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Temperature dependence of carrier capture by defects in gallium arsenide

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Temperature dependence of carrier capture by defects in gallium arsenide

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Abstract

This report examines the temperature dependence of the capture rate of carriers by defects in gallium arsenide and compares two previously published theoretical treatments of this based on multi phonon emission (MPE). The objective is to reduce uncertainty in atomistic simulations of gain degradation in III-V HBTs from neutron irradiation. A major source of uncertainty in those simulations is poor knowledge of carrier capture rates, whose values can differ by several orders of magnitude between various defect types. Most of this variation is due to different dependence on temperature, which is closely related to the relaxation of the defect structure that occurs as a result of the change in charge state of the defect. The uncertainty in capture rate can therefore be greatly reduced by better knowledge of the defect relaxation.

CONTENTS

1. INTRODUCTION

Displacement damage in minority carrier devices, such as bipolar junction transistors, decreases their gain due to carrier recombination at lattice defects. Models for the response of III-V heterojunction bipolar transistors (HBTs) to pulsed damage are being developed which include an atomistic description of carrier transport and recombination at defects [1]. A major uncertainty in such models is the rate of carrier capture by the defects. While many properties of defects in semiconductors, such as energies of formation and migration, have been calculated by Density Functional Theory (DFT) [1], calculation of carrier capture rates from first principles is still very challenging [2,3]. Atomistic simulations of carrier recombination at defects in GaAs presented in reference 1 used nominal, or typical values for carrier capture rates, for lack of defect specific information. However, the capture rates at room temperature can differ by several orders of magnitude for various defect types, as shown in figure 1. This variation introduces a large uncertainty in atomistic simulations of HBT response to damage. Most of the variation arises from different temperature dependence of capture rate, as pointed out by Henry and Lang [4-6]. This temperature dependence is closely related to the relaxation of the defect structure that occurs when the defect charge state changes. The uncertainty in capture rate can therefore be greatly reduced by improved knowledge of the defect relaxation.

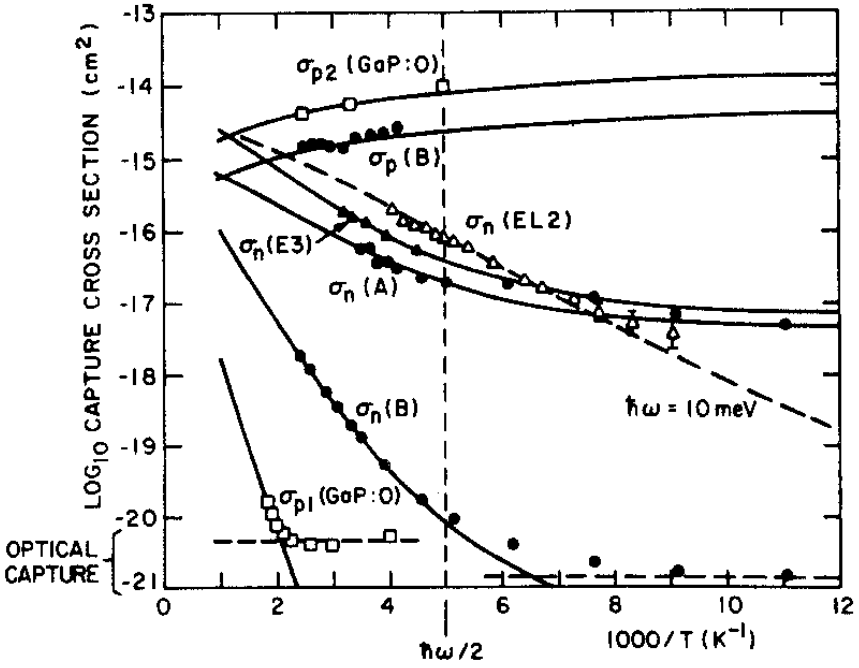

Figure 1 Temperature dependence of the cross section for carrier capture [6].

