

transitions like L_1 to L_1 (1.4 eV in Sc, not calculated for Gd and suppressed more deeply below E_F in Re) might account for further absorption. In all cases large volumes of reciprocal space may be involved, not just regions along symmetry lines. It is quite impossible to make even qualitative estimates of the origins of the higher-energy structures in A for both polarizations.

Thus, the data presented here not only allow tentative information concerning the bands of Y itself, but also provide support for the existing bands of Sc and Gd. Likewise, these data represent the only existing data on oriented crystals of Y. It is hoped

that a more detailed calculation of the bands of Y will follow as more experimental information becomes available for Y. More positive identifications than those presented here must await these bands and measurements in the vacuum ultraviolet of (probably) ultrahigh-vacuum-evaporated films of Y, which, when used in conjunction with our data, will make it possible to determine the optical constants.

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Hot-Electron Hall Transport in n -Type Germanium

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The hot-electron Hall coefficient in n -Ge is theoretically estimated incorporating the band nonparabolicity, the electron transfer to the $\langle 100 \rangle$ minima, and the effect of the magnetic field on the distribution function. A better agreement with the nature of the experimental curve at 200 °K is obtained when the nonparabolicity is considered than when it is ignored. A close fit with experiment requires the value of the deformation-potential constants for the optical and for the nonequivalent intervalley scattering to be 0.66×10^9 and 0.5×10^9 eV cm^{-1} , respectively.

I. INTRODUCTION

In an earlier paper,¹ calculations of the Hall factor in n -type germanium at high electric fields were reported taking into account the influence of the electron population in the $\langle 100 \rangle$ minima and that of the magnetic field on the valley distribution function. The nonparabolicity of the $\langle 111 \rangle$ bands was, however, not included in these calculations and the value of the optical-phonon deformation-potential constant D_0 required for an agreement with the experimental results at 200 °K was found to be unusually high. It may be mentioned that when parabolic bands are considered, there remain discrepancies in the values of D_0 obtained from various studies.¹ Incorporation of nonparabol-

icity has recently been found to reduce to a large extent the disparity in the D_0 values obtained from the conductivity results at high and low electric fields.^{2,3} It would be of interest to examine whether the hot-electron Hall-coefficient characteristic can also be explained with the same value of D_0 as that obtained from the conductivity data when the nonparabolic nature of the band structure is taken into account in addition to the carrier transfer to the $\langle 100 \rangle$ minima and the influence of the magnetic field on the carrier distribution function. In this paper we present the results of such calculations. We have also studied the effect of a change in the coupling constant for nonequivalent intervalley scattering D_{n1} and have determined the value required for a fit with the experimental results.

II. THEORETICAL FOUNDATION

The heating electric field F_x is assumed to be applied along the x direction of the chosen coordinate system which in the present situation coincides with the [100] crystallographic axis. The magnetic field B_z is applied along the z direction so that the Hall field F_y appears in the y direction.

The solution in the present case is made tractable by the assumption of a Maxwell-Boltzmann distribution function. Though this distribution may not be exactly attained, its assumption yields fairly accurate results in the case of germanium and at the same time vastly simplifies the calculations.^{1,3} The important scattering mechanisms at high electric fields affecting momentum and energy loss of the carriers are the intravalley acoustic and optic scattering and the nonequivalent intervalley scattering between the $\langle 111 \rangle$ and the $\langle 100 \rangle$ minima. All these scattering processes have been considered. The equations giving the carrier temperature and the relaxation time for the $\langle 111 \rangle$ electrons incorporating these scattering mechanisms and the band nonparabolicity and overlap factors have been given in Ref. 3 and will not be repeated here. The carriers in the $\langle 100 \rangle$ minima are assumed to thermalize at the lattice temperature because of their low mobility and the carrier density in these valleys is determined from the equation of detailed balance in intervalley scattering.³

