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ON THE EINSTEIN RELATION IN *n*-CHANNEL INVERSION LAYERS ON TERNARY SEMICONDUCTORS

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An attempt is made to derive a generalized expression of the Einstein relation in *n*-channel inversion layers on ternary semiconductors without any approximations of weak or strong electric field limits. It is found, taking *n*-channel inversion layers on $Hg_{1-x}Cd_xTe$ as an example, that the same ratio decreases continuously with increasing alloy composition and decreasing surface electric field, respectively, in the electric quantum limit. In addition, the corresponding results for inversion layers on parabolic semiconductors are also obtained from the expression derived.

I. INTRODUCTION

In recent years, there has been considerable interest in studying the various physical features of degenerate semiconductors having non-parabolic energy bands and obeying Kane's dispersion relation [1, 2]. The band non-parabolicity has been observed to influence many of these features resulting in special properties of these semiconductors. It is well known [3, 4] that the performance of 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 present in these devices. The simplest method of analysing semiconductor devices taking into account the degeneracy of the bands is to use the Einstein relation to express the performance at the device terminals and the switching speed in terms of a carrier concentration. Moreover, the relation for the diffusivity-mobility ratio of the carriers in semiconductors (hereafter referred to as DMR) is a very useful one since one can accurately determine from this relation the diffusivity by knowing the mobility and vice-versa. Furthermore, in recent years the connection of the DMR with the velocity autocorrelation function [5], the connection of this ratio with the screening of the carriers in semiconductors [6] and the various modifications of the Einstein relation under different physical conditions have extensively been investigated

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[8—15]. Nevertheless, it appears that, the generalized expression of the DMR in n-channel inversion layers on ternary semiconductors has yet to be theoretically worked out without any approximations of weak or strong electric field limits. This is very important since the various aspects of inversion layers on narrow-gap semiconductors are being increasingly investigated for their peculiar physical characteristics [16—18]. In particular, such studies for ternary semiconductors which have Kane-type energy bands would be interesting since the compound $Hg_{1-x}Cd_xTe$ is a very important optoelectronic material because its bandgap 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 crystals with specially prepared surface layers [20]. Furthermore, the same material is ideally suited for narrow-gap subband physics, because the relevant physical parameters are within easy experimental reach [20].

In what follows we shall first derive an expression of the surface electron concentration per unit area in n-channel inversion layers on ternary semiconductors without any approximations of weak or strong electric field limits. We shall then derive the DMR with the proper use of the electron statistics. Besides, we shall investigate theoretically the effects of alloy composition and carrier degeneracy on the DMR, respectively, taking n-channel inversion layers on $Hg_{1-x}Cd_xTe$ as an example.

II. THEORETICAL BACKGROUND

The DMR of the electrons in inversion layers on semiconductors can be expressed [8], in the electric quantum limit, as

$$\frac{D}{\mu} = \frac{1}{e}\cdot N_s\left[\frac{dN_s}{d(E_F - \epsilon_0)}\right]^{-1} \qquad (1)$$

where e is the electron charge, N_s is the surface electron concentration per unit area and ϵ_0 and E_F are the electric and electrochemical potentials, in the electric quantum limit, respectively, as measured from the edge of the conduction band on the surface. It appears then that the evaluation of the DMR using equation (1) requires an expression of the 2D electron statistics which, in turn, is determined by the corresponding density-of-states function. Incidentally, the dispersion relation of the 2D electrons in n-channel inversion layers on narrow-gap semiconductors can be written [16] as

$$\frac{1}{2}\left[\omega_0\sqrt{1+\omega_0^2} - \ln\left|1+\sqrt{1+\omega_0^2}\right|\right] = \left(a+\frac{1}{4}\right)^{-1} K(n), \qquad (2)$$

