The precision of the neutron measurements is such that a small moment on iridium, 0.2–0.3 μ_B, would just be detectable. However, it is known[2,6] that there exists a range of compositions for these and similar compounds over which the Laves phase structure is found. If a 3% weight loss on melting, as noted by Bozorth and coworkers, be attributed to loss of Tb then one would have to do with $Tb_{0.9}Ir_2$[7] rather than $TbIr_2$ and a moment differing by some 10% from that of the ideal compound would be inferred. It appears impossible to us to state at this time that iridium does or does not carry a small magnetic moment.

[6] J. H. Wernick and S. Geller, Trans. AIME **218**, 866 (1960).

[7] Direct chemical analysis of the $TbIr_2$ specimen investigated here gives a composition $Tb_{1.01}Ir_2$, which is not distinguishable, in our measurement, from the ideal composition. A change from the ideal composition of 10% Tb would, however, create fluctuations in the nuclear intensity which would be easily detectable.

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Galvanomagnetic Phenomena in High Electric Fields

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The Hall coefficient in a many-valley semiconductor is calculated for high electric fields and is shown to be independent of the electric field. For silicon we find $R_{100}/R_{111}=0.9$ and $R_{110}/R_{111}=0.85$, where R_{100} is the Hall coefficient for the current in the [100] direction, etc. For germanium we find $R_{111}/R_{100}=0.68$. Distribution functions for hot electrons in high magnetic fields are calculated at high and low temperatures for acoustical phonon scattering.

IN this paper we shall consider the galvanomagnetic properties of a system of electrons in a strong electric field. Sodha and Eastman[1] have calculated the electric-field dependence of the low-magnetic-field Hall coefficient for the case of a simple parabolic energy band and scattering by acoustical phonons.

Conwell[2] has used McClure's[3] solution of the Boltzmann equation to obtain general expressions for the Hall coefficient in a many-valley semiconductor in terms of the electron-distribution function. The conditions under which one may use McClure's treatment to describe a system of hot electrons have been discussed qualitatively by Conwell.

In this treatment we separate the general Boltzmann equation for a many-valley semiconductor into coupled equations for the isotropic and anisotropic parts of the distribution function. The equation for the anisotropic part is shown to be identical with McClure's equation except for an additional term which is shown to be negligible. The equation for the isotropic part allows one to calculate the electric and magnetic field dependence of the distribution function for arbitrary fields.

In Sec. II, we calculate the low-magnetic-field Hall coefficient using the hot-electron distribution obtained by Reik and Riskin.[4] Results are obtained for several current directions in silicon and germanium. In Sec. III we calculate the distribution function for hot electrons in high magnetic fields for acoustical phonon scattering.

[1] M. S. Sodha and P. C. Eastman, Phys. Rev. **110**, 1314 (1958).
[2] E. M. Conwell, Phys. Rev. **123**, 454 (1961).
[3] J. W. McClure, Phys. Rev. **101**, 1642 (1956).
[4] H. G. Reik and H. Riskin, Phys. Rev. **124**, 777 (1961).

I. THE BOLTZMANN EQUATION

The time-independent Boltzmann equation is given by

$$e(\mathbf{E}+\mathbf{V}\times\mathbf{B})\cdot\nabla_{\mathbf{K}}f=\hat{C}f, \tag{1}$$

where $\mathbf{E}$ and $\mathbf{B}$ are the electric and magnetic fields, $\hat{C}$ is the collision operator, and $\mathbf{K}$ and $\mathbf{V}$ are the wave vector and velocity, respectively. We consider a many-valley semiconductor with ellipsoidal constant energy surfaces. In the coordinate system of the principal axes of the valley under consideration, the electron energy is given by

$$\epsilon=K_x^2/2m_x+K_y^2/2m_y+K_z^2/2m_z. \tag{2}$$

Transforming these ellipsoidal surfaces into spheres, Eqs. (1) and (2) become

$$e(\mathbf{E}'+\mathbf{V}'\times\mathbf{B}')\cdot\nabla_{\mathbf{K}'}f=\hat{C}'f; \quad \epsilon=\mathbf{K}'^2/2m_0,$$

