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Hot Electron Diffusion in CdTe

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Abstract. The parallel and transverse components of diffusion constants of electrons in CdTe have been computed for fields of 30, 40, and 50 kV/cm using the Monte Carlo method. Results are presented for the velocity autocorrelation function and for the ac diffusion constants for two models of energy band structure and scattering constants, used earlier in the literature. The diffusion constants as obtained from the two models are significantly different, but none are in agreement with the available experimental results.

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Cadmium telluride is considered to be one of the important II–VI compound semiconductors as it has wide applications in different fields of electronics. Its properties being similar to those of other important III–V compound semiconductors used in high-field devices like Gunn oscillators and FET's, hot electron transport in this material has been the subject of extensive studies. The high-field velocity-field characteristics were experimentally determined by Canali et al. [1, 2]. The characteristics were calculated using the Monte Carlo technique by Jacoboni and Reggiani [3] and also by Ruch [4]. Close agreement between the experimental and calculated characteristics were obtained although two different models (hereinafter referred as Models I and II) were used in these two papers for the band parameters, particularly for the satellite valleys. It could not be established from these studies which of the models is more appropriate, apparently because the conductivity characteristic is not very sensitively affected by the choice of the satellite valley parameters [5]. Values of the diffusion constant, on the other hand, are likely to be critically dependent on the band model as the contribution of intervalley scattering is more prominent for this constant at high fields. The parallel hot electron diffusion constant in CdTe was experimentally determined by Canali et al. [6]. The experimental values are about three times higher than the values calculated earlier by Alberigi-Quaranta et al. [7] using Model I. It is, therefore, of interest to examine the results given by Model II.

The present authors developed a Monte Carlo program for the evaluation of the autocorrelation function of the velocity fluctuations of electrons, the ac diffusion constant and the spectral density of thermal noise current. Results obtained by using this program for InSb [8], GaAs, InP [9], and HgCdTe [10] have been reported earlier. We present results calculated for CdTe on the basis of the autocorrelation function and the two components (parallel and perpendicular) of the ac diffusion constant. Results are presented for the fields of 30, 40, and 50 kV/cm. The fields have been chosen to be in the range where the difference is expected to be the most pronounced. The results would also be most appropriate for the operating conditions of high-field devices which may be built with CdTe.

1. Results and Discussion

The method used for the evaluation of the ac diffusion constant and the autocorrelation function has been

Table 1. Physical constants

Parameter	Symbol	Unit	Model I		Model II	
			Γ Valley	L Valley	Γ Valley	L Valley
Effective mass ratio	m^*/m_e	–	0.0963	0.50	0.11	0.2
Acoustic deformation potential	E_1	eV	9.5	9.5	9.5	9.5
Non-equivalent intervalley scattering						
Equivalent temperature	$T_{\Gamma L}$	K	220	220	220	220
Coupling constant	$D_{\Gamma L}$	10^8 eV/cm	10	10	6	6
Equivalent intervalley scattering						
Equivalent temperature	T_{LL}	K	–	248	–	–
Coupling constant	D_{LL}	10^8 eV/cm	–	10	–	–
Non-polar optic scattering						
Equivalent temperature	T_0	K	–	–	–	248
Coupling constant	D_0	10^8 eV/cm	–	–	–	10
Static dielectric constant	ε_s	–	10.6		9.65	
Optical dielectric constant	ε_0	–	7.13		7.21	
Separation between valleys	ΔE	eV	1.5		0.51	
Non-parabolicity parameter	α	eV^{-1}	0.545	–	0.514	–
Density	ϱ	g/cm^3	5.86		6.06	
Velocity of sound	v_s	10^5 cm/s	3.448		3.39	

described in details in [8–10]. The relevant mathematical expressions are briefly included here for the convenience of presentation of the results.