where $\omega_0 \equiv \left(a_0 + \frac{1}{4}\right)^{-1}[\alpha\epsilon(1+\alpha\epsilon) - a_0]$, $a_0 \equiv \alpha\hbar^2 k_s^2/2m_0^*$, $\alpha \equiv 1/E_g$, E_g is the bandgap, $\hbar \equiv h/2\pi$, h is the Planck constant, $k_s^2 \equiv k_x^2 + k_y^2$, m_0^* is the effective electron mass at the edge of the conduction band, ϵ is the electron energy as measured from the edge of the conduction band on the surface, $K(n) \equiv$ $\equiv \left(n+\frac{3}{4}\right)\alpha\pi F_s(\alpha\hbar^2/2m_0^*)^{1/2}$, n $(= 0, 1, 2, \ldots)$ is the electric sub-band index, F_s $(= eN_s/\epsilon_{sc})$ is the surface electric field applied normal to the surface and ϵ_{sc} is the permittivity of the semiconducting substrate material.

Using equation (2) the density-of-states function is given by

$$P(\epsilon) = C\sum_{n=0}^{n_{max}}(1+2\alpha\epsilon)[1+\Phi(\omega_0, a_0)]^{-1} H(\epsilon - \epsilon_n), \qquad (3)$$

H is the Heaviside step function and ϵ_n is the energy corresponding to the bottom of the nth electric sub-band which can be obtained from equation (1) by putting $\epsilon = \epsilon_n$ and $a_0 = 0$ and the other symbols are defined in Appendix 1.1. Thus, combining equation (3) with the Fermi–Dirac occupation probability factor, the surface electron concentration per unit area can be expressed as

$$N_s = ck_BT\sum_{n=0}^{n_{max}}[\Psi_n]^{-1}[(1+2\alpha\epsilon_n)F_0(\eta_n) + 2\alpha k_BTF_1(\eta_n)], \qquad (4)$$

where k_B is the Boltzmann constant, T is the temperature and the other notations are defined in Appendix 1.1. Equation (4) is the generalized expression of the electron statistics in n-channel inversion layers on Kane-type semiconductors. Incidentally the expressions for the surface concentration under the weak and strong electric-field limits can respectively be expressed, using equation (4), as

$$N_s = ck_BT\sum_{n=0}^{n_{max}}\left[\left(1+\frac{2}{3}\alpha\epsilon_n\right)F_0(\eta_n) + 2\alpha k_BTF_1(\eta_n)\right], \qquad (5)$$

and

$$N_s = ck_BT\sum_{n=0}^{n_{max}}[(1+2\alpha\epsilon_n)F_0(\eta_n) + 2\alpha k_BTF_1(\eta_n)], \qquad (6)$$

where the various notations are defined in subsections 1.2 and 1.3 of the Appendix, respectively.

It may be mentioned in this context that equation (6) has already been derived elsewhere [15]. Thus using equations (4) and (1) we get

$$\frac{D}{\mu} = (N_s/e)[X - Y], \qquad (7)$$

where the notations are defined in Appendix 1.1.

The expressions for the DMR under the weak and strong electric-field limits can respectively be expressed using equation (7) as

$$\frac{D}{\mu} = \frac{k_B T}{e}\left[\frac{\left(1+\frac{2}{3}\alpha\epsilon_0\right)F_0(\eta_0) + 2\alpha k_B T F_1(\eta_0)}{\left(1+\frac{2}{3}\alpha\epsilon_0\right)F_{-1}(\eta_0) + \left(1+\frac{\Theta}{3}\right)2\alpha k_B T F_0(\eta_0)}\right], \qquad (8)$$

and

$$\frac{D}{\mu} = \frac{k_B T}{e}\left[\frac{(1+2\alpha\epsilon_0)F_0(\eta_0) + 2\alpha k_B T F_1(\eta_0)}{(1+2\alpha\epsilon_0)F_{-1}(\eta_0) + (1+\Phi)2\alpha k_B T F_0(\eta_0)}\right], \qquad (9)$$

where the various notations of equations (8) and (9) are defined in subsections 1.2 and 1.3 of the Appendix respectively. It must be noted that equation (9) was derived for the first time A. N. Chakravarti et al. [15].

