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Citation: Journal of Applied Physics **63**, 4536 (1988); doi: 10.1063/1.340151
View online: http://dx.doi.org/10.1063/1.340151
View Table of Contents: http://scitation.aip.org/content/aip/journal/jap/63/9?ver=pdfcov
Published by the AIP Publishing

The Einstein relation in Kane-type semiconductors

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(Received 8 June 1987; accepted for publication 9 December 1987)

An attempt is made to investigate the Einstein relation for the diffusivity-mobility ratio of the carriers in degenerate Kane-type semiconductors, taking n-Cd_3As_2 as an example, on the basis of a newly derived dispersion relation of the conduction electrons allowing various types of anisotropies in the band parameters within the framework of $\mathbf{k}\cdot\mathbf{p}$ formalism. It is found that the above ratio increases with increasing carrier degeneracy and is in quantitative agreement with the suggested experimental method of determining the Einstein relation in degenerate semiconductors having an arbitrary dispersion relation. In addition, the corresponding results for an isotropic three-band Kane model are also obtained from the expressions derived.

I. INTRODUCTION

It is well known that the Einstein relation for the diffusivity-mobility ratio of the carriers in semiconductors (here after referred to as DMR) is a very useful one since this is more accurate than any of the individual relations for the diffusivity or the mobility, which are considered to be the two most widely used parameters of carrier transport in semiconductors. It may also be noted that because of the performance of the semiconductor devices at the device terminals and the speed of operation of modern switching, semiconductor devices are significantly influenced by the degree of carrier degeneracy,[1,2] the simplest way of analyzing them would be to use the expression for the DMR, which in turn enables us to express the aforementioned features of semiconductor devices in terms of carrier concentration. In recent years, the connection of the DMR with the velocity autocorrelation function,[3] its relation with the screening of the carriers in semiconductors,[4] and the various modifications of the same ratio for degenerate semiconductors having different types of band structures have been investigated in the literature[5–10] under various approximations. Nevertheless, the generalized expression for such a ratio has yet to be investigated by formulating the generalized band structure. In this work, we shall take $A_3^{II}B_2^{V}$ type of narrow-gap semiconductors having tetragonal crystal structure.[11] Various types of device-oriented applications of $A_3^{II}B_2^{V}$ compounds having Kane-type energy bands have drawn the attention of the investigators to different physical properties of the said semiconductors.[12] Incorporating the crystal potential to the Hamiltonian and the special features of the above narrow-gap materials, Bodnar[13] proposed an E-$\mathbf{k}$ dispersion relation of the condition electrons in the same semiconductor using the assumption of an isotropic spin-orbit splitting parameter. It would, therefore, be of much interest to investigate the DMR in these materials by generalizing the above model within the framework of $\mathbf{k}\cdot\mathbf{p}$ formalism since the anisotropic spin-orbit splitting parameter is a significant physical feature of $A_3^{II}B_2^{V}$ semiconductors.[14]

In Sec. II A we shall generalize the Bodnar model by incorporating the anisotropy of the spin-orbit splitting parameter and using Kane's $\mathbf{k}\cdot\mathbf{p}$ method. We shall then formulate the DMR by deriving the appropriate electron statistics. In Sec. II B we shall obtain the corresponding results for isotropic three-band Kane model from our generalized expressions under certain limiting conditions. We shall also suggest a method of determining the DMR in degenerate semiconductors having an arbitrary dispersion relation from the experimental data of the thermoelectric power of the electrons in the presence of a classically large magnetic field in Sec. II C. We shall study the doping dependence of DMR by taking n-Cd_3As_2 for the purpose of numerical computation which is being increasingly used in Hall pickups and thermal detectors.

II. THEORETICAL BACKGROUND

A. Formulation of band structure and the subsequent derivation of the DMR in $A_3^{II}B_2^{V}$ semiconductors

The form of the $\mathbf{k}\cdot\mathbf{p}$ matrix for $A_3^{II}B_2^{V}$ semiconductors can be written, following Kildal,[15] as

$$H=\begin{bmatrix} H_1 & H_2 \\ H_2^{+} & H_1 \end{bmatrix}, \tag{1}$$

where

$$H_1\equiv\begin{bmatrix} E_g & P_{\parallel}k_z & 0 & 0 \\ P_{\parallel}k_z & -[\delta+(\Delta_{\parallel}/3)] & (\sqrt{2}/3)\Delta_{\perp} & 0 \\ 0 & (\sqrt{2}/3)\Delta_{\perp} & -\tfrac{2}{3}\Delta_{\parallel} & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

$$H_2\equiv\begin{bmatrix} 0 & 0 & f_- & f_+ \\ 0 & 0 & 0 & 0 \\ -f_- & 0 & 0 & 0 \\ f_+ & 0 & 0 & 0 \end{bmatrix},$$

where E_g is the band gap, $P_{\parallel}$ and $P_{\perp}$ are the momentum-matrix elements $\parallel$ and $\perp$ to the direction of the c axis, respectively, δ is the crystal-field splitting parameter, $\Delta_{\parallel}$ and $\Delta_{\perp}$ are the spin-orbit splitting parameters along and perpendic-

