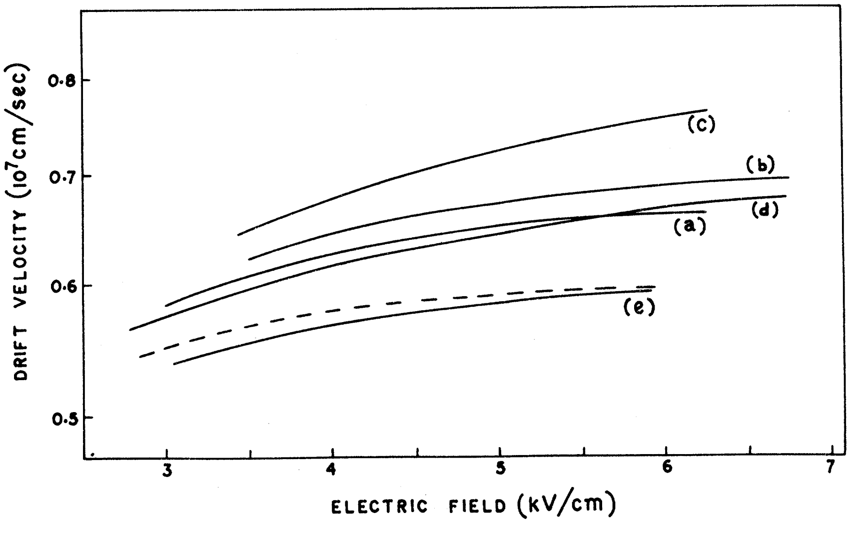

FIG. 1. Room-temperature velocity-field characteristics of n-Ge. Curve (a) is due to Dumke. Curves (b)–(e) are obtained in the present analysis. The effect of the ⟨100⟩ valleys is considered in (d) and (e), but neglected in (b) and (c). The acoustic-mode energy loss is properly included in all but curve (b). (d) corresponds to $D_0 = 0.66 \times 10^9$ eV cm^{-1}, $D_{12} = 0.5 \times 10^8$ eV cm^{-1}, and (e) to $D_0 = 0.6 \times 10^9$ eV cm^{-1}, $D_{12} = 0.2 \times 10^8$ eV cm^{-1}. The dashed line represents the experimental curve (Ref. 14).

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Semiconductor-to-Metal Transition in the Blue Potassium Molybdenum Bronze, $K_{0.30}MoO_3$; Example of a Possible Excitonic Insulator

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The electrical conductivity of the blue-phase potassium molybdenum bronze $K_{0.30}MoO_3$ has been extended down to 4 °K. Below 10 °K, σ is weakly metallic. Above 10 °K, there is an activation energy for conduction of 0.025 eV. Above 180 °K, σ becomes metallic again with a discontinuity only in the slope. Several models are suggested to account for the semiconductor-to-metal transition in the absence of an antiferromagnetic Néel point or heat effect at 180 °K. Included are the Mott-Hubbard model with a short-range electron-hole attraction proposed by Ramirez, Falicov and Kimball, and the excitonic-insulator model on the semimetallic side. The latter, although semiquantitatively consistent with the electrical conductivity, the Seebeck coefficient, and the weak temperature dependence of the magnetic susceptibility, cannot be distinguished from a correlation-free model involving only a simple lattice distortion on the semimetallic side. The exciton binding energy is calculated to be 0.021 eV in satisfactory agreement with the low-temperature-conductivity activation energy (0.025 eV).

I. INTRODUCTION

The term bronze has been given to a series of highly doped formally mixed-valence metal oxides which in some cases have a very high metallic luster.[1] The tungsten bronzes M_xWO_3, where M is usually an alkali or alkaline-earth metal, have been the most thoroughly studied. They form simple-cubic perovskite structures each cube corner being occupied by a WO_6 octahedron sharing corners with neighboring octahedra and with the doping atom M sitting in the center of the cube. They are highly metallic with a room-temperature conductivity $\sigma = 2.6\times10^4\ \Omega^{-1}\,\mathrm{cm}^{-1}$ for $K_{0.4}WO_3$ as an example. The conductivity is for the most part independent of the kind of dopant and only depends on the dopant's concentration.

The dopant donates its valence electron to the conduction band of the host which in the case of the tungsten bronzes contains states which are made up of a linear combination of antibonding tungsten $5d(t_{2g})$ orbitals and oxygen $2p_\pi$ orbitals. This bonding scheme for the tungsten bronzes was first suggested by Sienko[1] and further clarified by Goodenough[2] for the general class of perovskites. Within this general framework it was possible to understand the metallic electrical properties of the tungsten bronzes as arising from an almost-free electron interacting with polar modes of the lattice to form large polarons.[3]

The significant decrease in the radial extension of the wave function in going from $5d$ to $3d$ raised the question as to the importance of $d(t_{2g})$-p_π overlap for bronzes of the $3d$-transition-metal oxides. Based on a wealth of information it appears that for the vanadium bronzes $M_xV_2O_5$, the dopant again donates its valence electron to the host, but due to the absence of $d(t_{2g})$-p_π overlap,[4] the band-