Journal of Electron Devices, Vol. 15, 2012, pp. 1236-1240

Journal of Electron Devices
www.jeldev.org

MONTE-CARLO STUDY OF VELOCITY-FIELD CHARACTERISTICS AND TERAHERTZ GENERATION IN CdSe

Aniruddha Ghosal[1] and Arindam Biswas[2]
[1]Institute of Radio Physics and Electronics, University of Calcutta, 92 A.P.C. Road, Kolkata- 9.
[2]Dumkal Institute of Engineering and Technology, WBUT, Dumkal, Murshidabad, Pin-742406.
mailarindambiswas@yahoo.co.in

Received 29-08-2012, online 31-08-2012

ABSTRACT

Velocity-field characteristics of CdSe at different lattice temperatures, namely, 20K, 50K, and 77K have been theoretically investigated by solving the Boltzmann transport equation with the help of one-particle Monte-Carlo simulation. The deformation potential acoustic phonon, polar optical phonon, impurity and intervalley phonon scatterings have been incorporated in our analysis. The velocity-field curves of the electrons show a Negative Differential Resistance (NDR) effect at low electric fields for the lattice temperatures considered. Based on the NDR effect the self-oscillating frequencies of CdSe diodes of micron dimensions are calculated from the peak drift velocity of the electrons at 20K, and are found to be in the Terahertz frequency range. The variation of mobility with temperature has also been exhibited.

Keywords: Monte-Carlo Simulation, Polar Optical Phonon Scattering, Negative Differential Resistance.

I. INTRODUCTION

Electron transport in CdSe has received considerable attention in recent years due to the wide spectrum technological applications of the material in optoelectronic devices [1-6]. The high field and high frequency devices made from CdSe show promise for good performance characteristics due to its wide band gap [7].

The Monte-Carlo method is an age-old one which has been extensively used to obtain the velocity-field characteristics of various compound semiconductors [8]. Literature survey reveals that the velocity-field characteristics of bulk CdSe have not been studied in detail by any worker using the Monte Carlo simulation. So the authors have used the Monte Carlo method for solving the Boltzmann transport equation to obtain the velocity-field characteristics of CdSe, incorporating the various scattering processes, namely, the deformation potential acoustic phonon, polar optical phonon, impurity and intervalley phonon scatterings in the computations. The effect of screening due to the charge carriers has also been taken into account. The Monte-Carlo simulation has the merit that it provides a nearly exact solution of the Boltzmann transport equation by treating accurately the hot electron effects which cannot be accomplished by the drift diffusion models[9]. We have done the calculations at low temperatures as it is observed that in CdSe no perceptible change in the mobility value occurs with the applied electric field at room temperature [10-11].

II. THEORETICAL MODEL :

We have used the Monte-Carlo method to study the motion of one electron in momentum space encountering a large number of lattice scattering processes. The procedure used for following the motion of an electron requires random numbers to represent the time which the electron drifts before being scattered, and to represent the final state after the scattering event [8]. The probability distribution of these random numbers is correlated with the electric field strength and transition probabilities of the various scattering processes. A uniformly distributed random number r_1 between 0 and 1 is generated to calculate the time t for which the electron drifts freely in the applied field before being scattered. The random number r_1 is expressed as [8] :

$$r_1 = 1 - \exp[-\int_0^t \lambda[k(t^{'})dt^{'}]] \qquad (1)$$

where $k(t^{/}) = k_0 + eEt^{/}/\hbar$, k_0 is the wave vector at t = 0 at the beginning of the flight, E is the applied electric field and λ (k) is the total transition rate from the state k due to all the scattering mechanisms. The type of scattering is determined by a second random number r_2 uniformly distributed between 0 and 1 and satisfying the inequality

$$r_2 < \sum^{m} \frac{\lambda_q(k)}{\Gamma} \qquad (2)$$

for all m. The value of Γ is chosen greater than the maximum value of λ (k). Two more random numbers r_3 and r_4 are required to determine the final state after the scattering. The drift velocity of the electron is calculated from the following expression

$$v = \frac{\sum E_f - E_i}{[\hbar \sum (k_{zf} - k_{zi})]} \qquad (3)$$

where k_{zf} and k_{zi} are the initial and final values of the wave vector for a particular flight, E_f and E_i are the final and initial energies of the electron, and Σ represents the summation over all electron free flights. The authors have taken 15,000 collisions in order to obtain convergent results.

