YU ISSN 0015—3206
FZKAAA 20 (3) 311 (1988)

EINSTEIN RELATION IN n-CHANNEL INVERSION LAYERS ON TERNARY SEMICONDUCTORS

KAMAKHYA P. GHATAK and VASWATI MITRA*

Department of Electronics and Telecommunication Engineering, University of Jadavpur, Calcutta-700 032, West Bengal, India

Received 6 June 1988

UDC 538.93

Revised manuscript received 22 August 1988

Original scientific paper

An attempt is made to study the Einstein relations for the diffusivity-mobility ratios of the carriers in n-channel inversion layers on ternary semiconductors under both weak and strong electric field limits, taking n-channel inversion layers on $Hg_{1-x}Cd_xTe$ as an example. It is found, on the basis of the three band Kane model which has been studied in the literature to be the most valid model for bulk specimens of ternary semiconductors that the ratios increase with increasing surface electric fields for both the limits. We have also suggested an experimental method of determining the Einstein relation in degenerate semiconductors having arbitrary dispersion laws. In addition, the corresponding well-known results for isotropic two-band Kane model are also obtained from the expressions derived.

1. Introduction

The Einstein relation for the diffusivity-mobility ratio of the carriers in semiconductors (hereafter referred to as DMR) is known to be a very useful one since this is more accurate than any of the individual relations for the diffusivity or the mobility are considered to be the two most widely used parameters of carrier transport in semiconductors. Besides, since the performance of the semiconductor

* Office of the Controller of Examinations, University of Jadavpur, Calcutta-700032, India.

devices at the device terminals and the speed of operation of the modern switching devices are significantly influenced by the degree of carrier degeneracy, the simplest way of analysing them would be to use the expression for the DMR which in turn enables us to express the above features of the devices made of degenerate semiconductors in terms of carrier concentration[1,2]. Furthermore the connection of the Einstein relation with the velocity autocorrection function[3], the modification due to non-linear charge transport[4], the relation of this ratio with the screening of the carriers in semiconductors[5-6] and the different modifications of the DMR in degenerate semiconductors under various physical conditions have extensively been investigated in the literature[3-14]. Nevertheless, the DMR in n-channel inversion layers on ternary semiconductors has yet to be investigated for the more interesting case which occurs from the consideration of the three band Kane model since, in recent years, the inversion layers on semiconductors having non-parabolic and non-standard energy bands are being increasingly studied for their various device oriented applications[15-17] and also since the inversion layers on ternary semiconductors have been experimentally realized[17]. Besides, the above class of materials are being increasingly used as infrared detectors[15] and different technical applications. The conduction band in ternary semiconductors is strongly non-parabolic where $E/E_g \approx 1$ instead of being much less than unity as is often assumed in the literature[12] (E being the electron energy as measured from the edge of the conduction band and E_g being the band gap). It would, therefore, be of much interest to investigate the DMR in n-channel inversion layers of ternary semiconductors by using three band Kane model since it is the most valid model for above class of materials[18].

In what follows, in Sec. 1 of theoretical background we shall formulate the diffusivity-mobility ratios in n-channel inversion layers on ternary semiconductors for both weak and strong electric field limits. In Sec. 2 we shall obtain the corresponding well-known results for two-band Kane model from our generalized expressions under certain limiting conditions. Besides, we shall also suggest a method of determining the DMR in degenerate semiconductors for any arbitrary dispersion relation from the experimental data of the thermoelectric power of electrons in the presence of a classically large magnetic field in Sec. 3. We shall take n-channel inversion layers on $Hg_{1-x}Cd_xTe$ as an example for the purpose of numerical computations. It may be noted that the compound $Hg_{1-x}Cd_xTe$ is an important optoelectronic material because its band gap can be varied to over the entire spectral range from 0.8 μm to over 30 μm by adjusting the alloy composition[19]. Its use as an infrared detector material has spurred a $Hg_{1-x}Cd_xTe$ technology for the production of high mobility single crystal with specially prepared surface layers[20]. The same semiconductor is ideally suited for narrow-gap subband physics[20].