Henry and Lang (HL) developed a model for the temperature dependence of carrier capture, based on multi-phonon emission with harmonic potentials to represent the vibrational states of the defect [4-6] and the structural relaxation. This model was subsequently extended by Schenk to include the influence of electric field on carrier capture rates due to band-to-trap tunneling from nearby band states [7,8]. A formulation of band-to-trap tunneling by S.M. Myers, based on Schenk's model, was recently compared to carrier emission rates from defects in GaAs measured by Robert Fleming using DLTS, and was found to give good fits to the data with physically plausible parameter values [9]. The dependence of carrier capture on temperature can be obtained experimentally using new methods based on DLTS [9,10]. This temperature dependence could also be predicted using the MPE models with defect relaxation from DFT calculations. This report compares the models for carrier capture described by Henry and Lang, and by Schenk as implemented in [9], with particular attention on the predicted temperature dependence.

2. HENRY AND LANG

Following Huang and Rhys [11] HL give the following expression for the spectral lineshape (intensity vs photon energy *hv*) for photon absorption with carrier emission or photon emission with carrier capture, by a defect:

$$f(hv) = W_p/\hbar\omega_0 \tag{1}$$

where

$$W_p = \exp[-S(2f_B + 1)] \left(\frac{f_B+1}{f_B}\right)^{\frac{p}{2}} I_p(z) \tag{2}$$

or equivalently:

$$W_p = \exp\left[-S(2f_B + 1) + \frac{p\hbar\omega_0}{2kT}\right] I_p(z)$$

is a dimensionless temperature-dependent transition probability and

$$f_B = \frac{1}{\left(exp\left(\frac{\hbar\omega_0}{kT}\right)-1\right)},$$

$$z = 2S\sqrt{f_B(f_B + 1)}\,.$$

I_p is the modified Bessel function of the first kind of order p, and

$$S = \frac{E_r}{\hbar\omega_0}$$

is the Huang-Rhys factor. E_r is the lattice relaxation energy associated with the change in charge state of the defect. This expression uses a harmonic potential, or linear force model for the vibrational states of the defect with frequency ω_0, assumed to be the same for both charge states. The defect has vibrational states with energies $p\hbar\omega_0$ where p is the quantum number, or number of phonons. The optical lineshape *f*(*hv*) is obtained by evaluating equations 1 & 2 with

$$p\hbar\omega_0 = E_t - hv$$

where E_t is the binding energy of the carrier to the trap, or the energy difference between the free and bound states.

The lineshape is thus determined by three properties of the defect, E_t, $\hbar\omega_0$ and E_r or S. Figure 2 illustrates the various quantities in a configuration coordinate diagram in which the

lattice configuration is represented by a single effective coordinate Q, and the energy vs displacement is $E(Q)=1/2\ m\ \omega_0^2\ Q^2$.