where

$$\mathbf{K}'=\alpha\mathbf{K}, \quad \mathbf{B}'=R\mathbf{B}, \quad \mathbf{E}'=\alpha\mathbf{E}, \quad \mathbf{V}'=\mathbf{K}'/m_0,$$
$$\alpha=\begin{bmatrix} m_0/m_x & 0 & 0 \\ 0 & m_0/m_y & 0 \\ 0 & 0 & m_0/m_z \end{bmatrix}^{1/2},$$
$$R=\begin{bmatrix} m_x & 0 & 0 \\ 0 & m_y & 0 \\ 0 & 0 & m_z \end{bmatrix}^{1/2}\frac{m_0}{(m_xm_ym_z)^{1/2}}. \tag{3}$$

We now separate f into two parts S and A: $f=S+A$,

where S is the isotropic part of the expansion of f in spherical harmonics and A is the anisotropic part. Separating Eq. (3) into isotropic and anisotropic parts we find

$$e\mathbf{E}'\cdot\nabla_{\mathbf{K}'}S+\mathrm{An}\{e\mathbf{E}'\cdot\nabla_{\mathbf{K}'}A\}+(e/m_0)\mathbf{K}'\times\mathbf{B}'\cdot\nabla_{\mathbf{K}'}A=\hat{C}'A\,, \quad (4)$$

$$\mathrm{Is}\{e\mathbf{E}'\cdot\nabla_{\mathbf{K}'}A\}=\hat{C}'S, \quad (5)$$

where $\mathrm{An}\{X\}$ = anisotropic part of X, and $\mathrm{Is}\{X\}$ = isotropic part of X. We now make the following assumptions:

(a) $\mathrm{An}\{e\mathbf{E}'\cdot\nabla_{\mathbf{K}'}A\}$ is small;

(b) $\hat{C}'A=-A/\tau(\epsilon)$.

We shall verify *a posteriori* (see Appendix) that assumption (a) is valid. After making these assumptions, Eq. (4) becomes identical with McClure's linearized Boltzmann equation for this band structure, except that the equilibrium distribution is replaced by the more general isotropic function S. We find straightforwardly that

$$A=-\tau\frac{dS}{d\epsilon}\mathbf{V}'\cdot\left[\frac{e\mathbf{E}'+(e^2\tau^2/m_0^2)\mathbf{B}'\mathbf{B}'\cdot e\mathbf{E}'+(e\tau/m_0)\mathbf{B}'\times e\mathbf{E}'}{1+(e^2\tau^2/m_0^2)\mathbf{B}'^2}\right]. \quad (6)$$

Substituting this into Eq. (5) we find

$$-\frac{2(e\mathbf{E}')^2}{3m_0\epsilon^{1/2}}\frac{d}{d\epsilon}\left[\tau\epsilon^{3/2}\frac{dS}{d\epsilon}\left(\frac{1+\gamma_0^2\omega^2\tau^2}{1+\omega^2\tau^2}\right)\right]=\hat{C}'S, \quad (7)$$

where γ_0 is the direction cosine of $\mathbf{B}'$ with respect to $\mathbf{E}'$ and $\omega=e\mathbf{B}'/m_0$.