 0021-8979/88/094536-04$02.40

ular to the c axis, respectively, $f_{\pm} \equiv (P_1/\sqrt{2})(k_x \pm ik_y)$, and $i \equiv \sqrt{-1}$. Thus, neglecting the contributions of the higher bands and the free-electron energy, the diagonalization of the above matrix leads to the dispersion relation of the conduction electron in bulk specimens of $A_3^{II} B_2^{V}$ type of semiconductors as

$$C(E) = A(E)k_T^2 + B(E)k_z^2, \tag{2}$$

where

$$C(E) \equiv E(E+E_g)\left[(E+E_g)(E+E_g+\Delta_\parallel) + \delta(E+E_g+\tfrac{2}{3}\Delta_\parallel) + \tfrac{2}{9}(\Delta_\parallel^2 - \Delta_\perp^2)\right],$$

$$k_T \equiv \left[k_x^2 + k_y^2\right]^{1/2},$$

E is the energy as counted from the bottom of the conduction band,

$$A(E) \equiv \left[2m_\perp^*(E_g + \tfrac{2}{3}\Delta_\perp)\right]^{-1}\hbar^2 E_g(E_g+\Delta_\perp) \times \left[\delta(E+E_g+\Delta_\parallel) + (E+E_g) \times (E+E_g+\tfrac{2}{3}\Delta_\parallel) + \tfrac{1}{9}(\Delta_\parallel^2 - \Delta_\perp^2)\right],$$

$$B(E) \equiv \hbar^2 E_g\left[2m_{\parallel}^*(E_g+\tfrac{2}{3}\Delta_\parallel)\right]^{-1}(E_g+\Delta_\parallel) \times \left[(E+E_g)(E+E_g+\tfrac{2}{3}\Delta_\parallel)\right], \quad \hbar \equiv h/2\pi,$$

where h is the Planck's constant and $m_\parallel^*$ and $m_\perp^*$ are the longitudinal and transverse effective electron masses at the edge of the conduction band, respectively.

The use of Eq. (2) leads to the expression of the electron statistics as

$$n_0 = \int_0^\infty z(E)\left[1 + \exp\left(\frac{E-E_F}{K_B T}\right)\right]^{-1} dE, \tag{3}$$

where

$$z(E) \equiv \int_0^{k_{z\max}} \pi k_T^2 \, dk_z,$$

where E_F is Fermi energy as measured from the edge of the conduction band, K_B is the Boltzmann constant, and T is the temperature. Evaluating the above integral we get

$$n_0 = (3\pi^2)^{-1}\left[M(E_F) + + N(E_F)\right] \tag{4}$$

where

$$M(E_F) \equiv \left[C(E_F)\right]^{3/2}\left[A(E_F)\sqrt{B(E_F)}\right]^{-1},$$

$$N(E_F) \equiv \sum_{r=1}^{s} L(r,0)\left[M(E_F)\right],$$

$$L(r,J) \equiv 2(k_B T)^{2r}(1-2^{1-2r})\zeta(2r)\frac{d^{2r+J}}{dE_F^{2r+J}},$$

where r and J are the sets of real positive integers and $\zeta(2r)$ is the zeta function of order $2r$. Since the DMR of the electrons in semiconductors can, in general, be expressed[9] as

$$\frac{D}{\mu} = \frac{1}{e} n_0\left(\frac{\partial n_0}{\partial E_F}\right)^{-1}. \tag{5}$$