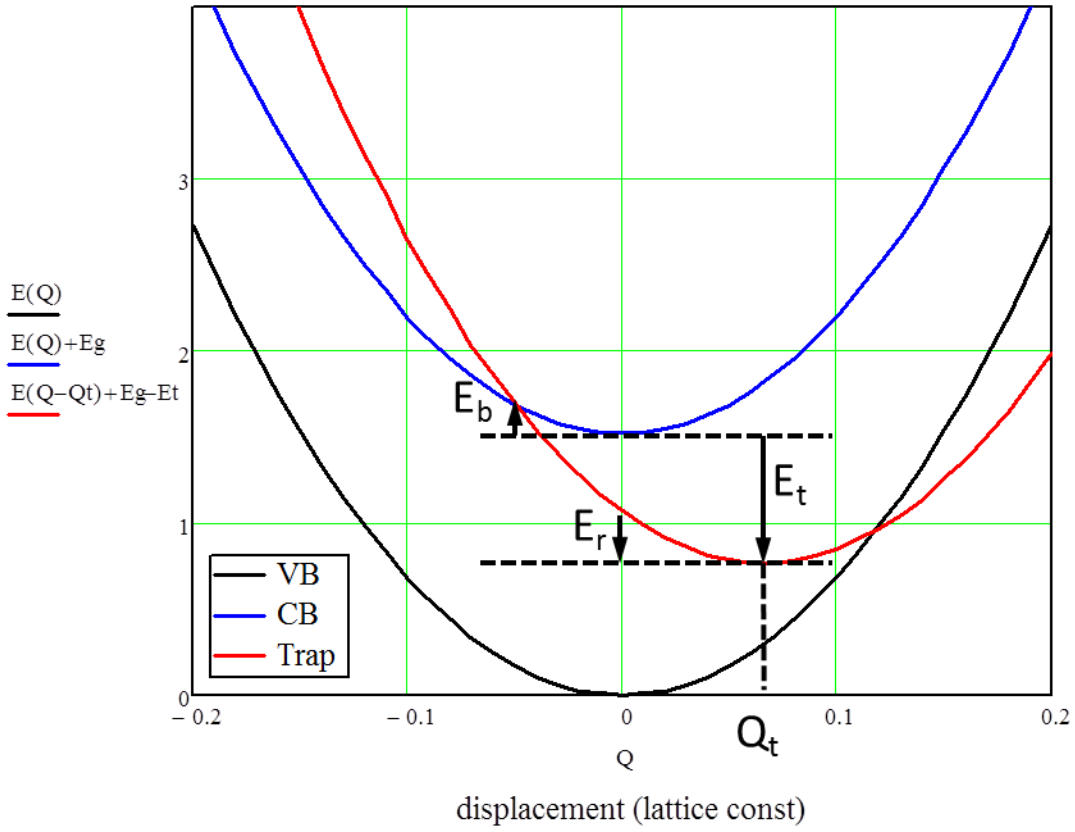

Figure 2. Configuration coordinate diagram for the EL2 defect discussed below.

In the high temperature limit kT>> $\hbar\omega_0$ the lineshape approaches a Gaussian centered on E_r:

$$W_g(p) = \frac{1}{\sqrt{2\pi}\,\sigma} \exp\left(-\frac{1}{2}\left(\frac{p-S}{\sigma}\right)^2\right) \qquad (3)$$

with $$\sigma = \sqrt{\frac{2\,S\,kT}{\hbar\omega_0}},$$

or equivalently $$W_g(E) = \frac{1}{\sqrt{2\pi}\,\sigma} \exp\left(-\frac{1}{2}\left(\frac{E-E_r}{\hbar\omega_0\,\sigma}\right)^2\right)$$

with $$\sigma = \frac{\sqrt{2\,E_r\,kT}}{\hbar\omega_0}$$

as illustrated in figure 3.

