

Novel electron mobility model for n-HgCdTe

S.D. YOO^{1*}, B.G. KO¹, G.S. LEE¹, J.G. PARK¹, and K.D. KWACK²

¹Advanced Semiconductor Material and Device Development Center, Hanyang University
Seoul 133-791, Korea

²Department of Electronic Engineering, Hanyang University, Seoul 133-791, Korea

In the conventional simulations for HgCdTe device, the empirical mobility model is used which lacks in generality. Especially, the field dependent mobility is found to be wrong by comparing Monte Carlo results. The semi-empirical electron mobility model for the simulator is proposed in this paper. Low field mobility consists of two terms related to ionised impurity and phonon scattering. It is calculated by using the relaxation time approximation, which gives the information on the dominant factors affecting the mobility. The ionised impurity mobility model is modified based on Brooks-Herring model to include the degeneracy effect and overlap integral. For field dependent mobility, a new formula is proposed to take into account features of the dominant scattering mechanism such as nonparabolic relation between energy and wave function at high field. Final formula is accomplished by introducing fitting parameters extracted from Monte Carlo simulation results. This new model retains more physical meaning than conventional model.

Keywords: HgCdTe, electron mobility, semi-empirical mobility model, field dependent mobility, relaxation time approximation.

1. Introduction

The study on HgCdTe has been concentrated on the material growth for many years, which makes it possible to realising various devices for infrared detectors. As for improving performance of the conventional device and exploiting new application areas, the computer simulation has an advantage in the view of cost and time. There are many commercial and in-house simulators all over the world. Most of the commercial tools are developed for Si and GaAs. It is, therefore, said that the commercial tools have drawbacks in analyzing HgCdTe photodetectors since those do not include the features of HgCdTe such as large nonparabolic factor and complex defect states. As a consequence, in-house tools are desirable for HgCdTe.

There are basic parameters which should be predefined in the numerical simulator. They contain mobility, effective mass, effective density of states, lifetime, and so forth. HgCdTe is characterised by small

band gap, large nonparabolic conduction band, and small electron effective mass. The conduction band is, then, easily degenerated. Those are the obstacles that render the calculation of carrier concentration hard to perform analytically. Many workers have devoted their efforts on the calculating the carrier concentration [1,2] and develop the expression [3,4]. As the mobility is closely related to scattering mechanism, the dominant scattering mechanism and its dependencies should be identified. That is why mobility calculation is much more difficult than the carrier concentration calculation. We face those problems to be solved for utilizing the numerical simulator.

This work aims to develop a mobility model for the simulator. The mobility must show the dependency of external environment such as doping profile and bias as well as that of internal functions such as potential or quasi-Fermi energy and carrier concentrations. It is the most important requirement that the first order derivative of the mobility over the variables of carrier concentration and potential should be continuous to ensure the convergence. The first principle of the mobility modeling is the theoretical approach based on the mi-

*e-mail: sangdy@shira.hanyang.ac.kr

macroscopic movement of the carriers. This can predict the effect of each scattering mechanism and scattering parameters on the mobility. Though this method retains physical meaning and shows the dependency of the external and internal variables, the result usually deviates from the experimental data. Furthermore, its formula is too complicated to use in the simulator. When an obscure mechanism or unknown parameters exist, the difference grows. The empirical method is more practical since it is based on real experimental data. The ultimate mobility formula modeled by this method is in a simple form and shows the macroscopic or external dependency clearly. If the experimental data of the samples exhibit large dispersion, this method loses its usefulness. There can be another method called semi-empirical method, in which the merits of two methods are combined by modifying the empirical model to consider the microscopic phenomena. Minute changing of the parameter value is required to predict and fit the experimental data, which is the attractive thing of this approach.

In the conventional numerical simulation [5,6] the empirical formula based on the Scott's data [7] has been commonly used. To consider the doping density effect the ionised impurity scattering mobility is added to the formula, which is developed from the relaxation time approximation (RTA). For the field dependent mobility the electron temperature model is adopted, where the electron temperature is calculated as a function of the field. In the case of conventional HgCdTe device simulation, it has been assumed that the dominant scattering mechanism responsible for energy exchange is acoustic phonon scattering. The acoustic phonon scattering is, however, known as having little roles on the mobility. Our approach follows the conventional one but propose a new mobility model which is more practical and capable of including HgCdTe features.