We can combine Eqs. (4) and (5) to obtain the generalized expression for the same ratio in degenerate $A_3^{II} B_2^{V}$ semiconductors as

$$\left(\frac{D}{\mu}\right) = \frac{1}{e}\left[M(E_F) + N(E_F)\right]\left[p(E_F) + q(E_F)\right]^{-1}, \tag{6}$$

where e is the electron charge,

$$p(E_F) \equiv \left(\frac{3}{2}\frac{C_1(E)\sqrt{C(E)}}{A(E)\sqrt{B(E)}} - \frac{A_1(E)C(E)^{3/2}}{A^2(E)\sqrt{B(E)}} - \frac{C^{3/2}(E)B_1(E)}{A(E)B^{3/2}(E)}\right)\Bigg|_{E=E_F},$$

$$C_1(E) = \{4E^3 + 3E^2(3E_g + \Delta_\parallel + \delta) + 2E\left[3E_g^2 + 2\Delta_\parallel E_g + 2\delta E_g + \tfrac{2}{3}\Delta_\parallel\delta + \tfrac{2}{9}(\Delta_\parallel^2 - \Delta_\perp^2)\right] + \left[E_g^3 + \Delta_\parallel E_g^2 + \delta E_g^2 + \tfrac{2}{3}\Delta_\parallel\delta E_g + \tfrac{2}{9}E_g(\Delta_\parallel^2 - \Delta_\perp^2)\right]\},$$

$$A_1(E) \equiv \hbar^2 E_g(E+\Delta_\perp)\left[2m_\perp^*(E_g+\tfrac{2}{3}\Delta_\perp)\right]^{-1} \times \left[2E + 2E_g + \delta + \tfrac{2}{3}\Delta_\parallel\right],$$

$$B_1(E) \equiv \hbar^2 E_g(E_g+\Delta_\parallel)\left[2m_\parallel^*(E_g+\tfrac{2}{3}\Delta_\parallel)\right]^{-1} \times (2E + 2E_g + \tfrac{2}{3}\Delta_\parallel)$$

and

$$q(E_F) \equiv \sum_{r=1}^{s} L(r,1)\left[M(E_F)\right].$$

B. Special case

Under the substitutions $\delta = 0$, $\Delta_\parallel = \Delta_\perp = \Delta$ (the isotropic spin-orbit splitting parameter), and $m_\parallel^* = m_\perp^* = m^*$ (the isotropic effective mass at the edge of the conduction band), Eq. (2) takes the form

$$\frac{\hbar^2 k^2}{2m^*} = \gamma(E),$$

$$\gamma(E) \equiv \frac{(E_g+\tfrac{2}{3}\Delta)E(E+E_g+\Delta)(E+E_g)}{E_g(E_g+\Delta)(E+E_g+\tfrac{2}{3}\Delta)}, \tag{7}$$

which is the standard dispersion relation for Kane-type semiconductors and is known as the three-band Kane model.[16] Using the above conditions, Eqs. (4) and (6) assume the forms

$$n_0 = (3\pi^2)^{-1}\left[r(E_F) + s(E_F)\right] \tag{8}$$

and

$$D/\mu = (1/e)\left[r(E_F) + s(E_F)\right]\left[a(E_F) + b(E_F)\right]^{-1}, \tag{9}$$

where

$$r(E_F) \equiv \left[\gamma(E_F)\right]^{3/2},$$

$$s(E_F) \equiv \sum_{r=1}^{s} L(r,0)\left[r(E_F)\right],$$

$$a(E_F) \equiv \tfrac{3}{2}\gamma_1(E_F)\sqrt{\gamma(E_F)},$$

$$\gamma_1(E_F) \equiv \gamma(E_F)\left[E_F^{-1} + (E_F+E_g)^{-1} + (E_F+E_g+\Delta)^{-1} - (E_F+E_g+\tfrac{2}{3}\Delta)^{-1}\right],$$

and

$$b(E_F) \equiv \sum_{r=1}^{s} L(r,1)\left[r(E_F)\right].$$

Equations (8) and (9) can be used as such for semiconductors where $\Delta \simeq E_g$ (e.g., n-InAs). Finally, we may remark that the well-known results for the electron statistics and the DMR for two-band Kane model and that of parabolic energy bands can be derived from Eqs. (8) and (9) under the conditions $\Delta \to \infty$ and $E_g \to \infty$, respectively.

C. Suggested experimental procedure of determining DMR

It is well known that the thermoelectric power of the electrons in semiconductors in the presence of a classically large magnetic field is independent of scattering mechanisms and is given by[17]

$$G_\infty = H_0/en_0 , \tag{10}$$

where H_0 is the entropy per unit volume. In this context we must note that in the presence of a classically large magnetic field the conditions $\hbar w_c \ll E_F$ (w_c is the cyclotron frequency) and $w_c\tau \gg 1$ (τ is the relaxation time) must be obeyed[17]; otherwise, the density-of-states function will be affected.[8] Therefore, Eq. (10) is valid under the two aforementioned inequalities. Following Tsidilkovski,[17] Eq. (10) can be expressed as

$$G_\infty = \left(\frac{\pi^2 K_B^2 T}{3en_0}\right)\left(\frac{\partial n_0}{\partial E_F}\right). \tag{11a}$$