The scattering rate for polar mode scattering in parabolic band approximation is given in accordance with [8] as

$$\lambda_{po}(k) = \frac{e^2 m^{*1/2} \omega_0}{4\sqrt{2}\pi\hbar \in_0}\left(\frac{1}{k_\infty} - \frac{1}{k_0}\right) E^{\frac{1}{2}} \times F_0(E, E^{'}) H \begin{cases} N_0 \,(absorption) \\ (N_0+1)(emission) \end{cases} \qquad (4)$$

where $$E^{'} = \begin{cases} E + \hbar\omega_0 \,(absorption) \\ E - \hbar\omega_0 \,(emission) \end{cases} \qquad (5)$$

$$F_0(E, E^{'}) = \ln \left| \frac{E^{\frac{1}{2}} + E^{'\frac{1}{2}}}{E^{\frac{1}{2}} - E^{'\frac{1}{2}}} \right| \qquad (6)$$

The factor H is unity for absorption and is equal to the Heavyside unit function H (E-$\hbar\omega_o$) for emission.The angle β between the initial state **k** and the final state **k′** has been obtained from the angular probability distribution $P_A(\beta)$ given in [8]:

$$\cos\beta = \frac{[(1+f)-(1+2f)^r]}{f} \qquad (7)$$

where $f = 2(E,E^{'})^{\frac{1}{2}}(E^{\frac{1}{2}} - E^{'\frac{1}{2}})^{-2}$ (8)

and r is the random number uniformly distributed between 0 and 1.We have included in our calculations the expressions for deformation potential acoustic phonon scattering, ionized impurity scattering and inter valley scattering as given in [8].

III. RESULTS AND DISCUSSION

The effective mass of the electrons for CdSe is taken as $m^* = 0.12m_0$, where m_0 is the rest mass of the electron. The other parameter values of CdSe used in our computations, are taken from the references [6].

Table 1. Materical parameters of CdSe used in the calculations

Parameters	Values
Static dielectric constant	9.4
Optic dielectric constant	6.1
Longitudinal elastic constant	7.37×10^{10} Nm^{-2}
Transverse elastic constant	2.459×10^{10} Nm^{-2}
Acoustic deformation potential constant	3.7 eV
Piezoelectric tensor component for parallel mode scattering	3.37×10^{9} Vm^{-1}
Piezoelectric tensor component for perpendicular mode scattering	2.36×10^{9} Vm^{-1}
Polar LO phonon temperature	303 K

Figure 1 shows the computer simulated results of velocity versus electric field for electrons at lattice temperatures of 20K, 50K, and 77K respectively.

It is found that at low electric fields there is an usual increase of velocity but as the field reaches about 5 kV/m, then velocity starts decreasing for all the temperatures showing an NDR effect. This may be attributed to the inter valley scattering effect of the electrons from low effective mass high mobility central valley to the high effective mass low mobility higher satellite valleys.

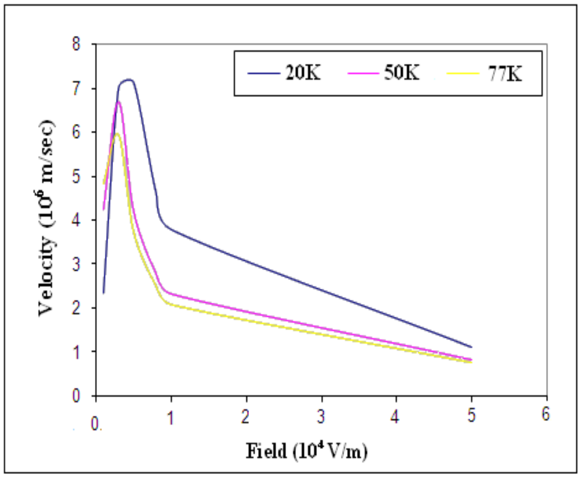

Fig.1: Velocity-field characteristics of CdSe at lattice temperatures of 20K, 50K and 77K.

The peak drift velocity is higher at lower temperatures because the scattering mechanisms particularly polar optical phonon scattering dominates at higher temperature limiting the velocity. Authors have utilized the NDR effect in CdSe for possible theoretical design of diodes of micron dimensions at Terahertz frequencies. The self oscillating frequencies (f) of the diodes of length l are calculated from the following relation :

$$v_p = f \times l \qquad (9)$$

where v_p is the peak drift velocity of the electrons. From the Figure 1, v_p is found to be 7.3 x 10^7 m/s at 20K, the corresponding frequencies of the diode are calculated from the relation (9), and they are found to be all in the Terahertz range for diode of micron dimensions. This has been shown in the Table 2 given below.