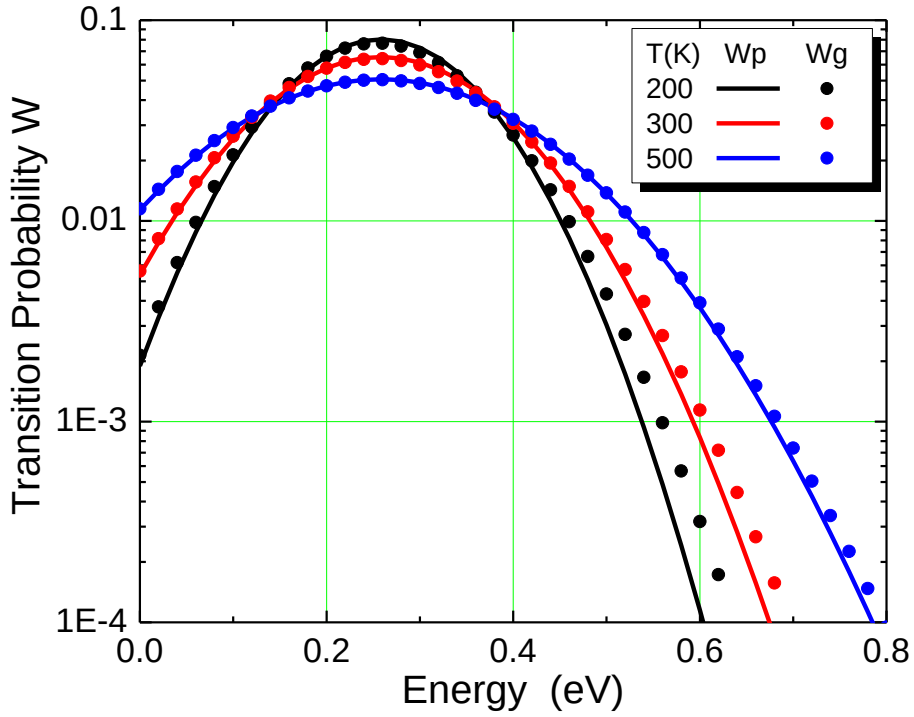

Figure 3. The transition probability vs energy for parameters of the EL2 defect, $\hbar\omega_0$ = 0.016 eV. In this case the peak at E_r=0.299 eV is lower in energy than the band edge at E_t=0.75 eV. Solid lines show W_p from eq.2 and symbols show the high-temperature Gaussian approximation from eq. 3.

The rate for non-radiative carrier capture κ is related to the transition probability by:

$$\kappa = A'\,f(h\upsilon = 0) = A'\,\frac{W_{HL}}{\hbar\omega_0} \qquad (4)$$

where $$A' = \frac{2\pi\Omega}{\hbar}\,|\langle c|\Delta V|t\rangle|^2 \qquad (5)$$

is a temperature independent prefactor depending on the matrix element for transition between band $|c\rangle$ and bound $|t\rangle$ states, and

$$W_{HL} = W_{p_t} \tag{6}$$

is the transition probability W_p from equation 2 evaluated for a vibrational state whose energy is equal to the binding energy of the carrier to the trap $p_t=E_t/\hbar\omega_0$. Figure 4 shows the transition probability W_{HL} versus 1/T , i.e. the temperature dependence of the non-radiative carrier capture rate for parameters E_t=0.75 eV, =0.016 eV and S=18.7 for the EL2 defect as discussed below. These values for $\hbar\omega_0$ and S were determined from a fit of the Schenk model to the data for EL2 (symbols).