The diffusion constant for any frequency ω for the α direction is given by [11]

$$D_\alpha(\omega) = \int_0^\infty C_\alpha(s) \cos \omega s \, ds, \tag{1}$$

where $C_\alpha(s)$ is the autocorrelation function for the interval s. The subscript α refers to the orientation of the direction of measurement in relation to that of the field. The parallel orientation is hereafter referred by subscript "p" and the transverse orientation by "t". $C_\alpha(s)$ is expressed in terms of velocity fluctuation $\Delta v_\alpha(t)$ as

$$C_\alpha(s) = \mathscr{L}\underset{T\to\infty}{t} \frac{1}{T} \int_0^T \Delta v_\alpha(t) \Delta v_\alpha(t+s) dt. \tag{2}$$

In our Monte Carlo method the trajectory of a single electron is computed by storing in the computer the instants of collision, the velocity components immediately after the collisions and the average acceleration in the inter-collision period. $C_\alpha(s)$ is obtained from the values of $\Delta v_\alpha(t)$ calculated by using the above data and $D_\alpha(\omega)$ is then computed using (1).

The scattering and energy-band parameters of the two models are given in Table 1. It may be pointed out that the main difference is in the values of the effective masses and band separation of the satellite valley, which are, respectively, taken to be $0.5m_e$ and 1.5 eV in Model I, and $0.2m_e$ and 0.5 eV in Model II. The central valley parameters are also slightly different; the effective mass is taken to be larger and the difference in dielectric constant values smaller in Model II. Some of the coupling constants for the different mechanisms are also taken to be different. It would appear from the parameter values that intervalley scattering would be more dominant in Model II, but the expected consequential reduction in mobility is compensated by choosing smaller values for the effective mass and for the coupling constants for the scattering mechanisms. As a result, both the models give identical velocity-field curves in spite of the differences.

We first present in Fig. 1 the velocity autocorrelation functions for the two models for a field of 50 kV/cm. The shape of the curves is identical to that for the III–V compounds reported earlier [8, 9]. The curves for the transverse components decrease monotonically with an approximately constant value of decay constant, while those for the parallel components decrease sharply, attain a negative maximum value and then reduce to zero. It may also be noted that the curves for the two models although similar in shape are quantitatively very different. The decay constant for Model I is less than for Model II. On the other hand, for the parallel component, the negative maximum is much larger for Model I.

The computed parallel and transverse diffusion constants for the two models for the field of 50 kV/cm are shown in Fig. 2. We find that the values as well as the shape of the curves, particularly for D_p are significantly different for Model I. D_t has a value of 260 cm²/s for lower frequencies, remains constant up to about 250 GHz and then decrease with increase in frequency attaining a value of about 95 cm²/s at 2500 GHz. The parallel component D_p starts from a very low value of about 4.0 cm²/s, increases with increase in frequency and attains a value nearly equal to that of D_t (i.e. 220 cm²/s) at 1250 GHz and decreases again. On the other hand, for Model II D_t has a value of about 110 cm²/s, almost independent of frequency up to 2500 GHz. The parallel component D_p starts from a value of 48 cm²/s, increases with frequency and attains a nearly frequency independent value equal to that of the transverse component (i.e. 120 cm²/s) at about 250 GHz. The significant features of the computed results are presented in Table 2. Some calculations were done excluding the effects of overlap integrals [12] for Model I, in order to assess its importance with a view to simplifying the calculations. These results are also given in the table for information. The overlap integrals are seen to affect the results very significantly and were therefore included in all other computations.

We find from Table 2, that the values of drift velocity for the two models are within 12%, whereas the diffusion constants as well as all its associated characteristic parameters differ by large factors, some parameters differ even in magnitudes. It is also seen that neither of the models give results in agreement with the experimental values of D_p.