2. Mobility formulation

The mobility can be calculated using RTA [3]

$$\mu = \frac{e}{m_e^*} \langle \tau_m \rangle \quad (1)$$

$$\langle \tau_m \rangle = \frac{2 \int_{-\infty}^{\infty} \tau_m \frac{\gamma^{3/2}(E)}{(1+2\alpha E)} \Delta_E f_0 dE}{3 \int_{-\infty}^{\infty} f_0 \sqrt{\gamma(E)} (1+2\alpha E) dE} \quad (2)$$

where e , m_e^* , and α denote the electron charge, electron effective mass, and nonparabolic factor, respec-

tively. $\gamma(E)$ represents the nonparabolic relation between the electron energy E and the electron wave vector k . The expression of nonparabolic factor and electron effective mass can be obtained from $\mathbf{k} \cdot \mathbf{p}$ method [8], τ_m is total momentum relaxation time

$$\frac{1}{\tau_m} = \sum_i \frac{1}{\tau_{mi}} \quad (3)$$

where τ_{mi} is the momentum relaxation time for i -th scattering mechanism. The scattering mechanisms considered are due to ionised impurity, alloy, polar optic phonon (POP), electron-hole, and neutral impurity. Equation (2) includes the nonparabolic conduction band, velocity degradation as electron energy increases, and band degeneracy.

The electron mobility calculated by RTA fits well with experimental data both in n-type and in p-type HgCdTe [8,9]. But, the relaxation time associated with each scattering mechanism has its own energy dependent, which leads the mobility formula being too complex to use in numerical simulator. What RTA calculation provides for mobility modeling is information on the dominant scattering mechanism affecting mobility and its dependency on temperature, mole fraction, and doping density. At below 50 K, the impurity scattering prevails over all other scatterings, while at above 100 K the polar optic phonon scattering is dominant. In the intermediate temperature ranges, alloy scattering has an influence on the mobility along with the POP and ionised impurity scattering. In the view of electron energy, high POP scattering rate is shown at higher energy region. Ionised impurity scattering rate is high at low energy region and is comparable to POP scattering rate at high-energy region.

3. Conventional model and drawbacks

There is a mobility formula widely used in numerical simulation [5,6]. It consists of low field mobility and field dependent mobility. For low field mobility, the following formula has been used

$$\frac{1}{\mu_0} = \frac{1}{\mu_{ii}} + \frac{1}{\mu_{other}} \quad (4)$$

where μ_{ii} represents the mobility by ionised impurity scattering and μ_{other} is for other scattering mechanisms, such as POP, alloy, and defects.

For ionised impurity scattering mobility, Brooks-Herring (BH) model has been used [10]

$$\mu_{ii}^{BH} = \frac{64\epsilon_0\epsilon_s(2k_B T)^{3/2}}{Z^2 e^3 N_I} \sqrt{\frac{\pi}{m_e^*} g_{BH} \left(\frac{24\pi\epsilon_0\epsilon_s(2k_B T)^2}{e^2 \hbar^2 (n+p)} \right)}, \quad (5)$$

where

$$g_{BH}(x) = \frac{1}{\ln(1+x) - x/(1+x)}. \quad (6)$$

The $g_{BH}(x)$ term related to scattering angle dependent varies slowly with energy under the above assumptions. \hbar is the reduced Planck constant. ϵ_0 and ϵ_s represent permittivity in free space and relative static dielectric constant, respectively. k_B is the Boltzmann constant, T is the lattice temperature, N_I is the ionised impurity density acting as scattering center, and Z the ionised degree of the impurity. n and p are the electron and hole concentrations, respectively. It is worth to note the assumptions underlying in developing the formula. First of all, the conduction band is assumed as parabolic band. In addition, the band is nondegenerated, which allows us to use Maxwell-Boltzmann statistics. The term is, then, to be located out of the integral in Eq. (2) with the energy $E_{avm} = 3k_B T$ at which the integrand is maximised [11].