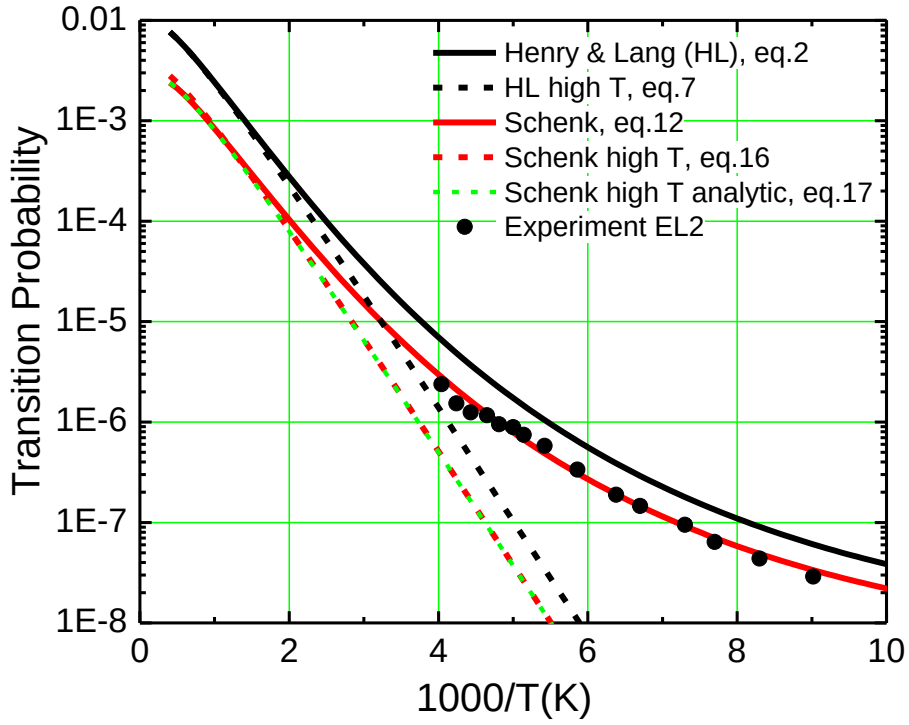

Figure 4. Transition probability from Henry and Lang and Schenk, and high temperature approximations. Symbols show values from measurements of capture rate for EL2 [6].

From equation 3, the transition probability in the high temperature limit is

$$W_{HLh} = W_g(E_t) = \frac{1}{\sqrt{2\pi}\,\sigma}\exp\left(-\frac{1}{2}\left(\frac{E_t-E_r}{\hbar\omega_0\,\sigma}\right)^2\right) = \frac{\hbar\omega_0}{\sqrt{4\pi E_r kT}}\exp\left(-\frac{E_b}{kT}\right) \tag{7}$$

where

$$E_b = \frac{(E_t-E_r)^2}{4E_r} \tag{8}$$

is the activation energy or barrier for carrier capture indicated in figure 2. This is the same

expression for the high temperature limit given by HL in eq. 28 of reference 5. This high temperature approximation (eq. 7) is compared to the full expression (eq. 2) in figure 4.

The matrix element term A' in equation 4 is related to the coefficient A used by HL (defined in equation 20 of reference 5) by $A' = A\, v_{th}$. Our formulation avoids the use of a carrier velocity in comparing the model to measured capture rates, which avoids ambiguity over what carrier velocity should be used when the carrier drift velocity becomes comparable to the thermal velocity, as may be the case in high field depletion regions near a pn junction. This also removes the temperature dependence in the thermal velocity from the prefactor. A carrier velocity v_{th} is only needed when the capture rate is expressed in terms of a cross section σ_c:

$$\kappa = \sigma_c \, v_{th} \tag{9}$$

Comparison between the model and experimentally measured capture rates require a value for the prefactor A' . This parameter is difficult to calculate from first principles [2,3,5]. Here we evaluate A' using the following expression proposed by HL for capture by a neutral defect:

$$A' = \frac{h^2}{(2m^*)^{3/2}} \sqrt{\varepsilon} \tag{10}$$

with ε=0.06 eV. For electrons in GaAs $m^*=0.067m_e$, eq. 10 gives A' = $6.3\text{x}10^{-6}$ cm^3 eV/s .

3. SCHENK

Schenk uses the same Huang-Rhys expression for the transition probability (eq. 2) to calculate carrier capture rates, but includes two extensions [7,8]. First, he includes a factor for enhancement of carrier capture by tunneling from nearby band states to vibrational states below the band edge. This increases the carrier capture rate in regions where the electric field is high. Here we are concerned only with the temperature dependence of carrier capture at zero field so we omit this term for band-to-trap tunneling in the following discussion. Secondly, Schenk includes capture of carriers from electronic states above the band edge, whereas HL only included capture at the band edge.