The current densities in the x and y directions for a particular valley are given, retaining only the terms up to the first order in B_z , by

$$J_x = \frac{ne^2}{m_0} \left((\alpha_{xx} F_x + \alpha_{xy} F_y) \langle \tau \rangle - \frac{e}{m_0} \beta_{zz} B_z F_y \langle \tau^2 \rangle \right) \quad (1)$$

and

$$J_y = \frac{ne^2}{m_0} \left((\alpha_{xy} F_x + \alpha_{yy} F_y) \langle \tau \rangle + \frac{e}{m_0} \beta_{zz} B_z F_x \langle \tau^2 \rangle \right), \quad (2)$$

where n is the carrier concentration in the valley, e is the electron charge, the α are the components of the reciprocal-mass tensor normalized by the free-electron mass m_0 , and $\beta_{zz} = \alpha_{xx} \alpha_{yy} - \alpha_{xy}^2$. The angular brackets $\langle \rangle$ represent the average quantities defined by

$$\langle \tau^n \rangle = \frac{8\sqrt{2}\pi m_T m_L^{1/2}}{3\hbar^3 I_n K_B T_e} \int_0^\infty \tau^n(E) \left(1 + \frac{2E}{E_g}\right)^{-n} E^{3/2} \times \left(1 + \frac{E}{E_g}\right)^{3/2} e^{-E/\kappa_B T_e} dE \quad (n=1, 2). \quad (3)$$

In this equation m_T , m_L represent the transverse and longitudinal effective masses, \hbar is the Dirac constant, I_n is the normalization integral, K_B is the Boltzmann constant, T_e is the electron temperature, τ is the relaxation time, E_g is the direct energy gap, and E is the carrier energy. It may be

noted that Eqs. (1) and (2) are similar to those obtained for parabolic bands. The inclusion of nonparabolicity only affects the average values defined by (3).

The magnetic field influences the valley distribution function by perturbing the values of n and T_e . The perturbations may be evaluated in the same way as for parabolic bands, leading to an expression for the Hall mobility having the same form as Eq. (1) of Ref. 1.

III. RESULTS AND COMPARISON WITH EXPERIMENTS

Numerical calculations have been performed with the values of the material constants given in Ref. 3. The value of $\langle \tau \rangle$ for the silicon-type $\langle 100 \rangle$ valleys was derived by assuming the mobility in these valleys is (1/5.5) times the low-field mobility of the $\langle 111 \rangle$ electrons.³ The value of $\langle \tau^2 \rangle$ for the $\langle 100 \rangle$ minima was also assumed to be equal to $\langle \tau \rangle^2$ without introducing any serious error.¹

In Fig. 1 we have shown the electric field variation of the Hall coefficient normalized by its low-field value. Curves (a) and (b) are drawn according to the present analysis incorporating the effects of nonparabolicity with a value of D_0 equal to 0.66×10^9 eV cm⁻¹. This value corresponds to the temperature variation of weak-field mobility and is close to that obtained from the hot-electron conductivity data.^{2,3} We have used in curve (a) $D_{n1} = 0.2 \times 10^8$ eV cm⁻¹ and in curve (b) $D_{n1} = 0.5 \times 10^9$ eV cm⁻¹. The former value corresponds to the high-field conductivity characteristic³ and the latter to the resistivity measurements under hydro-

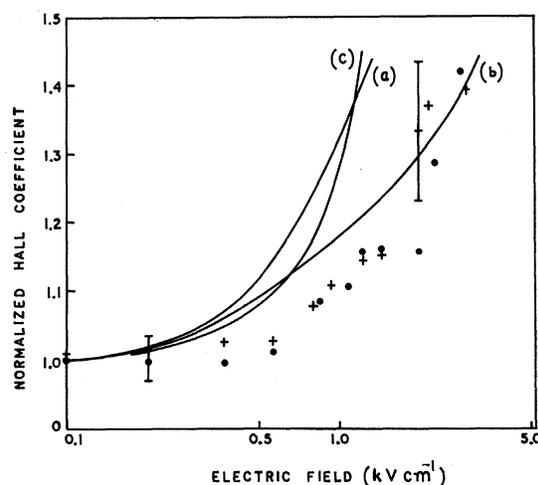


FIG. 1. Normalized Hall coefficient vs electric field. Curves (a) and (b) represent the results of the present analysis with $D_0 = 0.66 \times 10^9$ eV cm⁻¹. In curve (a) $D_{n1} = 0.2 \times 10^8$ eV cm⁻¹ and in curve (b) $D_{n1} = 0.5 \times 10^9$ eV cm⁻¹. Curve (c) is calculated for parabolic bands (Ref. 1) with $D_0 = 1 \times 10^9$ eV cm⁻¹ and $D_{n1} = 1 \times 10^8$ eV cm⁻¹. The ● and + are the experimental points of Heinrich *et al.* (Ref. 4).

