# Enhanced multiphonon capture of hot electrons by deep centers with strong lattice coupling: A Monte Carlo study of InP:Fe

Mark Isler and Dennis Liebig

Technische Universität Hamburg-Harburg, Arbeitsbereich Hochfrequenztechnik, Denickestrasse 22, D-21073 Hamburg, Germany

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The free-carrier energy dependence of the nonradiative multiphonon capture mechanism in semiconductors is investigated in the case of weak and strong lattice coupling of the deep center, considering high and low lattice temperatures. It is shown that in the case of strong coupling, the multiphonon capture probability is resonantly enhanced for hot electrons. This effect is even more pronounced at low temperatures. Consequently, enhanced capture of hot electrons by DX or other deep centers can be explained in a very general way. Incorporating the analytically calculated energy dependent multiphonon capture probability into a Monte Carlo transport simulation of InP, the electric field dependence of the effective electron capture cross section is calculated. By varying the Huang-Rhys coupling constant over a wide range of magnitude, the cases of weak and strong electron-lattice interaction are investigated. For strong coupling, an enhancement of the capture cross section in the presence of a high electric field is found, in accordance with the experimental data for Fe-doped InP. By attributing the capture of electrons to the excited state  $Fe^{2+}({}^{5}T_{2})$ , excellent agreement is obtained between the theoretical calculation and the experimental data for both the temperature and the electric field dependence of the capture cross section. The calculated temperature dependence reveals a lowering of the capture barrier induced by the electric field.

### I. INTRODUCTION

Until now, the enhanced capture of hot electrons, experimentally observed in the presence of an accelerating electric field, has not been explained satisfactorily. While an increase of the capture rate with electric field strength at low temperatures can be attributed to the Sommerfeld factor in the case of a repulsive center (Ref. 1, p. 118, and references therein), the reported strong enhancement of the nonradiative capture cross section in an electric field,<sup>2</sup> irrespective of the charge state of the defect, is not well understood. Moreover, the reported high field capture cross section shows a near independence of lattice temperature, whereas the capture cross section in a zero electric field shows a pronounced thermally activated behavior.<sup>2</sup> Recently, a similar temperature and electric field dependence of the electron capture cross section has been observed for the Fe impurity in InP.<sup>3</sup> Since Fe doped InP is used as a semi-insulating substrate material electronic for speed high devices such as  $In_rAl_{1-r}As/In_vGa_{1-v}As$  high-electron-mobility transistors (HEMT's) and optoelectronic devices, an understanding of the electronic behavior of InP:Fe is essential for the improvement of these devices. Regarding transport modeling, the general use of the thermal capture cross section, for example, in drift-diffusion models, becomes questionable considering the reported strong electric field dependence of the cross section. Thus, it is of primary interest to take into account the electric field dependence of the capture cross section of a deep level in transport models, or more fundamentally, to consider the free-carrier energy dependence of the capture probability.

A popular example of hot electron capture is the capture to DX centers in  $Al_xGa_{1-x}As$ .<sup>4</sup> These centers are the cause of several deleterious effects on the electrical characteristics of a HEMT, such as, for example, the threshold voltage shift<sup>5</sup> or the collapse of the low field conductance.<sup>6</sup> Since it is widely accepted that DX centers exhibit large lattice relaxation, it is important to resolve how the lattice coupling of the deep center is related to hot electron capture. Moreover, it is still controversial whether the multiphonon theory is able to describe hot electron capture,<sup>2</sup> whereas there is no doubt that it is the appropriate framework to explain the thermally activated behavior of the thermal capture cross section for a variety of deep levels.<sup>7</sup> For this reason, the free-carrier energy dependence of the multiphonon capture probability is investigated in this work with particular attention to the influence of the Huang-Rhys coupling constant which specifies the strength of the electron-lattice interaction of a deep level. Furthermore, the deduced energy dependence of the multiphonon capture probability is incorporated into a Monte Carlo transport simulation, allowing an accurate study of hot electron effects. By performing Monte Carlo simulations of *n*-type InP, the electron capture cross section is calculated by varying the electric field strength and the Huang-Rhys coupling constant over a wide range of magnitude. The results are used for a comparison of the electric field and temperature dependence of the electron capture cross section in iron-doped InP with the experimental data of Ref. 3.