The total transition rate is the sum of W_p over states above the band edge, weighted by the density of carriers at each energy:

$$W_S = \frac{1}{n}\sum_{p>p_t} \rho\left(E_p\right) F\left(E_p\right) W_p \tag{11}$$

where ρ(E) is the density of electronic states and F(E) is the state occupancy and $p_t=Et/\hbar\omega_0$ is the quantum number of the vibrational state at the band edge. We convert the sum over p to an integral over energy from the band edge at $E=E_t$:

$$W_S = \frac{\int_{E_t}^{\infty} \rho(E)\, F(E)\, W_p\, dE}{\int_{E_t}^{\infty} \rho(E)\, F(E)\, dE} \tag{12}$$

where $p=E/\hbar\omega_0$ is used in the evaluation of W_p using eq. (2) . The denominator in eq. 12 provides the correct normalization for number of carriers. Apart from energy independent factors which cancel in the ratio, the density of states is

$$\rho(E) = \sqrt{E - E_t} \tag{13}$$

for $E \geq E_t$ for a parabolic band, and the occupancy is

$$F(E) = \exp\left(-\frac{E}{kT}\right) \tag{14}$$

for Boltzmann carrier statistics. Fermi-Dirac occupancy could be used here instead, although the capture rate then becomes dependent on the Fermi level of the carriers.

Schenk's initial equation for the multiphonon transition probability (eq 11 in reference [8]) includes a factor of $(p\pm S)^2/S$, however, later in that paper the factor is omitted, so consistent with his usage and that of HL and in ref [9] we also do not include it here.

For convenience of evaluation, Schenk [8] proposes an approximation for the Bessel function in equation 2

$$I_p(z) = \frac{1}{\sqrt{2\pi}\,(p^2+z^2)^{\frac{1}{4}}} \exp\left(\sqrt{p^2+z^2} - p\, ln\left(\frac{p}{z} + \sqrt{1+\frac{p^2}{z^2}}\right)\right). \tag{15}$$

This approximation is used in reference 9. Comparison between equation 15 and values for the Bessel function from standard math libraries show eq. 15 to be an accurate approximation in the relevant range of parameter values. Equations 12-15 give the same result as equation 6 in

reference [9] for the temperature dependence of capture rate at low field. Reference 9 avoids the use of the poorly known scaling factor A' relating the transition probability W to the capture rate (eq. 4) by considering the ratio of capture rate to the value at T=300K. Here we compare W calculated by the various models. This comparison does not use the parameter A', which is only used in comparing the models to measured values of capture rates.

Figure 4 shows the transition probability W_S evaluated using eqs. 2,12-14. Integration over states above the band edge makes a significant difference from the HL values. The difference depends on the energy derivative of the lineshape function at the band edge. Since W_p peaks near $E=E_r$, as shown in figure 3, the integration above the band edge makes $W_S > W_{HL}$ when $E_t < E_r$ and $W_S < W_{HL}$ when $E_t > E_r$.

Figure 4 also shows the high temperature approximation to the Schenk expression obtained using the Gaussian approximation eq. 3, instead of eq 2 for W_p;

$$W_{Sh} = \frac{\int_{E_t}^{\infty} \rho(E)\, F(E)\, W_g(E)\, dE}{\int_{E_t}^{\infty} \rho(E)\, F(E)\, dE}\,. \qquad (16)$$

Unfortunately, eq. 16 does not reduce to a simple analytic expression for $W_{Sh}(T)$ as for the case of eq. 7. However, we have derived a correction factor to eq. 7 which gives a good analytic approximation to the Schenk result in the high temperature limit;

$$W_{Sha} = \left(\frac{2E_r}{E_t+E_r}\right)^{3/2} \frac{\hbar\omega_0}{\sqrt{4\pi E_r kT}} \exp\left(-\frac{E_b}{kT}\right) \qquad (17)$$

This approximation to the high temperature limit is also shown in figure 4.
We note that the expression proposed by Schenk (eq.53 of ref. [8]) for the high temperature limit has a different dependence on temperature.