Besides, for $\alpha \to 0$ as for inversion layers on parabolic semiconductors equations (5) and (8) get simplified into

$$N_s = ck_B T \sum_{n=0}^{n_{max}} F_0(\eta_n) \qquad (10)$$

and

$$\frac{D}{\mu} = \frac{k_B T}{e} F_0(\eta_0)/F_{-1}(\eta_0). \qquad (11)$$

Finally, for $\eta_0 \ll 0$, as for nondegenerate electron concentration, the equations (7), (8), (9) and (11) reduce to the conventional Einstein relation $\frac{D}{\mu} = k_B T/e$ as they should.

III. RESULTS AND DISCUSSION

Using equations (5) and (10) together with parameters [21—23]

$$E_g(x) = [-0.30 + 1.73x + 5.6\times 10^{-4}(1-2x)T + 0.25x^4]\,\mathrm{eV} \qquad (12)$$

$$m_0^*(x) = E_g(x)[0.1m_0] \qquad (13)$$

$$\epsilon_{sc}(x) = [20.262 - (14.812x) + 5.279x^2]\epsilon_0' \qquad (14)$$

where ϵ_0' is the free space permittivity and taking $F_s = 3\times 10^4$ V/m (such that the conditions $K(0) \ll 1$ and $\alpha\epsilon_0 \ll 1$ are fairly satisfied), we have obtained the alloy composition dependence of the DMR in *n*-channel inversion layers on $Hg_{1-x}Cd_xTe$ at 4.2 K under the weak electric field limit as shown in plot a of Fig. 1, in which the same dependence is also plotted by using the generalized expressions, i.e. by using equations (4) and (7) respectively, as shown by plot (b) of the same figure for the purpose of comparison. The simplified limiting case of the DMR in *n*-channel inversion layers on isotopic parabolic energy bands by using equations (10) and (11) has been shown in plot *c* so that the nature of variation of the above ratio for complicated non-parabolic energy bands can be assessed.

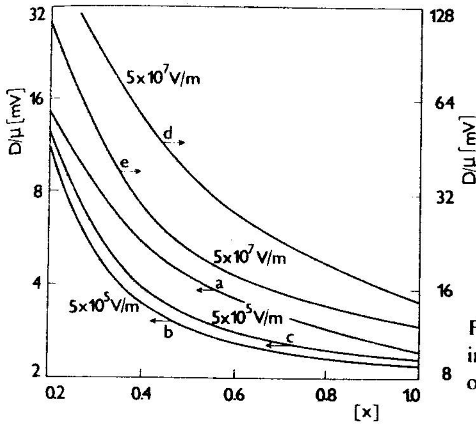

Fig. 1. Dependence of the DMR of the carriers in *n*-channel inversion layers on $Hg_{1-x}Cd_xTe$ on the alloy composition at 4.2 K under various physical conditions.

Thus following the same procedure and taking the parameters as used in a weak field case together with $F_s = 6\times 10^8$ V/m (such that the conditions $K(0) \gg 1$ and $\alpha\epsilon_0 \gg 1$ are fairly satisfied), we have determined the same dependence by using the equations (6) and (9) under the strong field limit as shown in plot d in Fig. 1, in which the same dependence is also plotted by using the generalized expressions as shown by plot e. In Fig. 2, the surface electric field dependence of the DMR has been shown for various cases for $x = 0.26$. It appears from the figures that the DMR decreases with increasing alloy composition and decreasing surface electric field, though the rates of variations are different in different plots of figures 1 and 2 respectively.

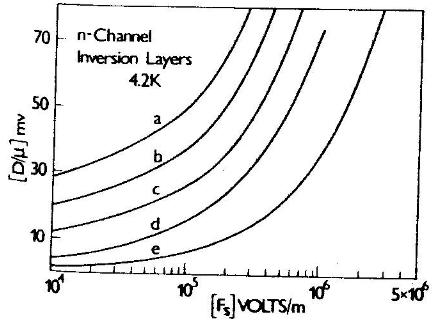

Fig. 2. Dependence of the DMR of the carriers in *n*-channel inversion layers on $Hg_{1-x}Cd_xTe$ on the surface electric field at 4.2 K under various conditions.