The conduction band of HgCdTe is highly nonparabolic. Since HgCdTe is easily degenerated, the integral becomes complex Fermi integral function. Furthermore, the energy in the out-located angle dependent term is not equal to $3k_B T$ due to nonparabolic band effect. Therefore, the assumptions made in the conventional model are no longer valid for HgCdTe.

For the second term in low field mobility μ_{other} , the following formula has been used

$$\mu_{other} = \frac{9 \times 10^8 b}{T_T^{2a}}, \quad (7)$$

where

$$a = \left(\frac{0,2}{x}\right)^{0.6}, \quad b = \left(\frac{0,2}{x}\right)^{0.75}, \quad (8)$$

x denotes Cd mole fraction, and T_T is given by

$$T_T = \frac{118 \times 10^5}{2600 - |T - 35|^{2.07}} \quad (T < 50 \text{ K}) \quad (9)$$

$$T_T = T \quad (T \geq 50 \text{ K}). \quad (10)$$

They are obtained from Scott's Hall measurement data [7]. For $T < 50 \text{ K}$, it represents defects and native doping effects on the mobility. The expression for $T \geq 50 \text{ K}$ explains the phonon and alloy scattering effects. The samples have about $2 \times 10^{15} \text{ cm}^{-3}$ impurities [7]. So, it can be said that Eq. (9) can not be applied to other samples with different density. As a consequence, the formula lacks in generality.

The field dependent mobility has been widely used in the conventional simulation in the following form

$$\mu_f = \mu_o \sqrt{\frac{T}{T_e}}, \quad (11)$$

where

$$\frac{T_e}{T} = \frac{1}{2} + \frac{1}{2} \left[1 + \frac{3\pi}{8} \left(\frac{\mu_o E}{C_s} \right)^2 \right]^{1/2}. \quad (12)$$

Here μ_o is the low field mobility, C_s is the longitudinal sound or acoustic velocity being $2.8 \times 10^5 \text{ cm/s}$, E is the electric field strength, and T_e is the electron temperature. Equation (11) implies that dominant scattering mechanism depends on $E^{1/2}$. Equation (12) is developed for the case that acoustic phonon scattering is responsible for the energy exchange at high fields. Figure 1 shows electron mobility and temperature as a function of electric field. Since few experimental data for field dependent mobility is available, the mobility calculated with the formula compares with Monte Carlo (MC) simulation result. MC data shows well-known behaviour of mobility and electron temperature. Electron mobility and temperature are in the equilibrium state at low field. Further increase in electric field strength results in higher electron energy and electron temperature. The mobility decreases from the electric field at which electron energy increases. The conventional mobility, however, is continuously reduced as electric field increases as shown in Fig. 1(a). What we concern is not the value of low field mobility but its slope. The conventional model shows gentle slope while MC results have steep slope. Fig. 1(b) shows that the electron temperature of the conventional model increases continuously and is higher in the value than that in MC results. From those two figures, we find that the simple $-1/2$ power of the electron temperature can not predict the field dependent mobility. Furthermore, the electron tem-