The symbols in figure 4 show data reported by Lang [6] for the EL2 arsenic antisite defect from measurements of the variation in height of the DLTS peak versus duration of the majority carrier filling pulse. To compare the reported values of capture cross section to calculated values of transition probability, we use equations 4 and 9 above with the value $A' = 6.3\text{x}10^{-6}$ cm^3 eV/s from equation 10 for electrons in GaAs and average thermal velocity

$$v_{th} = \sqrt{\frac{8\,kT}{\pi m^*}}\,. \qquad (18)$$

where m*, the effective mass of the carrier =0.067m_e for electrons in GaAs. The use of the thermal velocity in conversion from cross section to capture rate is justified in this case because majority carrier capture during the filling pulse is occurring in a low-field neutral region of the diode, so the carrier drift velocity will be low. The DLTS measurements gave a value of E_t=0.75 eV which is in good agreement with recent DFT calculations [12]. Figure 4 shows calculated values of W_s from our fit to the EL2 data obtained by adjusting values of $\hbar\omega_0$ and $S = E_r/\hbar\omega_0$. This fit gave values of $\hbar\omega_0$ =0.016 eV and S=18.7, or E_r=0.299 eV.

The midgap level of EL2 is a (0/+) transition, in which the electron is captured by a positively charged defect. In this case Coulomb attraction will increase the electron density at the defect and therefore also the capture rate. This increase is dependent on temperature [2, 5,13,14]. This increase was estimated to be about an order of magnitude at room temperature for capture of holes by a negative defect in GaP [5] and GaN [2].

The dependence on temperature and field of carrier emission rate, and by detailed balance also the capture rate, was recently determined for several defects in GaAs from DLTS measurements [9]. In that work the prefactor was determined from fits to the data, along with E_t, $\hbar\omega_0$ and S for each defect. Table 1 shows the values obtained from the fit for the three electron capture/emission reactions examined, labeled E2, E3 and E5. The defect corresponding to these DLTS peaks is not known. Table 1 also includes parameters from the fit to the data of Lang and Logan for EL2 [6] using two values of the prefactor, the value proposed by HL (eq. 10) for a neutral defect, and a value one order of magnitude larger to approximate the effect of Coulomb attraction. These values both give good fits to the data, but with different values of S and $\hbar\omega_0$. Table 1 also shows the value of the scale factor A' used in the fit in the case of EL2, or obtained from the fit in the case of E2, E3 and E5. Figure 5 shows the transition probability vs 1/T from the Schenk model for the E2, E3, E5 and EL2 (parameters in the top row of table 1) defects. Figure 5 also shows that above room temperature, the analytic high temperature approximation (eq. 17) is within about a factor of 2 of the general expression (eq 16) for these defects.