Besides, though the theoretical formulation is valid for the band Kane model, our present numerical computation is valid for $x > 0.17$ since for $x < 0.17$ the band-gap becomes negative in $Hg_{1-x}Cd_xTe$ leading to the semi-metallic state. It may be remarked that the theoretical studies covered in this paper are based on the following two assumptions:

(i) The profile of the potential well at the oxide-semiconductor interface has been assumed to be triangular for the calculation of the energy eigenvalue and,

(ii) in the theoretical calculations, the condition of the electric quantum limit has been considered. Under this condition the Fermi level is below the lower edge of the second electric subband so that only one subband is occupied by the electrons [2].

The approximation of the potential well at the surface by a triangular well introduces some errors, as, for instance, the omission of the free charge contribution to the potential. This kind of approach is reasonable if there are only few charge carriers in the inversion layers but is responsible for an over estimation of the splitting when the inversion carrier density exceeds that of the depletion layer. But it is observed that the maximum error due to the triangular potential well approximation is tolerable in a practical sense, as for the actual calculation one needs a self-consistent solution which is very difficult for non-parabolic energy bands without exhibiting a widely different qualitative behaviour. The second assumption of the electric quantum limit is valid in the range of low temperatures. Thus, whenever the condition of an electric quantum limit has been applied, the temperature has been assumed to be low enough so that the above assumption becomes well grounded, because at low temperatures where the quantum effects become prominent one can assume that nearly all the electrons are on the lowest electric subbands [24]. Though the hot-electron effect, the formation of band-tails and the effect of electron-electron interactions have not been considered in this simplified analysis, the basic qualitative features of this theoretical formulation will not alter significantly even after the necessary above modifications. It may also be noted that, since the available noise power is directly proportional to the DMR as discussed elsewhere [25], the experimental results on the thermal noise of degenerate semiconductors will provide an experimental check for the predictions of the above ratio and also a technique for probing the band structure in degenerate semiconductors. Finally, it may be stated that the basic purpose of the present paper is not solely to demonstrate the effect of the alloy composition on the DMR in n-channel inversion layers on Kane-type semiconductors, but also to formulate the generalized density-of-states function since the various transport phenomena and the analytical formulation of different important physical parameters are based on the density-of-states function in such materials.

APPENDIX

1.1. The symbols c, $\varphi(w_0, a_0)$, Ψ_n, $F_j(\eta_n)$, X and Y are defined as follows:

$$c = m_0^*/\pi h^2 \tag{1.1a}$$

$$\varphi(w_0, a_0) = \left\{w_0^2 - \left\{w_0\left(a_0 + \frac{1}{4}\right)\right\}^{-1} \{2k(n)\sqrt{1 + w_0^2}\}\right\} \tag{1.1b}$$

$$\Psi_n = [\ln(G_n + \sqrt{1 + G_n^2})]/[G_n(1 + G_n^2)^{-1/2}] \tag{1.1c}$$

$$F_j(\eta_n) = (\sqrt{j + 1})^{-1} \int_0^\infty t^j[1 + \exp(t - \eta_n)]^{-1}\,dt \tag{1.1d}$$

$$X = k_B T \delta \Psi_0[(1 + 2\alpha\epsilon_0) F_{-1}(\eta_0) + 2\alpha k_B T F_0(\eta_0)]^{-1} \tag{1.1e}$$

$$Y = [2K(0)\sqrt{1 + G_0^2}][\alpha G_0(1 + 2\alpha G_0)]^{-1}, \tag{1.1f}$$

where

$$G_n \equiv 4\alpha\epsilon_n(1 + \alpha\epsilon_n), \qquad \eta_n \equiv (k_B T)^{-1}(E_F - \epsilon_n),$$