Thus, combining Eqs. (11a) and (4) we get

$$D/\mu = (\pi^2 K_B^2 T)/3e^2 G_\infty . \tag{11b}$$

Since the classically large magnetic field does not alter the density-of-states function,[8] the DMR in the presence of classically large magnetic field will therefore be equal to the same ratio in the absence of that field. Thus, we can experimentally determine DMR for any arbitrary dispersion relation by knowing G_∞, which is an easily measurable experimental parameter.[18]

III. RESULTS AND DISCUSSION

For n-Cd_3As_2 using Eqs. (4) and (6) and taking the parameters[11,13] $E_g = 0.095$ eV, $\Delta_\parallel = 0.24$ eV, $\Delta_\perp = 0.29$ eV, $m_\parallel^* = 0.03\, m_0$, $m_\perp^* = 0.04\, m_0$, $\delta = 0.085$ eV, and $T = 4.2$ K we have computed the DMR as a function of the electron concentration as shown in Fig. 1 in which the same dependence is also plotted by using (11b) and taking the experimental values of the thermoelectric power of the electrons in n-Cd_3As_2 in the presence of a classically large magnetic field as given elsewhere.[18] In the same figure the plots corresponding to the degenerate three-band Kane model, two-band Kane model, and that for a parabolic energy band are also shown for the purpose of comparison. Besides, the dotted plot corresponds to $\delta = 0$. It appears from the figure that the DMR increases with increasing carrier degeneracy as expected for degenerate semiconductors, and is in good agreement with the suggested experimental method of determining the same ratio for arbitrary dispersion law. Although the DMR also increases nonlinearly with electron concentration in other limiting cases, the rates of increase are different from that in the proposed band model. The classical value of the DMR is $k_B T/e$ and is equal to 0.36 mV at 4.2 K. This is, therefore, not shown in the same figure as it would be senseless in such a figure.

In recent years, the mobility of the electrons in small-gap semiconductors has been extensively investigated, but the diffusion constant (a very important device parameter which can not be easily experimentally determined) of such materials has relatively been less studied. Thus, the theoretical results of our paper will be useful in determining the diffusion constants even for parabolic energy bands. Although the many-body effects, the formation of band tails in degenerate semiconductor, and the variation of the diffusion constant with the concentration gradient[6] have not been considered in the theoretical formation, this simplified analysis exhibits the basic features of the DMR in degenerate semiconductors and the agreement between the theory and the suggested experimental method of determining the same ratio becomes rather significant in spite of the above simplications. Finally, it can be stated that the basic purpose of this paper is not solely to investigate the DMR in $A_3^{II} B_2^{V}$ semiconductors but also to formulate the generalized carrier statistics by including the various types of anisotropies in the energy spectrum since the various electronic properties and the analytical formulation of different important physical parameters in semiconductors are based on the temperature-dependent carrier statistics in such materials.

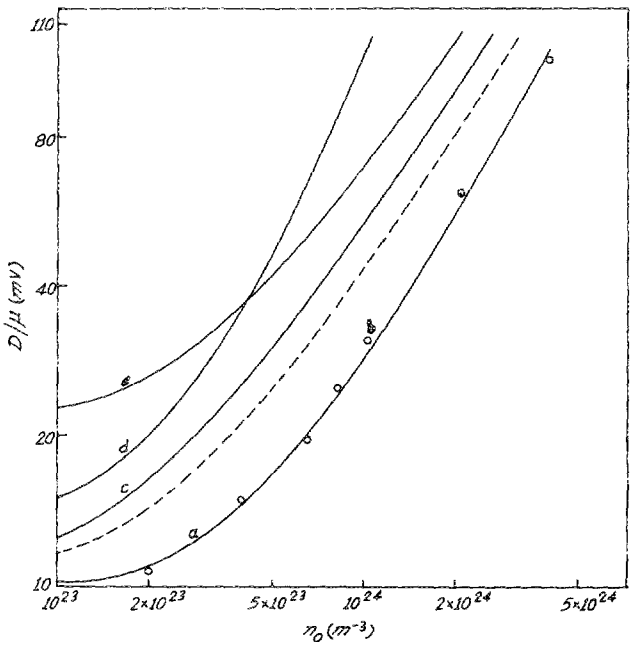

FIG. 1. Plot of the DMR as a function of the electron concentration at 4.2 K in degenerate n-Cd_3As_2 by using (a) the proposed dispersion relation, (b) the experimental values of the thermoelectric power of the electrons in a classically large magnetic field, (c) three-band Kane model, (d) two-band Kane model, and (e) isotropic parabolic energy bands. The dotted line corresponds to $\delta = 0$.

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