2. *Theoretical background*

2.1. *The derivation of the 2D-DMRs in n-channel inversion layers on ternary semiconductors*

The expressions of the surface electron concentration per unit area under weak and strong electric field limits in n-channel inversion layers on ternary semiconductors whose energy band structures are defined by three band Kane model can, respectively, be expressed[21] as

$$N_{s\omega} = (m_0^*/\pi \hbar^2) \sum_{n=0}^{n_{max}} [p(E_{F\omega}) + q(E_{F\omega})] \tag{1a}$$

and

$$N_{ss} = (m_0^*/\pi \hbar^2) \sum_{n=0}^{n_{max}} [r(E_{Fs}) + s(E_{Fs})] \tag{1b}$$

where E_F is the Fermi energy under low electric field limit as measured from the edge of the conduction band at the surface and E_{Fs} is the corresponding energy under high electric field limit. Besides, the function $p(E_{F\omega})$, $q(E_{F\omega})$, $r(E_{Fs})$ and $s(E_{Fs})$ are defined in the Appendix 1.1.

Incidentally, the DMR of the electrons in inversion layers on semiconductors can be expressed[9], in the electric quantum limit, as

$$\frac{D}{\mu} = \frac{N_{s0}}{e} \left[\frac{\mathrm{d}\, N_{s0}}{\mathrm{d}(E_{F0} - E_0)} \right]^{-1} \tag{2}$$

where e is the electron charge, N_{s0} is the surface electron concentration at the electric quantum limit, E_{F0} is the Fermi energy at the electric quantum limit as measured from the edge of the conduction band at the surface and E_0 is the energy of the lowest electric subband as measured from the edge of the conduction band at the surface.

Thus, combining Eqs. (1a), (1b) and (2), the expressions for the DMR's under weak and strong electric field limits can, respectively, be expressed as

$$\left(\frac{D}{\mu}\right)_\omega = (N_{s\omega 0}/e)\, [P(E_{F\omega 0})]^{-1} \tag{3a}$$

$$\left(\frac{D}{\mu}\right)_s = (N_{ss0}/e)\, [R(E_{Fs0})]^{-1} \tag{3b}$$

where the subscript indicates the physical parameter at the electric quantum limit. Besides, the functions $P(E_{F\omega 0})$ and $R(E_{Fs0})$ are defined in Appendix 1.1.

2.2. *Special cases*

Under the substitutions $\Delta \to \infty$ and $S_n \to \left[\frac{3\pi}{8}(4n+3)\right]^{2/3}$ (for large values of n)[24] in the above equations, the expressions for the electron statistics and the DMR in n-channel inversion layers on Kane type semiconductors whose energy band structures are defined by two-band Kane model can, respectively, be expressed, for both the limits, as

$$N_{s\omega} = \left(\frac{m_0^* k_B T}{\pi \hbar^2}\right) \sum_{n=0}^{n_{max}} \left[\left(1 + \frac{2}{3} \alpha E_\omega\right) F_0(\eta_\omega) + 2\alpha\, k_B T F_1(\eta_\omega)\right] \tag{4a}$$

$$N_{ss} = \left(\frac{m_0^* k_B T}{\pi \hbar^2}\right) \sum_{n=0}^{n_{max}} [(1 + 2\alpha E_s) F_0 (\eta_s) + 2\alpha k_B T F_1 (\eta_s)] \tag{4b}$$

$$\left(\frac{D}{\mu}\right)_\omega = \frac{k_B T}{e} \left[\frac{\left(1 + \frac{2}{3} \alpha E_{\omega 0}\right) F_0 (\eta_{\omega 0}) + 2\alpha k_B T F_1 (\eta_{\omega 0})}{\left(1 + \frac{2}{3} \alpha E_{\omega 0}\right) F_{-1} (\eta_{\omega 0}) + 2\alpha' k_B T F_0 (\eta_{\omega 0})} \right] \tag{5a}$$

$$\left(\frac{D}{\mu}\right) = \frac{k_B T}{e} \left[\frac{(1 + 2\alpha E_{s0}) F_0 (\eta_{s0}) + 2\alpha k_B T F_1 (\eta_{s0})}{(1 + 2\alpha E_{s0}) F_{-1} (\eta_{s0}) + (1 + \Theta) 2\alpha k_B T F_0 (\eta_{s0})} \right] \tag{5b}$$

where

$$E_\omega (1 + \alpha E_\omega) = \left[\frac{3}{2} \pi \hbar e F_s (1 + 2\alpha E_\omega) (2m_0)^{-1/2}\right]^{2/3},$$

$$E_s (1 + \alpha E_s) = \left[2 \pi \hbar e F_s \left(n + \frac{3}{4}\right) (2E_g m_0^*)^{-1/2}\right], \quad \alpha' \equiv \left(1 + \frac{1}{3} \Theta\right),$$

$$\eta_\omega \equiv (k_B T)^{-1} [E_{F\omega} - E_\omega], \qquad \eta_s \equiv (k_B T)^{-1} [E_{Fs} - E_s],$$