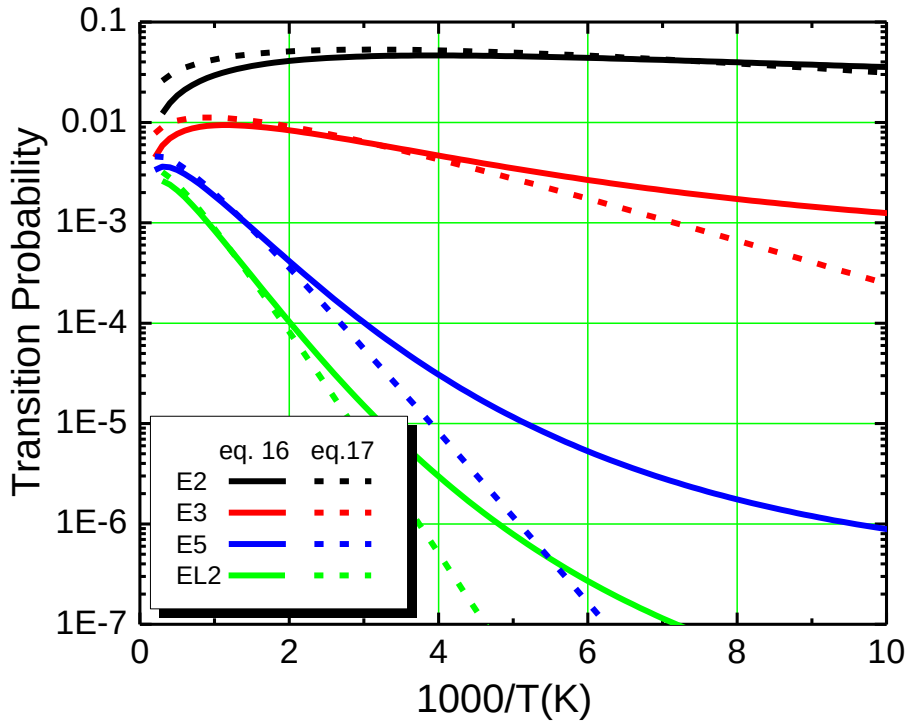

Figure 5. Transition probability vs 1/T for the defects listed in table 1 from the Schenk model (solid lines, eq. 16) and the analytic expression for the high temperature limit (dashed lines, eq. 17).

Figure 5 shows that the transition probability, and hence capture rates, can vary over several orders of magnitude at room temperature, but in the high temperature limit the spread in values is less than an order of magnitude. This illustrates the point that by including the temperature dependence, the uncertainty in values at room temperature can be greatly reduced.

Table 1. Parameters from fits to measured capture rates.

Defect	E_t (eV)	$\hbar\omega_0$ (meV)	S	E_r (eV)	κ(300K) (10^{-6} cm^3/s)	A' (10^{-6} cm^3 eV/s)	E_b (eV)
EL2	0.75	16	18.7	0.299	0.020	6.3	0.170
EL2	0.75	19	13.6	0.258	0.028	63	0.234
E2	0.12	16.5	14.2	0.234	6.8	2.44	0.014
E3	0.30	15	9.2	0.138	1.11	2.88	0.048
E5	0.66	20	12.2	0.244	0.45	135	0.177

Finally, we note that the three parameters E_t, E_r, and $\hbar\omega_0$ which determine the temperature dependence of carrier capture rates in the multi-phonon emission model with harmonic approximation, could be obtained from DFT calculations. The binding energy E_t has already been calculated for a variety of defects and charge states [1]. The lattice relaxation energy E_r can be obtained from DFT calculations in which the lattice configuration is first held fixed during a charge change reaction, and then allowed to relax to the minimum-energy configuration. This has been done by Alan Wright for the arsenic antisite defect in GaAs (EL2) [15]. Wright calculated a relaxation energy of 0.08 eV for the EL2 0/+ transition, which is about a factor of 3 smaller than the value obtained from the fit of the model to the capture data of Lang and Logan [6]. In this case the relaxation is of the "breathing mode" type in which the local coordination and symmetry remains the same and only the interatomic distances change. The reason for this factor of 3 discrepancy has not yet been identified. The DFT calculations could be further extended to follow the formation energy along the configurational path between the two equilibrium configurations. This might provide a value for the force constant and vibrational energy $\hbar\omega_0$ for the two configurations, and indicate whether the harmonic approximation assumed in the model is valid. In other charge-change reactions the local lattice reconfiguration is not small, for example in the (0/+1) or (+1/+2) reactions of the arsenic interstitial in GaAs. In such cases a more sophisticated treatment is needed for the influence of lattice reconfiguration on carrier capture rates, as described in reference 1.

4. CONCLUSION

The temperature dependence of carrier capture by defects in GaAs at zero field, predicted by the MPE models by Henry and Lang [5] and by Schenk [8], were compared and were found to be very similar. The main difference being that HL evaluate the capture rate for states at the band edge, whereas Schenk's model integrates over all occupied band states. Schenk's formulation should be physically more realistic. Analytic approximations were also presented for the capture rate in the high temperature limit ($kT > \hbar\omega_0$) for both models. The capture rate was evaluated for defects examined in a recent DLTS study [9] and for the EL2 defect [6]. These calculations demonstrate that the influence of temperature on capture rate can be included if the MPE parameters of the defect are known, thereby reducing the uncertainty in their values.

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