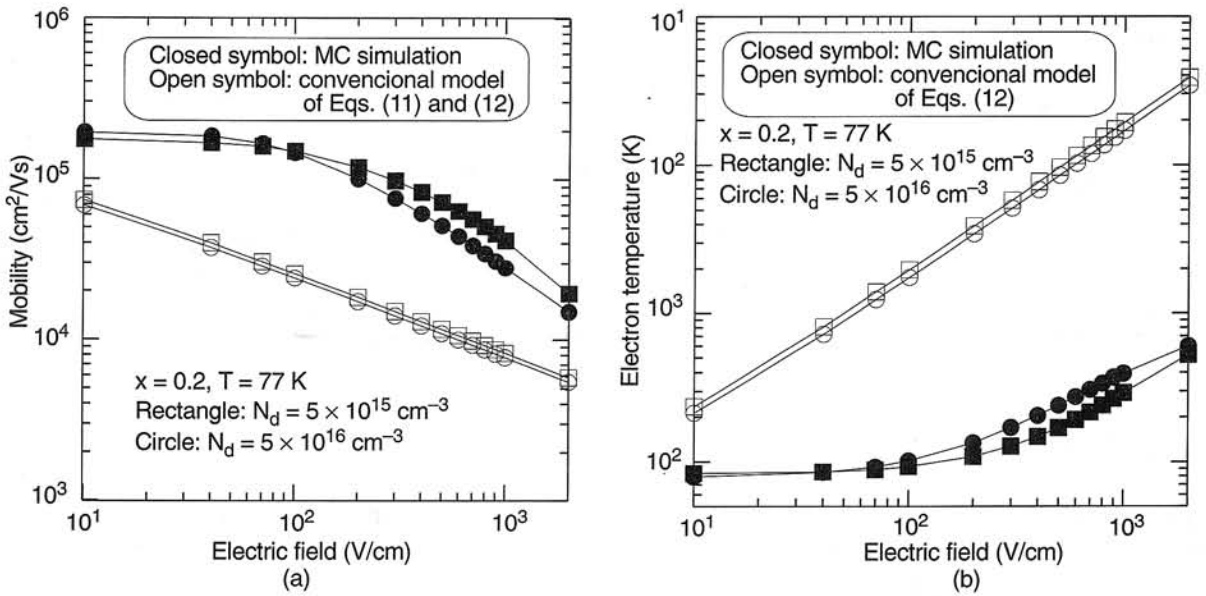


Fig. 1. Electron mobility (a) and electron temperature as a function of electric field (b).

perature behaviour with electric field can not be described by equation (12).

4. New model

A new model is required since the approximations underlying in the conventional model are proved to be invalid for HgCdTe. For impurity scattering mobility in the low field model, the band effects of non-parabolicity and degeneracy should be taken into account. The relaxation time for ionised impurity scattering is calculated by using BH model. Some assumptions have made to formulate the mobility. At first, overlap integral is assumed as a slowly varying function with the energy as in conventional model, which allows it to be out of the integral. Secondly, because ionised impurity scattering is dominant at low energy region, the nonparabolic relation can be reduced to parabolic relation. It results in more simple expression of the integral. With the reduced energy and the fact of electron temperature being equal to lattice temperature at low field, $\eta = E/k_B T$, the mobility can be given by

$$\mu_{ii} \equiv \frac{64 \epsilon_o^2 \epsilon_s^2 m_e^* (k_B T)^3}{3 \pi \hbar^3} \frac{1}{N_I e^3 n} \frac{1}{O_{io}(x)} \int \eta^3 \frac{\partial f}{\partial \eta} d\eta \quad (13)$$

$$= \frac{64 \epsilon_o^2 \epsilon_s^2 m_e^* (k_B T)^3}{3 \pi \hbar^3} \frac{1}{N_I e^3 n} \frac{1}{O_{io}(x)} \Gamma(4) F_2(\eta), \quad (14)$$

where n comes from the denominator of Eq. (2). It is calculated according to Ref. 12. O_{io} is the overlap integral

$$O_{io} = O_{io}^{BH} + O_{io}^{npe}. \quad (15)$$

O_{io}^{BH} is the same form as the denominator of $g_{BH}(x)$, and O_{io}^{npe} appears due to nonparabolic band

$$O_{io}^{BH} = \ln(\zeta + 1) - \frac{\zeta}{\zeta + 1}, \quad (16)$$

$$O_{io}^{npe} = -2(B + 2C) \left[1 + \frac{2}{\zeta} \ln(\zeta + 1) + \frac{\zeta}{\zeta + 1} \right] + 2C \left[1 - \frac{4}{\zeta} + \frac{6}{\zeta^2} \ln(\zeta + 1) - \frac{2}{\zeta(\zeta + 1)} \right] \quad (17)$$

The coefficients B and C are related to the band structure, which are the function of the electron energy [8]. And, $\zeta = 4k^2 \lambda^2$, where λ is screening length [13]. The screening length is to be Debye length when the conduction band is parabolic and nondegenerate, which is used in conventional model. The energy in out-located O_{io} is determined at which the integrand is maximized.

$$\eta = \frac{\eta_e + 3 \pm \sqrt{(\eta_e - 3)^2 + 48}}{2}, \quad (18)$$

where $\eta_e = E/k_B T_e$. The minus term is discarded because it can lead the negative energy. The η obtained