We see from Eq. (7) that when B is sufficiently small we can neglect $\omega^2\tau^2$ compared to unity and we obtain the same S as in the absence of the magnetic field. A becomes simply

$$A=-\tau\frac{dS}{d\epsilon}\mathbf{V}'\cdot\left[e\mathbf{E}'+\frac{e\tau}{m_0}\mathbf{B}'\times e\mathbf{E}'\right]. \quad (8)$$

II. THE HALL COEFFICIENT

If we limit ourselves to small magnetic fields ($\omega^2\tau^2\ll1$) we need only insert the hot-electron distribution in Eq. (8) and, thus, calculate the current and Hall coefficient. We shall consider a many-valley semiconductor in a strong electric field. In this case Reik and Riskin[4] have shown that the isotropic part of the distribution function in each valley is approximately Maxwellian and is given by

$$S=e^{-\epsilon/kT_e};\quad T_e\sim E^2\left(\frac{\alpha^2}{m_x}+\frac{\beta^2}{m_y}+\frac{\gamma^2}{m_z}\right), \quad (9)$$

where α,β,γ are the direction cosines of the electric field with respect to the ellipsoid axes. Taking into account the intervalley scattering to zeroth order they found that the number of electrons in a given valley is simply

$$n_i\sim1/T_i^{1/2}, \quad (10)$$

where T_i is the temperature of the valley.

We shall now see that the Hall coefficient is, in general, anisotropic, in contrast to the weak electric field case, and that it becomes independent of the electric fields for large fields. The saturation of the Hall coefficient for large electric fields could provide an experimental method for verifying if the isotropic part of the distribution becomes Maxwellian at high electric fields. Erlbach and Gunn[5] have studied the shape of the isotropic part of the distribution function by making noise experiments on hot electrons, but their experiments were not in the range of very large electric fields.

We shall now outline the calculation of the Hall coefficient. The current in a given valley is calculated by putting Eq. (9) into Eq. (8). Taking the longitudinal axis of the ellipsoid as the x axis and the transverse axes as y, z axes we find

$$V_x{}^i=\frac{eE_x}{m_l}n_i\langle\tau_i\rangle-e^2n_i\langle\tau_i{}^2\rangle\left[\frac{B_y{}^iE_z{}^i}{m_lm_t}-\frac{B_zE_y}{m_lm_t}\right], \quad (11)$$

where

$$\langle x\rangle\equiv\int_0^\infty x\epsilon^{3/2}e^{-\epsilon/kT_e}d\epsilon\Big/\int_0^\infty\epsilon^{3/2}e^{-\epsilon/kT_e}d\epsilon$$

and similar equations for the y and z components. We consider the applied field $\mathbf{E}_A$ in a given direction, the magnetic field $\mathbf{B}$ perpendicular to $\mathbf{E}_A$, and we wish to calculate the Hall field in a direction $\mathbf{E}_\perp$, perpendicular to $\mathbf{E}_A$ and $\mathbf{B}$. The current in each valley is resolved into components parallel to $\mathbf{E}_A$, $\mathbf{B}$, and $\mathbf{E}_\perp$, and the current is summed over all the valleys. We then require that the current in the $\mathbf{E}_\perp$ and $\mathbf{B}$ directions be zero, and determine the Hall field in terms of the current in the $\mathbf{E}_A$ direction. We neglect terms in B^2 throughout.

The calculation is simplest in silicon where we have two ellipsoids in each of the cube edge directions. We take the electric field in the [100] direction and the magnetic field in the [001] direction. Taking x, y, z axes in the [100], [010], [001], respectively, we find

$$V_y=2eE_y\left[\frac{n_1\langle\tau_1\rangle}{m_t}+\frac{n_2\langle\tau_2\rangle}{m_l}\right]-2e^2BE_x\left[\frac{n_1\langle\tau_1{}^2\rangle}{m_lm_t}+\frac{n_2\langle\tau_2{}^2\rangle}{m_lm_t}+\frac{n_2\langle\tau_2{}^2\rangle}{m_t{}^2}\right], \quad (12)$$

$$V_z=0, \quad (13)$$

where n_1, τ_1 refer to the [100] valleys and n_2, τ_2 refer to the remaining four valleys, since by symmetry these latter valleys all have the same n_i, $\langle\tau_i\rangle$ and $\langle\tau_i{}^2\rangle$. Setting

[5] E. Erlbach and J. B. Gunn, Phys. Rev. Letters **8**, 280 (1962).