Since it is established that iron introduces two levels in the energy gap of InP, the ground state  $Fe^{2+}({}^{5}E)$  at  $E_{C}$ -0.6 eV and the excited state  $Fe^{2+}({}^{5}T_{2})$  at  $E_{C}$  $-0.3 \text{ eV},{}^{8}$ we investigated whether the apparent capture cross section is due to the capture of electrons by the ground state, or by the excited state followed by an internal relaxation.

## II. ENERGY DEPENDENCE OF THE MULTIPHONON CAPTURE PROBABILITY

To examine the free-carrier energy dependence of the multiphonon capture mechanism, it is helpful to consider first the so-called configuration coordinate diagram, which will be briefly reviewed here. As a result of the linear coupling between a bound state and one phonon mode with fre-

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FIG. 1. Configuration coordinate diagram for the electron-lattice system for small (a) and large (b) lattice relaxation energy  $E_R = S\hbar \omega$  representing the weak and strong coupling cases. The capture barrier  $E_B$  is defined with respect to the bottom of the conduction band ( $\Gamma$ ).  $E_T$  denotes the energy depth of the defect. The broken parabola illustrates the case of a hot electron in the *L* valley.

quency  $\omega$ , generally assumed in multiphonon theory, a system composed of a bound state and lattice vibrations behaves as a harmonic oscillator. In the case of a free electron, the electron-lattice system represents a harmonic oscillator that is shifted in the lattice coordinate Q depending on the value of the Huang-Rhys coupling constant S. This is shown in Fig. 1 in the configuration coordinate diagram,<sup>9</sup> which depicts the total energy of the electron-lattice system for the bound and free carrier states in the cases of weak and strong coupling, respectively.

The energy  $E_B$  in Fig. 1 specifies the capture barrier (with respect to the bottom of the conduction band), resulting in a thermally activated capture cross section at high temperatures. Considering a high energy electron in the configuration coordinate diagram, for example, an electron in the L valley, means simply that the upper parabola for the case of a free carrier is shifted vertically upward in energy space, since the total energy of the electron-lattice system is considered. Obviously, the capture barrier increases with the electronic energy in the case of weak coupling, whereas, for strong coupling, the capture barrier first decreases, vanishes for a carrier energy  $\varepsilon_{res} = S\hbar \omega - E_T$ , and increases again for higher free-carrier energies. This means that a resonant energy dependence of the capture probability exists. For a center with strong electron-lattice coupling, it is hence expected that hot electrons are more likely captured than low energetic electrons. This is in sharp contrast with the generally used picture of capture occurring mainly from the bottom of the conduction band.

Keeping this qualitative understanding in mind, the multiphonon capture probability is now to be examined with respect to its free-carrier energy dependence. Using perturbation theory for the calculation of the capture probability, a system composed of electron and lattice vibrations has to be considered. In a Born-Oppenheimer approximation, the initial delocalized state  $|i,n\rangle$  and the final localized state  $|f,n'\rangle$ are products of an electronic wave function  $\psi$  and a vibrational wave function  $\chi_n$ , which is the normalized wave function of a harmonic oscillator. The capture probability  $P_{cap}$ then reads

$$P_{cap} = \frac{2\pi}{\hbar} A v_n \sum_{n',f} |\langle i,n|H_{int}|f,n'\rangle|^2 \delta(E_{i,n} - E_{f,n'}), \quad (1)$$

where  $Av_n$  denotes a thermal average over the initial vibrational states. As we are interested in calculating the energy dependent capture probability, i.e., the capture probability of one specific initial electronic state  $|i\rangle$ , there is no averaging with respect to *i*. The sum occurring in Eq. (1) is performed over all possible final states.  $H_{int}$  specifies the interaction Hamiltonian.  $E_{i,n} = \hbar \omega (n + \frac{1}{2}) + \varepsilon$  is the total energy of the initial state and  $E_{f,n'} = \hbar \omega (n' + \frac{1}{2}) - E_T$  the total energy of the final state,  $\varepsilon$  denoting the free-carrier energy and  $E_T$  the energy depth of the deep level with respect to the conduction band.