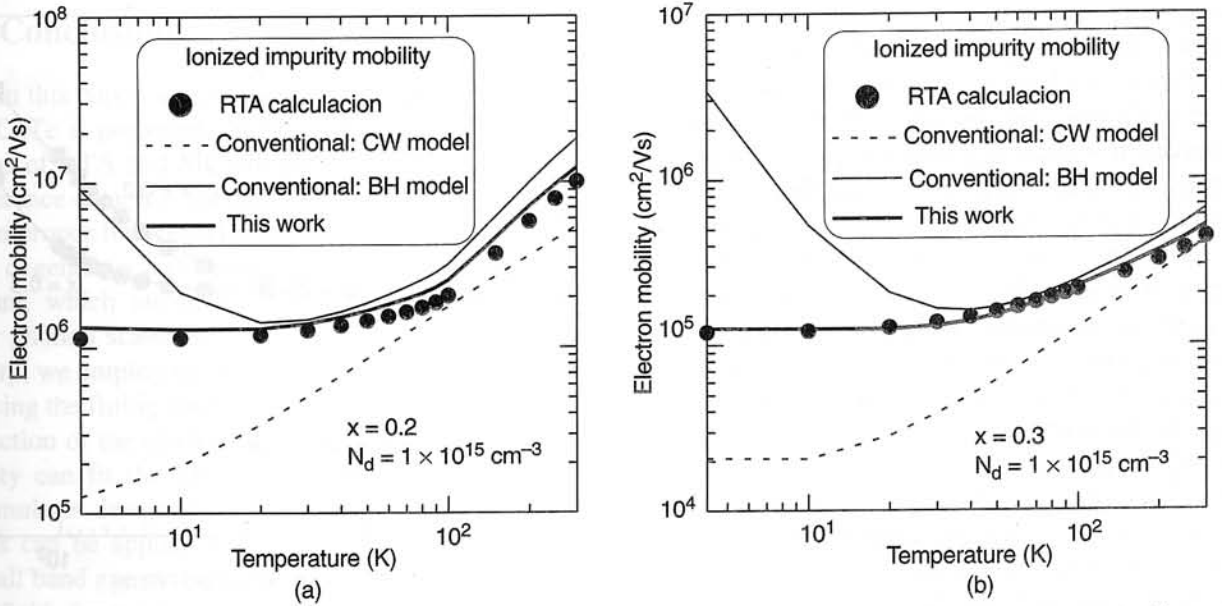


Fig. 2. Electron mobility as a function of temperature: (a) 0.2, and (b) 0.3 Cd mole fraction with $N_d = 1 \times 10^{15} \text{ cm}^{-3}$.

from Eq. (18) gives reasonable values for both the strong degenerate and nondegenerate cases.

Figure 2 shows the calculated results according to the ionised impurity models. At low temperature, where the band is heavily degenerated, the curves of conventional models largely deviate from those of RTA formula. In the intermediate temperature range where HgCdTe is operated, the BH model is close to the RTA calculation. The difference is observed again at high temperature, where the band becomes nondegenerate. It is thought that the difference is originated from nonparabolic band effect. For the higher

doping density the BH model deviates largely from RTA calculation. As the mole fraction increases, the band becomes less nonparabolic. The degree of discrepancy is reduced except BH model at low temperature. When the value of x in $g_{BH}(x)$ is small, g_{BH} becomes infinite since the denominator goes to 0. That is the demerit of BH model. The proposed model gives relatively good results for all temperature ranges. The figure indicates that the conventional model can not predict the ionised impurity mobility for all cases.

For the term μ_{other} in the low field mobility, the conventional formula of Eq. (10) is used for overall