$$\delta \equiv (ck_B T)^{-1} + Z(\Psi_0)^{-1}[(\Psi_0)^{-1} - 2\alpha F_0(\eta_0) - (k_B T)^{-1} \times$$
$$\times \{2\alpha k_B T F_0(\eta_0) - (1 + 2\alpha\epsilon_0) F_{-1}(\eta_n)\}],$$

$$Z = 4k(0) G_0^{-2}(1 + G_0^2)^{1/2}[G_0^{-1} - \Psi_0(G_0)^{-1} + \Psi_0 G_0(1 + G_0^2)^{-1}],$$

j is the set of set numbers and t is a dummy variable.

1.2. The symbols ϵ_n and Θ for weak electric field limit are defined as follows:

$$\alpha\epsilon_n(1 + \alpha\epsilon_n) - \left(\alpha\epsilon_n + \frac{1}{2}\right)^{2/3}[3K(n)]^{2/3} = 0 \tag{1.2a}$$

and

$$\Theta = (A_1 A_2 - 1)^{-1}, \tag{1.2b}$$

where

$$A_1 \equiv \frac{3}{2} N_S^{1/3}\left(1 - \frac{2}{3}\alpha\epsilon_0\right) D_0^{-1}, \qquad D_0 \equiv \left(\frac{3}{2} A_0\right)^{2/3},$$

$$A_0 \equiv (3/4)(\pi e^2/\epsilon_{sc})(\hbar^2/2m_0^*)^{1/2},$$

$$A_2 \equiv \left[(\pi h^2/m_0)(1 + \Delta)\left[\left(1 + \frac{2}{3}\alpha\epsilon_0\right) F_{-1}(\eta_0) + 2\alpha k_B T F_0(\eta_0)\right]^{-1}\right],$$

$$\Delta = [2m_0^*\epsilon_0(1 + \alpha\epsilon_0)/3\pi\hbar^2 N_s I]\left[\left(1 + \frac{2}{3}\alpha\epsilon_0\right) F_{-1}(\eta_0) + \frac{4}{3}\alpha k_B T F_0(\eta_0)\right]$$

and

$$I = \left[1 + 2\alpha\epsilon_0 - \frac{4}{3}\alpha\epsilon_0(1 + \alpha\epsilon_0)(1 + 2\alpha\epsilon_0)^{-1}\right].$$

1.3. The symbols ϵ_n and φ for a high-electric field limit are defined as follows:

$$\epsilon_n = (2\alpha)^{-1}\{-1 + \sqrt{1 + 8K(n)}\} \tag{1.3a}$$

and

$$\varphi = (\beta_1 \beta_2 - 1)^{-1}, \tag{1.3b}$$

where

$$\beta_1 = (2A_0\sqrt{\alpha})^{-1}(1 + 2\alpha\epsilon_0)$$

and

$$\beta_2 = \frac{\pi h^2}{m_0^*}\left[1 + 2A_0\sqrt{\alpha}\cdot\frac{m_0^*}{\pi h^2} F_{-1}(\eta_0)\right][(1 + 2\alpha\epsilon_0) F_{-1}(\eta_0) + 2\alpha k_B T F_0(\eta_0)]^{-1}.$$

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О СООТНОШЕНИЯХ ЭЙНШТЕЙНА В *n*-КАНАЛОВЫХ ИНВЕРСИОННЫХ СЛОЯХ НА ТЕРНАРНЫХ ПОЛУПРОВОДНИКАХ

Сделана попытка вывести обобщенные выражения для соотношений Эйнштейна в *n*-каналовых инверсионных слоях на тернарных полупроводниках, не прибегая к приближениям слабых или сильных электрических полей. На примере *n*-каналовых инверсионных слоев на $Hg_{1-x}Cd_xTe$ показано, что то же отношение плавно уменьшается при возрастании сплавового состава и уменьшении поверхностного электрического поля. Наряду с этим получены соответствующие результаты для инверсионных слоев на параболических полупроводниках.