$V_y=0$ and expressing E_x in terms of J_x, we find

$$E_y=\frac{J_xB}{2n_2e}\left[\frac{(n_1/n_2)\langle\tau_1^2\rangle+(K+1)\langle\tau_2^2\rangle}{((n_1/n_2)\langle\tau_1\rangle+2K\langle\tau_2\rangle)((n_1/n_2)\langle\tau_1\rangle+(1+1/K)\langle\tau_2\rangle)}\right], \tag{14}$$

where $K=m_l/m_t$. Taking $\tau=A\epsilon^{-s}$ we obtain from Eqs. (9), (10), and (11)

$$\begin{aligned}\langle\tau_{1,2}\rangle&=A\Gamma(\tfrac{5}{2}-s)(kT_{1,2})^{-s}/\Gamma(\tfrac{5}{2}),\\ \langle\tau_{1,2}^2\rangle&=A^2\Gamma(\tfrac{5}{2}-2s)(kT_{1,2})^{-2s}/\Gamma(\tfrac{5}{2}),\\ n_1/n_2&=(T_2/T_1)^{1/2}=K^{1/2};\quad n_2=n/2(2+K^{1/2}).\end{aligned} \tag{15}$$

Substituting Eq. (15) into (14) we obtain

$$\begin{aligned}E_y&=\frac{J_xB}{ne}rR_{100};\quad r=\frac{\langle\tau^2\rangle}{\langle\tau\rangle^2}=\frac{\Gamma(\frac{5}{2})\Gamma(\frac{5}{2}-2s)}{\Gamma^2(\frac{5}{2}-s)};\\ R_{100}&=\frac{(K^{2s+1/2}+K+1)(2+K^{1/2})}{(K^s+2K^{1/2})(K^{s+1}+K^{1/2}+K^{-1/2})}.\end{aligned} \tag{16}$$

With the applied electric field in the [111] direction the n_i, $\langle\tau_i\rangle$ and $\langle\tau_i^2\rangle$ are the same for all valleys and the Hall field is simply

$$E=(JB/ne)rR_{111};\quad R_{111}=3K(K+2)/(2K+1)^2. \tag{17}$$

Taking $s=\frac{1}{2}$ for phonon scattering and $K=5.1$ for silicon we obtain

$$R_{100}/R_{111}=0.9. \tag{18}$$

If we take the electric field in the [110] direction and the magnetic field in the [001] direction we find

$$R_{110}=\frac{(2+K\gamma^{4s+1})(2+\gamma)}{(K+1+K\gamma^{2s+1})(1+1/K+\gamma^{2s+1})}, \tag{19}$$

where

$$\gamma=\left(\frac{1+1/K}{2}\right)^{1/2}.$$

For $s=\frac{1}{2}$, $K=5.1$ we have

$$R_{110}/R_{111}=0.85. \tag{20}$$

The anisotropy of the Hall coefficient in germanium is greater than in silicon since $K=20$ for germanium. With the electric field in the [111] direction and the magnetic field in the $[1\bar{1}0]$ direction we find

$$R_{111}=\frac{3(3+\gamma)(5+4K+3\gamma^{4s+1})}{(1+8K+3\gamma^{2s+1})(5+4/K+3\gamma^{2s+1})}, \tag{21}$$

where

$$\gamma=\tfrac{1}{3}(1+8K)^{1/2}.$$

Taking $s=\frac{1}{2}$, $K=20$ we have

$$R_{111}/R_{100}=0.68. \tag{22}$$

Our results imply that it should be possible to measure the ratio of the effective masses by measuring the hot-electron Hall coefficient, but it should be remembered that all the calculations are based on a Maxwellian distribution function in each valley and have treated intervalley scattering only to zeroth order.