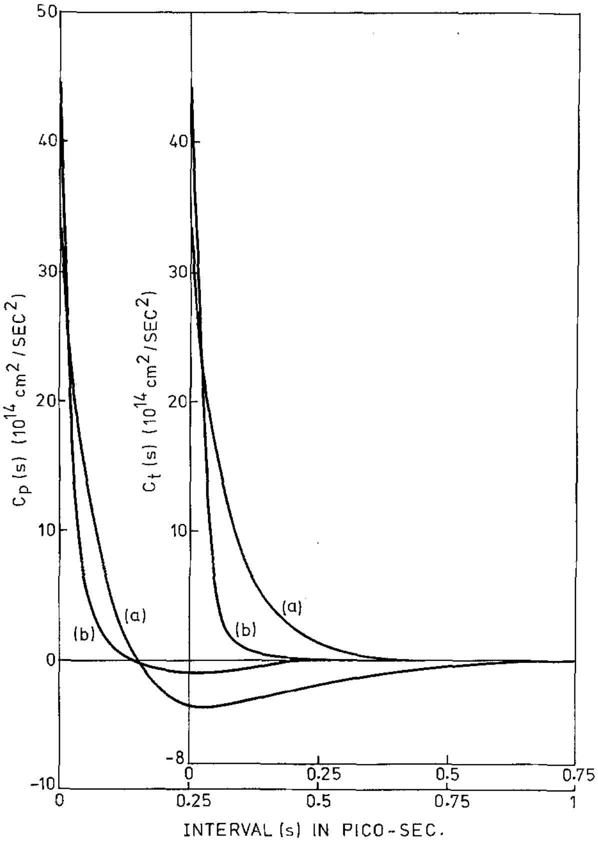

Fig. 1a and b. Transverse and parallel autocorrelation functions for electric field of 50 kV/cm. (a) Model I, (b) Model II

Some trial calculations were also done to find a model which would give the experimental values of D_p. We chose the parameter values for the central valley in accordance with Model I, as these are supported by

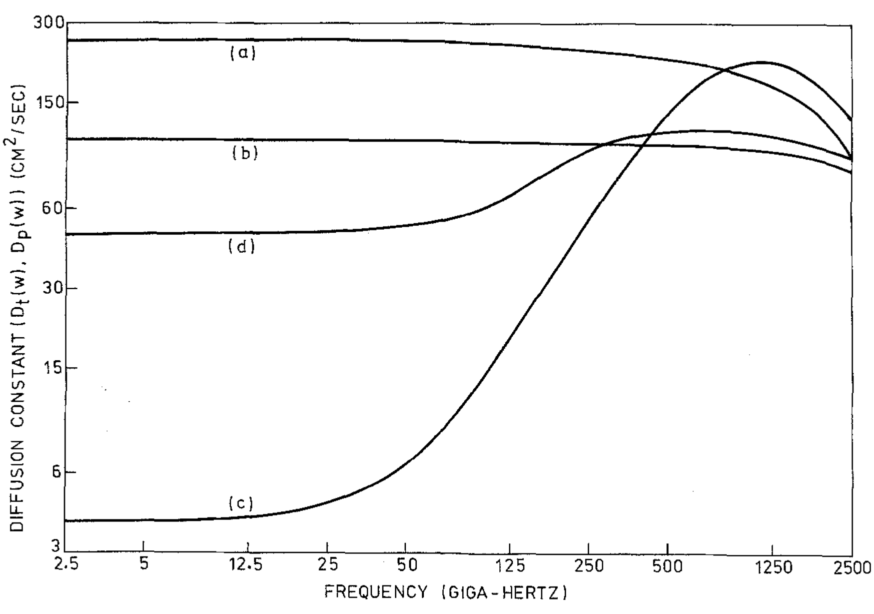

Fig. 2a–d. Transverse and parallel diffusion constants vs. frequency for electric field of 50 kV/cm. $D_t(\omega)$: (a) Model I, (b) Model II. $D_p(\omega)$: (c) Model I, (d) Model II