$F_j (\eta)$ is the one-parameter Fermi-Dirac integral of order j as defined by Blakemore[22] and the other notations are defined in Ref. 11.

2.3. *Suggested experimental procedure for determining DMR*

Following Ghatak et al.[21] the thermoelectric power of the 2D electrons in the presence of a classically large magnetic field can be expressed, in the electric quantum limit, as

$$G_\infty (\pi^2 k_B^2 T/3N_{s0}) \left[\frac{\mathrm{d} N_{s0}}{\mathrm{d} (E_{F0} - E_0)}\right]. \tag{6}$$

Thus combining Eqs. (6) and (2) we get

$$\frac{D}{\mu} = \pi^2 k_B^2 T/3e^2 G_\infty. \tag{7}$$

Since the classically large magnetic field does not change the density-of-states function therefore the DMR in the presence of a classically large magnetic field will be equal to the same ratio in the absence of that field[12]. Thus we can experimentally determine the DMR for any arbitrary dispersion relation by knowing G_∞.

3. Results and discussion

Using Eqs. (3a) and (6a) together with the parameters[15,23]

$$E_g(x) = [-0.303 + 1.73x + 5.6 \times 10^{-4}(1 - 2x)\,T + 0.25x^4]\ \text{eV}$$

$$m_0^*(x) = [3\,\hbar^2\, E_g(x)/4P^2(x)], \quad P(x) = [(\hbar^2/2m_0)\,(18 + 3x)]^{1/2},$$

$$\Delta = 0.9\,\text{eV}, \quad \varepsilon_{sc} = [20.262 - 14.812x + 5.2795x^2]\,\varepsilon_0$$

as appropriate for n-$Hg_{1-x}Cd_xTe$ we have plotted the DMR under weak electric field limit at 4.2 K for n-channel inversion layers on $Hg_{1-x}Cd_xTe$ as a function of the surface electric field taking $x = 0.21$ as shown in plot a of Fig. 1 in which the plots b and c exhibit the same dependence in accordance with two band Kane model and that of parabolic energy bands. Using the same parameters as used in obtaining the Fig. 1 and using Eqs. (3b) and (6b) we have plotted the DMR under strong electric field limit at 4.2 K as shown in plot a of Fig. 2. in which the other

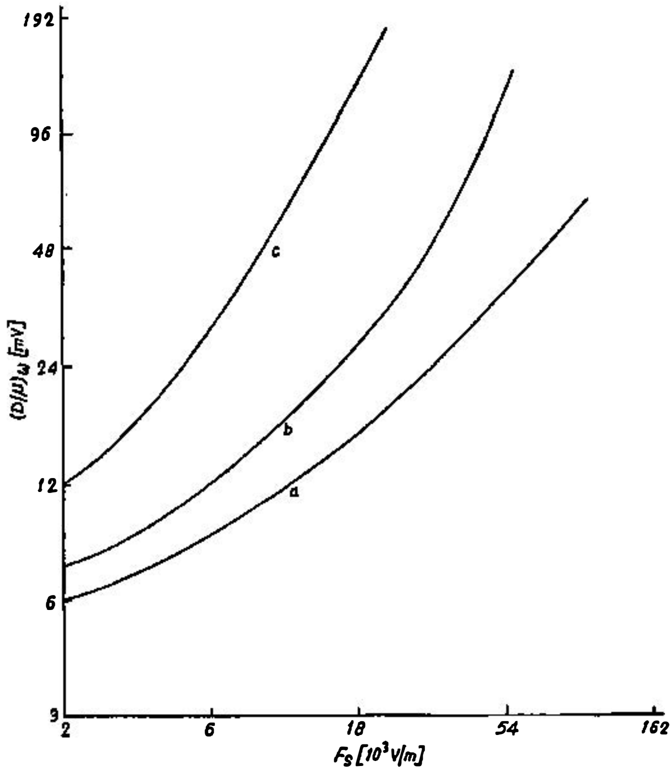

Fig. 1. Plot of the DMR as a function of the surface electric field under low electric field in n--channel inversion layers on $Hg_{1-x}Cd_xTe$ at 4.2 K by using (a) the three-band Kane model, (b) the isotropic two-band Kane model and (c) the parabolic energy bands.