III. LARGE MAGNETIC FIELDS

When $\omega^2\tau^2$ cannot be neglected compared to unity we must solve Eq. (7). Let us first consider the case of scattering by acoustical phonons. If we assume that equipartition holds for the acoustical phonons and that S varies little over the energy of a phonon, one[4,6] can derive the following expressions:

$$\begin{aligned}\hat{C}'S&=C_1/\epsilon^{1/2}\frac{d}{d\epsilon}\left[\epsilon^2\left(\frac{S}{kT}+\frac{dS}{d\epsilon}\right)\right];\quad \tau=C_2/\epsilon^{1/2}\\ C_1&=\frac{2^{11/2}\pi^3m_0^{3/2}m_tkT}{\rho h^4\det\alpha}\Sigma_d^2\left[1+\frac{1}{3}\left[\left(1+\frac{\Sigma_u}{\Sigma_d}\right)^2K-1\right]\right];\\ C_2&=\rho h^4C_l^2\det\alpha/2^{9/2}\pi^3m_0^{3/2}kT\Sigma_d^2\\ &\quad\times\left[1.31+1.61\frac{\Sigma_u}{\Sigma_d}+1.01\left(\frac{\Sigma_u}{\Sigma_d}\right)^2\right];\end{aligned} \tag{23}$$

where ρ is the density, C_l is the longitudinal velocity of sound, and Σ_d and Σ_u are the deformation potentials for dilation and uniaxial shear. Substituting Eq. (23) into (7) we obtain

$$S=\exp\left[-\int_0^\epsilon d\epsilon\frac{\epsilon/kT}{\epsilon+(2C_2(e\mathbf{E}')^2/3m_0C_1)((\epsilon+\gamma_0^2\omega^2C_2^2)/(\epsilon+\omega^2C_2^2))}\right]. \tag{24}$$

[6] R. Stratton, Proc. Roy. Soc. (London) **242**, 355 (1957).

This can be integrated to obtain

$$S=e^{-\epsilon/kT}\left[\left(\frac{\epsilon}{kT}\right)^2+\frac{b\epsilon}{(kT)^2}+\frac{C'}{(kT)^2}\right]^{p/2}\times\exp\left(-\frac{M(b^2-2C'-b\omega^2C_2^2)}{2(kT)^2}\right), \quad (25)$$

where

$$b=\omega^2C_2^2+\frac{2C_2(e\mathbf{E}')^2}{3m_0C_1}, \quad C'=\gamma_0^2\omega^2C_2^2pkT, \quad p=\frac{2C_2(e\mathbf{E}')^2}{3m_0C_1kT},$$

$$M=\int_0^{\epsilon/kT}\frac{d\epsilon}{\epsilon^2+b\epsilon+C'}$$

$$=\frac{2kT}{(4C'-b^2)^{1/2}}\tan^{-1}\left(\frac{2\epsilon+b}{(4C'-b^2)^{1/2}}\right); \quad 4C'-b^2>0$$

$$=\frac{kT}{(b^2-4C')^{1/2}}\ln\left|\frac{2\epsilon+b-(b^2-4C')^{1/2}}{2\epsilon+b+(b^2-4C')^{1/2}}\right|; \quad b^2-4C'>0.$$

When $\omega^2\tau^2$ can be neglected compared to unity we find the well known Yanashita-Watanabe[7] type solution

$$S=[\epsilon/kT+p]^pe^{-\epsilon/kT}. \quad (26)$$

If on the other hand $\omega^2\tau^2$ is large compared to unity we find from Eq. (24) that

$$S=\exp\left[-\int_0^\epsilon d\epsilon\frac{\epsilon/kT}{\epsilon+\gamma_0^2pkT}\right]$$

$$=[\epsilon/kT+\gamma_0^2p]^{\gamma_0^2p}e^{-\epsilon/kT} \quad (\gamma_0\neq0). \quad (27)$$

If $\gamma_0=0$, Eq. (24) becomes

$$S=\exp\left[-\int_0^\epsilon\frac{d\epsilon/kT}{1+pkT/(1+\omega^2\tau^2)\epsilon}\right].$$

If we now neglect unity compared to $\omega^2\tau^2$ we find

$$S=e^{-\epsilon/kT_e}; \quad T_e=T\left[1+\frac{pkT}{\omega^2C_2^2}\right]. \quad (28)$$

Thus, if we believe the validity of the Boltzmann equation[8] for $\omega^2\tau^2\gg1$ we find that for a large magnetic field perpendicular to the electric field, S becomes a simple Maxwellian whose temperature decreases with increasing magnetic field.