Table 2.: Self-oscillating frequencies at Terahertz range for CdSe diodes of micron dimensions.

DIODE LENGTH (μm)	SELF OSCILLATING FREQUENCY(THz)
1	7.3
2	3.65
4	1.825

Table 2 provides a theoretical insight regarding the design parameters of CdSe diodes at Terahertz frequencies.

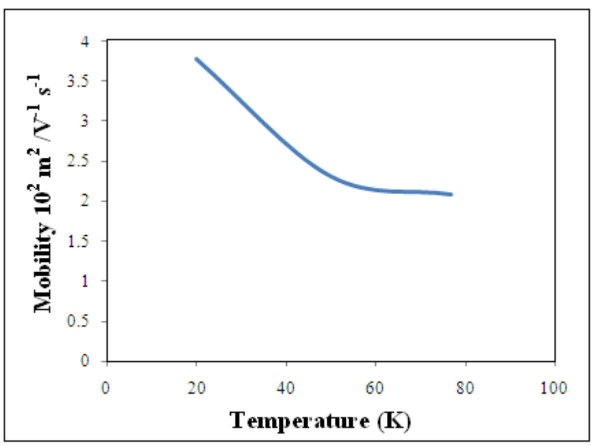

Fig. 2: Variation of electron drift mobility with lattice temperature.

Figure 2 shows the plot of electron drift mobility with lattice temperature. The mobility decreases with temperature due to the effect of polar optic phonon scattering which is found to be the predominant scattering mechanism over the temperature range considered.

IV. CONCLUSION

We have theoretically investigated with the help of Monte Carlo simulation the velocity –field characteristics of bulk CdSe at lattice temperatures of 20K, 50K and 77K respectively, incorporating all relevant lattice scatterings as shown in the Figure 1. The curves in the Figure 1 show a NDR effect with the velocity peaks being more prominent at lower temperatures. This is due to the fact that scattering effects come into play at higher lattice temperatures. The NDR effect has been used by the authors to predict theoretically the dimensions of CdSe diodes in micron range at Terahertz frequencies as given in Table 2. The mobility variation with lattice temperature as exhibited in the Figure 2 shows a decreasing nature being mainly limited by the polar optic phonon scattering.

References

[1] N.Samarth, H.Luc, J.K.Furdyna, R.G.Alonso, Y.R.Lee, A.K.Ramdas, S.B.Qaon and N.Otsuk, "Molecular beam epitaxy of $Zn_{1-x}Cd_xSe$ epilayers and $ZnSe/Zn_{1-x}Cd_xSe$ superlattices", Appl. Phys. Lett. **56**, 1163 (1990).

[2] G.Landwehr, A.Waag, F.Fischer, H.J.Lugauer, and K.Schull, "Blue emitting heterostructure laser diodes" Physica E **3** 158 (1998).

[3] H.K.Ng, Y.A.Leem, R.Knobel, I.P.Smorchkova, A.A.Sirenko, N.Samarth, "Cyclotron resonance in modulation-doped $ZnSe/Zn_{1-x}Cd_xSe$ and ZnTe/CdSe single quantum wells " Appl. Phys. Lett. **75** 3662 (1999).

[4] A.Ghosal and D.Chattopadhyay, "Low-temperature electronic transport in CdSe single quantum wells", Indian J. Phys.,**78**, 915 (2004)

[5] A.Ghosal and D.Chattopadhyay, "Diffusion thermopower in CdSe single quantum wells" Indian J. Phys., **80**, 405 (2006).

[6] P.K.Ghosh, A.Ghosal, D.Chattopadhyay, "Magneto-electronic transport of two dimensional electron gas in CdSe single quantum wells" Pramana J. of Phys. **72**, 399 (2009).

[7] Nag B R , "Electron Transport in Compound Semiconductor "Springer-Verlag, Berlin (1980).

[8] Fawcett W, Boardman A D and Swain S "Monte-Carlo determination of electron transport in gallium arsenide.",J. Phys. Chem. Solids, **31**, 1963 (1970).

[9] H. Arabshahi , "Potential performance of SiC and GaN based metal semiconductor field effect transistors" Brazilian J. of Phys., **39**, 35 (2009).

[10] D Mukhopadhyay, "Hot-electron conduction in cadmium selenide" Indian J. Phys., **53A**, 528 (1979).

[11] D Mukhopadhyay and D P Bhattacharya, "Electron transport in II–VI compound semiconductors" J. Phys. Chem. Solids, **45**, 393 (1984).