simplified cases have further been demonstrated. In Fig. 3 we have plotted the DMR versus x for both the limits in accordance with three and two band Kane models, respectively

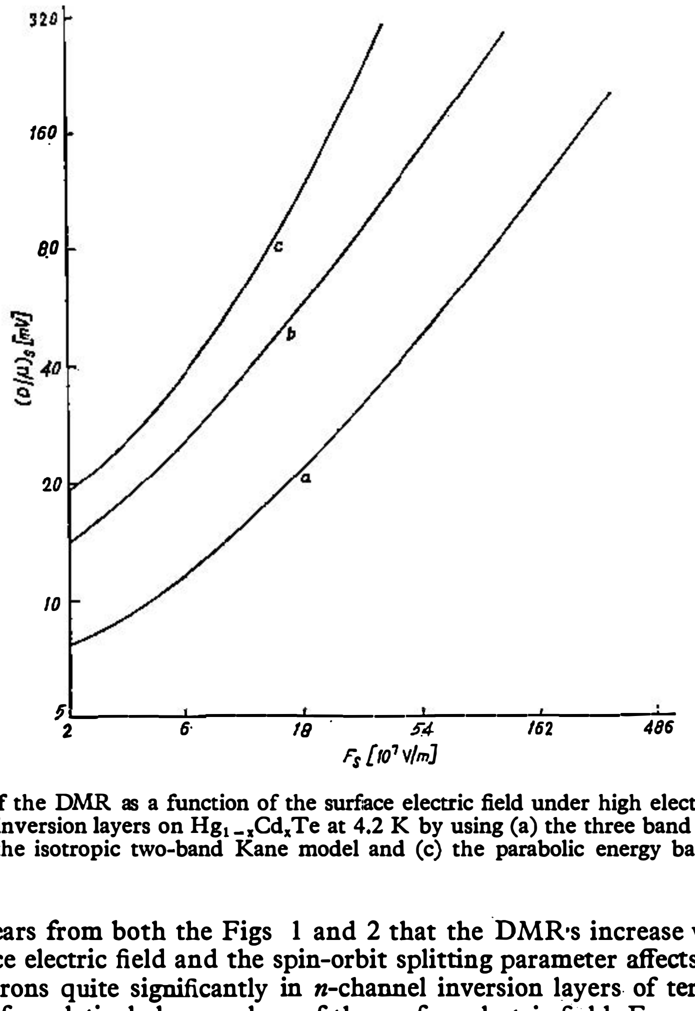

Fig. 2. Plot of the DMR as a function of the surface electric field under high electric field limit in n-channel inversion layers on $Hg_{1-x}Cd_xTe$ at 4.2 K by using (a) the three band Kane model, (b) the isotropic two-band Kane model and (c) the parabolic energy bands.

It appears from both the Figs 1 and 2 that the DMR's increase with increasing surface electric field and the spin-orbit splitting parameter affects the DMR of the electrons quite significantly in n-channel inversion layers of ternary semiconductors for relatively large values of the surface electric field For a fixed value of the surface electric field, the DMR of the electrons in accordances with three band Kane model is smaller as compared to that in two band Kane model in the whole range of fields considered for both the limits. Though the DMR also increases non-linearly with surface fields for both the limits in two band Kane model and also that of parabolic energy bands, the rates of increase are different from that in the three band Kane model. The classical value of DMR is $k_B T/e$ and is equal to 0.36 mV at 4.2 K. This is, therefore, not shown in both the figures as it would be senseless in such figures. From Fig. 3 it appears that the DMR decreases with increasing alloy composition in a monotonous manner for both the limits.