The condition $\omega^2\tau^2\gg1$ requires enormous magnetic fields (see Appendix) except at very low temperatures. At low temperatures, however, the equipartition of acoustical phonons is no longer true and Eq. (23) is no longer valid. Stratton[6] has calculated $\hat{C}S$ for acoustical phonon scattering and spherical constant energy surfaces. The results can be modified by using the transition probabilities for ellipsoidal energy surfaces given by Herring and Vogt.[9] We consider the case of spherical constant energy surfaces for which Stratton finds

$$\hat{C}S=\frac{4mC^2}{lkT(2m\epsilon)^{1/2}}\frac{d}{d\epsilon}\left[\epsilon^2\left(S+\tfrac{4}{5}(2mC^2)^{1/2}\epsilon^{1/2}\frac{dS}{d\epsilon}\right)\right], \quad (29)$$

$$\tau=5kTl/8\epsilon C,$$

where C is the velocity of sound and l is the mean free path for acoustical phonon scattering. This equation is only valid if $\epsilon/kT\gg kT/mC^2$ and, thus, only for electric fields large enough such that most of the electrons lie in this range. Putting Eq. (29) into (7) we find

$$S=\exp\left[-\frac{mC^2}{kT}\int_0^\epsilon\frac{\epsilon^2d\epsilon}{\frac{2}{5}((2mC^2)^{1.5}/kT)\epsilon^{2.5}+(5(eEl)^2kT(2m\epsilon)^{1/2}/48mC)N}\right], \quad (30)$$

$$N=(1+\gamma_0^2\omega^2\tau^2)/(1+\omega^2\tau^2).$$

When we consider optical phonons it is no longer generally possible to replace the optical-phonon operator by a simple differential operator as we did in Eqs. (23) and (29). However, when the electric field is sufficiently strong most of the electrons have energies greater than the optical-phonon energy and one can derive a differential operator for the optical phonons. In this case we can again write a differential equation for S, but the equation is fairly complicated and we shall not consider it here.

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APPENDIX

We have supposed throughout that $An\{e\mathbf{E}'\cdot\nabla_{K'}A\}$ is small. We notice that this term is at least quadratic in the electric field and is thus negligible for small fields. Thus, we need only consider the intermediate- and strong-field ranges.

Assuming for simplicity that **E** is perpendicular to **B**,

[7] J. Yamashita and M. Watanabe, Progr. Theoret. Phys. (Kyoto) **12**, 443 (1954).

[8] P. Argyres, Phys. Rev. **112**, 1115 (1958).

[9] C. Herring and E. Vogt, Phys. Rev. **101**, 944 (1956).

we find

$$\mathrm{An}\{e\mathbf{E}'\cdot\nabla_{\mathbf{K}'}A\}=\frac{(e\mathbf{E}')^2}{m}\left\{\frac{dS}{d\epsilon}\left[\frac{2\epsilon\omega}{3}\frac{d}{d\epsilon}\left(\frac{\tau^2}{1+\omega^2\tau^2}\right)P_2^2(\cos\theta)\sin\phi-\frac{4\epsilon}{3}\frac{d}{d\epsilon}\left(\frac{\tau}{1+\omega^2\tau^2}\right)P_2^0(\cos\theta)\right]\right.$$
$$\left.+\frac{d^2S}{d\epsilon^2}\left[\frac{2\epsilon\omega\tau^2}{3(1+\omega^2\tau^2)}P_2^2(\cos\theta)\sin\phi-\frac{4\epsilon\tau}{3(1+\omega^2\tau^2)}P_2^0(\cos\theta)\right]\right\}. \quad \text{(A1)}$$