Table 2. Computed results

Parameter unit \ Field	Model I 30 kV/cm	Model I 40 kV/cm	Model I 50 kV/cm	Model II 30 kV/cm	Model II 40 kV/cm	Model II 50 kV/cm
Drift velocity	–	–	7.1[a]	9.9	8.75	7.9
10^6 cm/s	(17.4	13.4	11.2)[b]			
Population in valleys Γ %	–		78.9[a]	47.2	38.0	34.6
	(95.1	90.2	86.5)[b]			
L %	–	–	21.1[a]	52.8	62.0	65.4
	(4.9	9.8	13.5)[b]			
Chord mobility	–	–	142[a]			
cm^2/Vs.	(580	335	224)[b]	330	218.8	158
Diff. mobility	–	–	–			
cm^2/Vs.	(−593	−288	−157)[b]	−128	− 91.4	− 63.0
Mean Sq. Vel. fluctuation:						
Transverse	–	–	32.86[a]	21.3	32.0	42.9
10^{14} cm^2/s^2	(32.9	34.5	34.3)[b]			
Parallel	–	–	32.57[a]	21.3	32.3	44.0
10^{14} cm^2/s^2	(35.1	35.9	35.3)[b]			
Correlation time	–	–	0.072[a]	0.048	0.030	0.028
10^{-12} s	(0.129	0.117	0.104)[b]	0.092	0.060	
Interval s for						
(a) $C_t(s)=0$	–	–	0.5[a]	0.34	0.32	0.30
10^{-12} s	(1.60	1.56	1.40)[b]			
(b) $C_p(s)=0$	–	–	0.15[a]	0.18	0.14	0.14
10^{-12} s	(0.40	0.30	0.26)[b]			
Low frequency diffusion coefficient						
Transverse D_t	–	–	259.9[a]	109.8	103.7	110.5
cm^2/s	(409.0	366.5	334.3)[b]			
	285	256	230[c]			
Parallel D_p	–	–	3.99[a]	25.9	38.7	48.2
cm^2/s	(19.0	3.63	–)[b]	40 (Expt)	20 (Expt)	15 (Expt)
	10	5	2[c]			
Max. value of	–	–	218.6[a]	103.5	103.6	110.6
$D_p(\omega)$ cm^2/s	(410.4	382.6	325.4)[b]			
Freq. for max	–	–	1250[a]	500	600	750
value of (D_p) GHz	(650	900	1250)[b]			

[a] Present calculation including the effect of overlap integral
[b] Present calculation excluding the effect of overlap integral
[c] Result of [7]

later experiments [13]. The results of the computations are given in Table 3. It was not possible to arrive at any definite conclusion as the number of unknown parameters is too large and the computation time required is rather long. It is, however, evident from these computations that D_p is not very sensitive to the choice of ΔE and m_2^*. The values of D_p converge very slowly as positive and negative parts of $C_p(s)$ are nearly equal in magnitude. Quoted values are the averages. However, the disagreement with the experiment is definitely a factor of about 3 and unless new data are available for D_p confirming the only experiment reported, it is not worthwhile to carry out such computations.

The values of drift velocity are not also significantly affected by the choice of the parameters. The difference is within 16% for the different combinations of values of ΔE and m_2^*. Hence, study of velocity-field characteristics is not helpful in resolving the problem. The transverse diffusion constant, D_t, is, on the other hand, significantly different for the different models. It really differs by a factor of about 7. Unfortunately, no

Table 3. Computed results for a field of 50 kV/cm using Model I with different values of satellite valley separation and effective mass ratio

Parameters	Unit	Values			
Satellite valley separation [ΔE]	eV	1.5	1	0.5	0.5
Effective mass ratio for the satellite valley [m_2^*/m_e]	–	0.5	0.5	0.5	0.35
Drift velocity [v_d]	10^6 cm/s	7.1	6.69	5.97	7.1
Low frequency diffusion coefficient					
Transverse D_t	cm^2/s	259.9	158.2	37.0	55
Parallel D_p	cm^2/s	3.99	2.7	3.4	3
Experimental value of $D_p \sim 15$					

experimental results are available for D_t. In view of the results presented here, it would be worthwhile to determine experimentally the values of D_t, for determining the satellite valley parameters.

2. Conclusion

Monte Carlo values of hot-electron diffusion constants in CdTe are different for the two models of energy band and scattering used earlier. The available experimental results on D_p do not agree with the values for either of the models. The values of D_p for a field of 50 kV/cm are also found to be not much dependent on the satellite valley parameters, but the values of D_t are found to vary significantly. Further experiments on hot electron diffusion in CdTe would be useful for meaningful application of the results of this paper in the clarification of energy band and scattering models.

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