It is worth remarking that since most of the carriers occupy the lowest electric sub-band at low temperatures for which the effects of electric quantization become more pronounced, it is sufficiently accurate for such temperatures to consider the

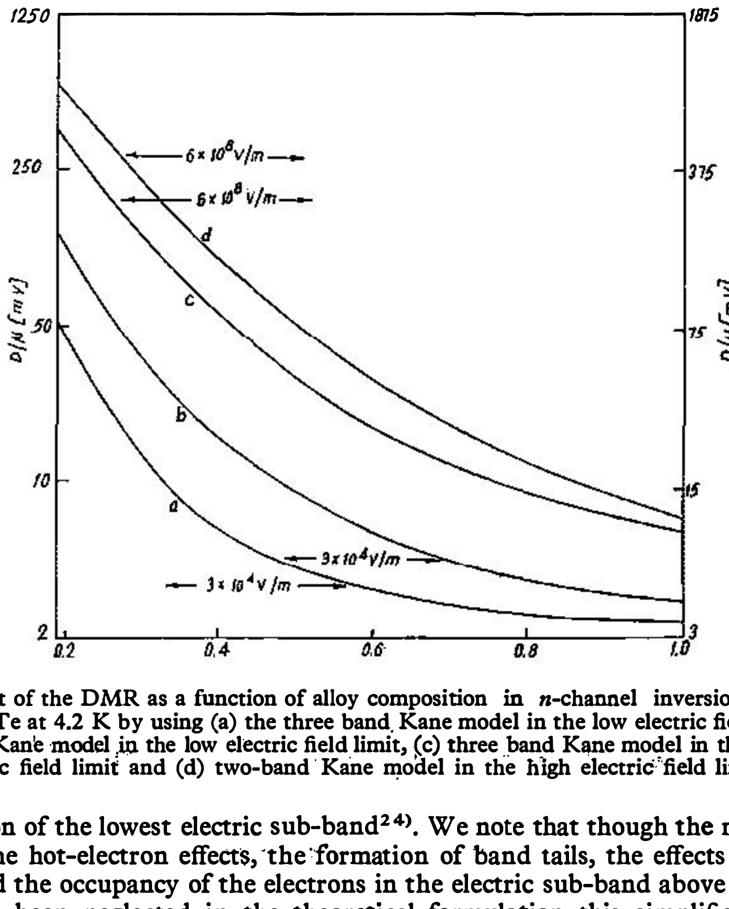

Fig. 3. Plot of the DMR as a function of alloy composition in n-channel inversion layers on $Hg_{1-x}Cd_xTe$ at 4.2 K by using (a) the three band Kane model in the low electric field limit, (b) two band Kane model in the low electric field limit, (c) three band Kane model in the high electric field limit and (d) two-band Kane model in the high electric field limit.

occupation of the lowest electric sub-band[24]. We note that though the many-body effects, the hot-electron effects, the formation of band tails, the effects of surface states and the occupancy of the electrons in the electric sub-band above the lowest one have been neglected in the theoretical formulation this simplified analysis exhibits the basic qualitative features of the DMR in n-channel inversion layers on semiconductors. Since the experimental data of the thermoelectric power in n-channel inversion layers on ternary semiconductors in the presence of a classically large magnetic field is not available to the best of our knowledge, we can not compare our theoretical results with the proposed experiment. Since the above power decreases with increasing surface electric field, from Eq. (7) we can conclude that the DMR will increase with increasing surface field as it should. The experimental result of G_∞ for inversion layers on ternary semiconductors will provide an experimental check on the above ratio and also a technique for probing the band structure in degenerate materials.

In recent years, the mobility of the electrons in inversion layers on small gap semiconductors has been extensively investigated but the diffusion constant (a very important device parameter which cannot be easily experimentally determined) of such 2D electron gases has yet to be investigated. Thus the theoretical results of our paper will be useful in determining the diffusion constant even for n-channel inversion layers on parabolic semiconductors. The general features of the effects of surface electric field on the DMR in n-channel inversion layer as discussed here would also be valid for most of the inversion layers on small-gap semiconductors since these semiconductors have non-parabolic energy bands are generally described by two-band Kane model whereas the present analysis is based on three band Kane model. Finally, it may be remarked that the basic purpose of the present paper is not solely to investigate the diffusivity-mobility ratios in n-channel inversion layers on ternary semiconductors but also to formulate the generalized carrier statistics by using the generalized three band Kane model for both the limits since the various transport phenomena and the derivation of the expressions of physical parameters of 2D semiconductor devices are based on the carrier statistics in such materials.