static pressure.⁵ We have also included in the figure the curve obtained in Ref. 1 assuming parabolic bands and $D_0 = 1 \times 10^9$ eV cm⁻¹, $D_{n1} = 1 \times 10^8$ eV cm⁻¹. It is evident that inclusion of nonparabolicity reduces the rise of the Hall coefficient at high fields and thus gives a better agreement with the trend of the experimental variation. Furthermore, it is found that for a fit with the experimental re-

sults, D_{n1} should be close to 0.5×10^9 eV cm⁻¹ in agreement with the value indicated from pressure experiments.

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Density of Electronic States in Liquid Beryllium

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The density of electronic states in liquid beryllium is calculated for both a random and a correlated distribution of atoms using the approach of independent pseudoatoms due to Rousseau *et al.*

In this paper we report the result of calculation of the electronic density of states in liquid beryllium using the model of independent pseudoatoms proposed by Rousseau *et al.*¹ These authors have calculated the density of states of liquid beryllium using a screened Coulomb potential corresponding to a charge $Z = 4$ in a Fermi gas. Recently, we have calculated the density of states of liquid aluminum² using the above formulation but with a form of the potential as given by Green *et al.*³ Although the present calculational scheme is the same as in Ref. 2 the motivation, unlike that for aluminum, is that there is only one bound state in beryllium and the problem due to orthogonalization of the effective potential matrix⁴ is less serious. We outline below only the essential steps of the formulation of Rousseau *et al.* which are relevant for the discussion of the results of our calculation.

The model of independent pseudoatoms enables one to write the diagonal elements of the density matrix as¹

$$C(\vec{r}, \vec{r}; \beta) = C_0(\vec{r}, \vec{r}; \beta) \prod_{\vec{R}_i} e^{-\beta U(\vec{r} - \vec{R}_i; \beta)}, \quad (1)$$

where $C_0(\vec{r}, \vec{r}; \beta)$ is the free-particle density matrix, \vec{R}_i is the position of the i th ion, and U is an "effective potential matrix" introduced by Hilton

*et al.*⁴ The essential advantage of this formulation is that $U(\vec{r}; \beta)$ is a much more slowly varying function than the actual potential $V(\vec{r})$ from which it is obtained. By a straightforward integration and configurational averaging, one arrives at the following expression for the partition function $Z(\beta)$:

$$Z(\beta) = (2\pi\beta)^{-3/2} \left(1 + \int d\vec{r}_1 \frac{f(\vec{r}_1; \beta) \{\exp[\rho G(\vec{r}_1)] - 1\}}{G(\vec{r}_1)} \right), \quad (2)$$

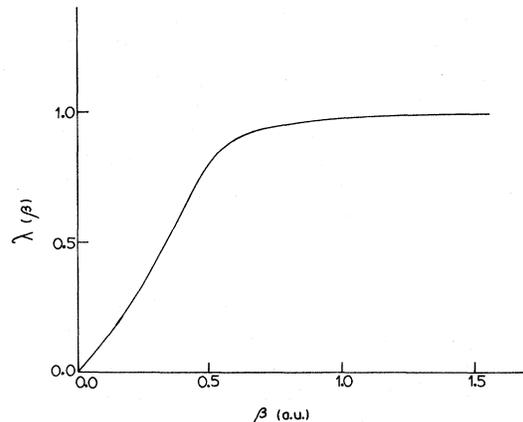


FIG. 1. Orthogonalization parameter $\lambda(\beta)$ is shown as a function of β .