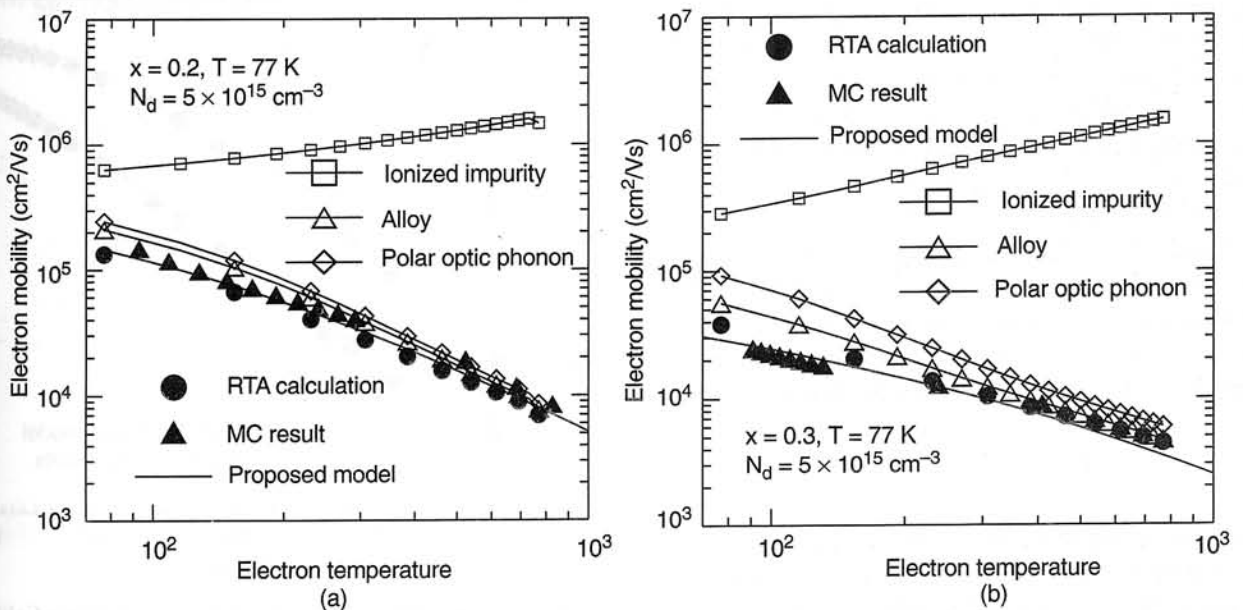


Fig. 3. Electron mobility as a function of electron temperature, (a) for $x = 0.2$, and (b) $x = 0.3$.

temperature in this work. The defect related mobility can be explained by the ionised impurity scattering mobility if the characteristics of the defect is well defined [8,9]. And, because at the high temperature the dominant scattering is phonon scattering which is independent on the doping density, the conventional formula is adequate.

The modeling process for field dependent mobility begins with changing formula as a function of the electron temperature. Solving the energy balance equation, then, follows to get the relation between electron temperature and electric field. For the first step, the dominant scattering mechanism in high field should be specified to determine the energy dependency of mobility. Fig. 3 represents the electron mobility as a function of electron temperature for the mechanisms which scattering rates are high. For n-HgCdTe, ionised impurity, alloy, and polar optic phonon scattering are in high scattering rate at high energy. Ionised impurity is an elastic scattering, and proportional to temperature. So, its contribution to the high field mobility is negligible. Alloy and polar optic phonon show identical trend on the temperature because they have the same energy dependency of $\gamma^{1/2}(E)(1 + 2\alpha E)$. From the inspection of the scattering mechanism the field dependent mobility is formulated as

$$\mu_f = \frac{\mu_o}{a_{mf}\alpha k_B \sqrt{T_e(1 + b_{mf}\alpha k_B T_e)} \times (1 + 2b_{mf}\alpha k_B T_e)} \quad (19)$$

The parameters of a_{mf} and b_{mf} are introduced to represent the energy and electron temperature relation. If the conduction band is parabolic, the formula becomes the conventional one, Eq. (11). In the figure the RTA calculation considering all scattering mechanisms and MC results are also shown. The value of the coefficient b_{mf} is not varied as the doping density and mole fraction. b_{mf} is to be 2.74. a_{mf} is 2 for the case of $x = 0.2$ and 6 for $x = 0.3$.