Appendix

1.1. The functions $P(E_{F\omega})$, $q(E_{F\omega})$, $r(E_{Fs})$, $s(E_{Fs})$, $P(E_{F\omega 0})$ and $R(E_{Fs0})$ are defined as follows:

$$p(E_{F\omega}) = \gamma(E_{F\omega}) - S_n [\hbar e F_s \psi(E_{F\omega})(2m_0^*)^{-1/2}]^{2/3} \tag{1.1a}$$

$$q(E_{F\omega}) = \sum_{Z=1}^{t} \nabla_t [p(E_{F\omega})] \tag{1.1b}$$

$$r(E_{Fs}) = \gamma(E_{Fs}) - S_n^{3/2} \left[\frac{4}{3} \hbar e F_s \sqrt{L(E_{Fs})}\,(2E_g m_0^*)^{-1/2}\right] \tag{1.1c}$$

$$s(E_{Fs}) = \sum_{Z=1}^{t} \nabla_t [r(E_{Fs})] \tag{1.1d}$$

$$P(E_{F\omega 0}) = \frac{m_0^*}{\pi\hbar^2}[p_1(E_{F\omega 0}) + q_1(E_{F\omega 0})]$$

$$\left[1 - \frac{m_0^*}{\pi\hbar^2}\{p_1(E_{F\omega 0}) + q_1(E_{F\omega 0})\}.\right.$$

$$\frac{2}{3} N_{s\omega 0}^{-1/3} \psi^{2/3}(E_{F\omega 0}) [\gamma_1(E_{F\omega 0}) S_0^{-1} \left\{\frac{\hbar e^2}{\varepsilon_{sc}} (2m_0^*)^{-1/2}\right\}^{-2/3} - \tag{1.1e}$$

$$\left. - \frac{2}{3} \psi_1(E_{F\omega 0}) \psi^{-1/3}(E_{F\omega 0}) N_{s\omega 0}^{2/3}]^{-1}\right]^{-1}$$

and

$$R(E_{Fs0}) = [r_1(E_{Fs0}) + s_1(E_{Fs0})]\left[\frac{m_0^*}{\pi\hbar^2}\right]$$

$$\left[1 - \frac{m_0^*}{\pi\hbar^2}\{r_1(E_{Fs0}) + s_1(E_{Fs0})\}\sqrt{L(E_{Fs0})}\;\cdot\right.$$

$$\left.\cdot\left[\frac{3\varepsilon_{sc}}{4\hbar e^2}\gamma_1(E_{Fs0})(2m_0^* E_g)^{1/2} S_0^{-3/2} - \frac{N_{ss0} L_1(E_{Fs0})}{2\sqrt{L(E_{Fs0})}}\right]^{-1}\right]^{-1} \tag{1.1f}$$

where

$$\nabla_t \equiv 2(k_B T)^{2t}(1 - 2^{1-2t})\,\zeta\,(2t)\frac{d^{2t}}{dE_F^{2t}},$$

k_B is Boltzmann constant, T is the temperature and $\frac{d}{dE}[f(E)] = f_1(E)$, where $f(E)$ is any differentiable function of energy.

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EINSTEINOVA RELACIJA U *n*-KANALNIM INVERZIONIM SLOJEVIMA NA TERNARNIM POLUVODIČIMA

KAMAKHYA P. GHATAK i VASWATI MITRA

Department of Electronics and Telecommunication Engineering, University of Jadavpur, Calcutta--700 032, West Bengal, India

UDK 538.93

Originalni znanstveni rad

Razmatrana je Einsteinova relacija za omjer difuzivnosti i pokretljivosti nosilaca naboja u *n*-kanalnim inverzionim slojevima na ternarnim poluvodičima u limesu jakih i slabih električnih polja. Kao primjer uzet je *n*-kanalni inverzioni sloj na $Hg_{1-x}Cd_xTe$. Nađeno je, na osnovi Kaneovog modela s tri vrpce da omjer difuzivnosti i pokretljivosti raste porastom površinskog električnog polja u oba limesa.