Comparing this with the other terms in Eq. (4) we find that for $\omega^2\tau^2\ll1$ the neglect of $\mathrm{An}\{e\mathbf{E}'\cdot\nabla_{\mathbf{K}'}A\}$ is equivalent to neglecting $e\mathbf{E}l/\epsilon$ compared to unity for the cases where phonon equipartition is valid. From Eq. (26) we see that $e\mathbf{E}l/\epsilon\sim(mC_l^2/kT)^{1/2}$, while for the hot Maxwellian distribution, Eq. (9), we find $e\mathbf{E}l/\epsilon\sim e\mathbf{E}l/kT_e$. In both cases the terms are very small compared to unity. When $\omega^2\tau^2\gg1$ one can neglect the $\mathrm{An}\{e\mathbf{E}'\cdot\nabla_{\mathbf{K}'}A\}$ term for the high-temperature case (equipartition of acoustical phonons) if

$$1\gg\left(\frac{pmC_l^2}{\omega C_2^2[1+pkT/\omega C_2^2]}\right)^{1/2}\sim\frac{(pkT/\omega C_2^2)^{1/2}(mC_l^2/kT)^{1/2}}{(1+pkT/\omega C_2^2)^{1/2}}\sim(mC_l^2/kT)^{1/2}. \quad \text{(A2)}$$

The condition $\omega^2\tau^2\gg1$ is only realized in high magnetic field in this case, since the average relaxation time decreases because the electrons populate higher energy ranges in the presence of a strong electric field.

If we consider the number of electrons per unit energy range we find that the maximum of this function is displaced towards the higher energies because of the electric field, while the magnetic field displaces the peak towards the thermal equilibrium value. Thus, the electric field "heats" the electrons while the magnetic field "cools" them. Similar results hold for the low-temperature case.

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Effect of Alloying and Pressure on the Band Structure of Germanium and Silicon*

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The pseudopotential method has been used to compute the band structure of germanium-silicon alloys and the band structure of germanium under high pressure. In the former case the parameters were chosen from a linear interpolation between the parameters used previously for pure germanium and pure silicon, while in the latter case a simplified expression for the pseudopotential parameters based on the orthogonalized plane wave method was used to estimate their variation with lattice constant. The results are in reasonable agreement with experimental observations on the variation with pressure and alloying of the principal band edges. The calculations also indicate that the first absorption peak due to direct transitions should have a much larger pressure coefficient in Ge than in Si.

I. INTRODUCTION

A VERY useful way of obtaining detailed information on the band structure of simple semiconductors has been to study the change produced in their physical properties by alloying one semiconductor with another. Johnson and Christian[1] studied the change of the energy gap of Ge-Si alloys as a function of silicon concentration. The energy gap increases rapidly up to ~15% Si and from there on the increase is slow until the value in pure silicon is reached. Herman[2] speculated that this result is due to the role of two different minima in the conduction band: up to ~15% Si the L_1 state at $\mathbf{k}=(2\pi/a)(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ is the absolute minimum of the conduction band and when more silicon is added the absolute minimum is shifted to a point along the [100] direction near the state X_1 at $\mathbf{k}=(2\pi/a)(1,0,0)$ which is practically insensitive to addition of silicon. This interpretation was confirmed most strikingly by Glicksman,[3] who was able to determine the symmetry of the conduction minima for varying alloy concentration from the properties of the magnetoresistance

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[1] E. R. Johnson and S. M. Christian, Phys. Rev. **95**, 560 (1954); A. Levitas, C. C. Wang, and B. H. Alexander, *ibid.* **95**, 846 (1954).
[2] F. Herman, Phys. Rev. **95**, 847 (1954).
[3] M. Glicksman, Phys. Rev. **100**, 1146 (1955); **102**, 1496 (1956).