Though the electron temperature is a function of electric field, the formula is not obtained easily by solving energy balance equation because of the non-parabolic band effect. In this work, the relation is obtained by fitting the MC results as shown in Fig. 4

$$T_e = T + a_{te}E + b_{te}E^2 \quad (20)$$

The second and third terms are for warm and hot electrons, respectively. The coefficients of a_{te} and b_{te} are a function of the low field mobility. a_{te} is found to be 0.18484 for the case of $x = 0.2$ and 0.0152131 for

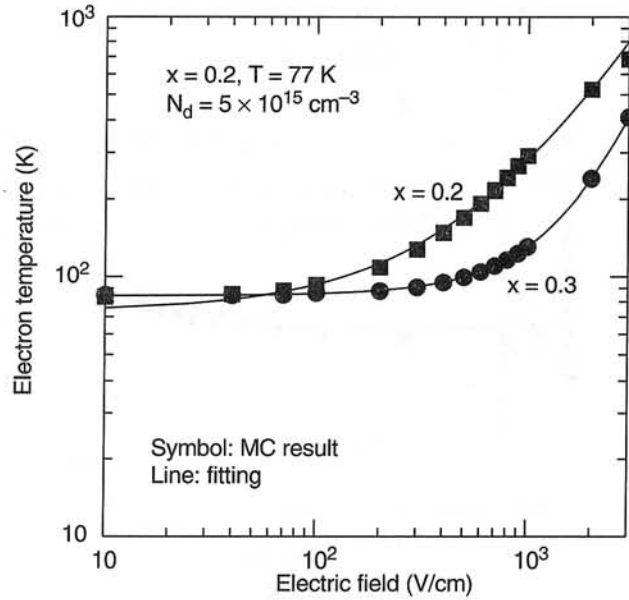


Fig. 4. Electron temperature as a function of electric field.

$x = 0.3$. b_{te} is 1.97817×10^{-5} for $x = 0.2$ and 3.10955×10^{-5} for $x = 0.3$. In the electric field range of the figure, the second order polynomial fitting is sufficient. At low mole fraction the second order term has negligible effect. Then, the conventional formula of Eq. (12) can be used by changing the proportional constant. But, at the high mole fraction the second term has an influence. Drift velocity of $v_d = \mu_f E$ is in well agreement with MC data as shown in Fig. 5. The figure certifies the formulation of field dependent mobility being appropriate.

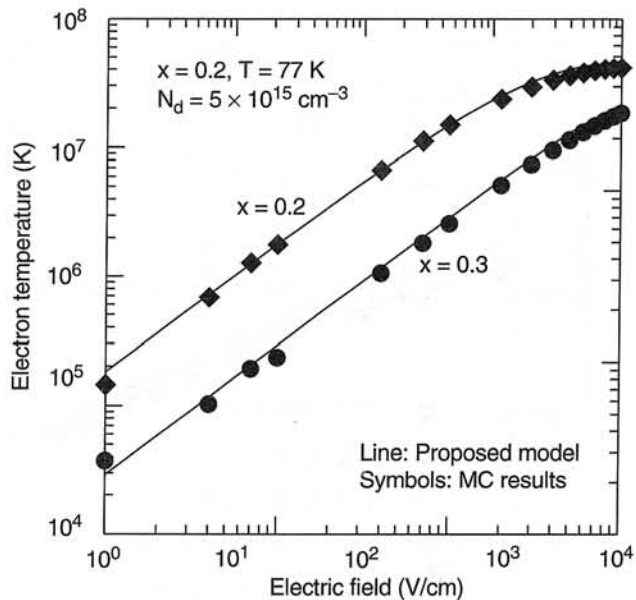


Fig. 5. Electron drift velocity as a function of electric field.

5. Conclusions

In this paper, a new model of electron mobility for HgCdTe is proposed. At first the theoretical calculations of RTA and MC are performed to provide as a reference data. It is found that the conventional model is improper for HgCdTe. For ionised impurity mobility, degeneracy and overlap integral are taken into account, which are neglected in conventional model. For phonon scattering related terms in low field mobility, we employ the previously used form. By introducing the fitting formula of electron temperature as a function of the electric field, the field dependent mobility can fit the MC results. Though the proposed formula is designed for HgCdTe, the modeling process can be applied to other materials, especially to small band gap material. There is something to do left in field dependent mobility. The real experimental data is not available for the drift mobility. It implies that the fitting parameters should be carefully chosen. Especially, the form of Eq. (20) should be testified under the higher fields. And, the physical properties are separated from the parameters. We think low field mobility is fairly good but field dependent mobility needs more inspection on the parameters.

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