Using a static scheme, the electronic wave functions are calculated at some given lattice coordinate. Evaluating the sum on account of the  $\delta$  function  $\delta(E_{i,n} - E_{f,n'})$ , the capture probability consists approximately of a pure electronic matrix element  $|\langle \psi_i | H_{int} | \psi_f \rangle|^2$  and an averaged vibrational overlap integral  $Av_n |\langle \chi_n | \chi_{n'} \rangle|^2$ . The last quantity can be calculated by using the well-known wave functions of a harmonic oscillator, and is given by<sup>7,10</sup>

$$Av_{n}|\langle\chi_{n}|\chi_{n+m}\rangle|^{2} = \exp\left[\frac{m\hbar\omega}{2k_{B}T} - S\coth\left(\frac{\hbar\omega}{2k_{B}T}\right)\right]I_{m}\left(\frac{S}{\sinh(\hbar\omega/2k_{B}T)}\right),$$
(2)

where, in the case considered here, *m* is given by  $(E_T + \varepsilon)/\hbar \omega$ .  $I_m$  denotes the modified Bessel function of order *m* which can be approximated for large values of *m* by

$$I_m(x) \approx \frac{e^{\sqrt{m^2 + x^2}}}{\sqrt{2\pi}(m^2 + x^2)^{1/4}} e^{-m \sinh^{-1}(m/x)}.$$
 (3)

For deep levels, this approximation is valid in general.

For a neutral center, the energy dependence of the electronic matrix element can be neglected in a first approximation: The error is expected to be of the order of  $O(E_T/\varepsilon)$ , which can be recognized by approximating the free state as  $|f\rangle \propto e^{ikr}/kr$ . The expected error is therefore small in comparison with the dominating exponential energy dependence of the overlap integral.

In the case of a charged deep center, the energy dependence of the electronic matrix element, due to the interaction of the electronic wave function with the long range Coulomb field, can be taken into account to a certain extent by the Sommerfeld factor<sup>11,12</sup>

$$s_{k}^{Z} = \frac{2\pi Z/a_{B}k}{1 - \exp[-2\pi Z/a_{B}k]}.$$
 (4)

Here, the electronic state is specified by the wave vector k.  $a_B$  is the effective Bohr radius and Z the charge state (in units of e) of the deep center. The Sommerfeld factor expresses the effect of an additional attractive or repulsive Coulomb tail of the defect potential on the capture probability. It takes the value of unity for a neutral center, as is the case for the Fe<sup>3+/2+</sup> electron capture transition in InP considered later on.

Restricting ourselves to a neutral center, we finally obtain for the energy dependent multiphonon capture probability  $P_{cap}(\varepsilon)$ 



FIG. 2. Free-carrier energy dependence of the multiphonon capture probability for different coupling strengths  $\eta := S\hbar \omega/E_T$  at T = 300 K. The high temperature approximation is depicted for one coupling strength (dotted line).

$$P_{cap}(\varepsilon) = A \exp\left[\frac{E_T + \varepsilon}{2k_B T} - S \coth\left(\frac{\hbar\omega}{2k_B T}\right)\right] \\ \times I_{(E_T + \varepsilon)/\hbar\omega}\left(\frac{S}{\sinh(\hbar\omega/2k_B T)}\right), \quad (5)$$

where the Bessel function can be approximated as above. The quantity A is an adjustable factor which does not depend on temperature. In the case of charged centers the Sommerfeld factor can be included in this expression as a first approximation.

It has to be pointed out that the expression for the energy dependent multiphonon capture probability that we obtained does not show any restrictions on the free-carrier energy, the strength of the electron-lattice coupling, or the temperature. It can be shown that the given expression is identical to the result in Ref. 11 in the weak coupling limit and for low carrier energies. Moreover, it reduces to the result given in Ref. 1 (p. 142ff) for low temperatures and weak coupling. Finally, it is comparable to the form obtained by Ridley,<sup>12</sup> who uses the adiabatic approach and considers the low temperature and weak coupling cases. In this way, we overcome previous limitations on the coupling strength and the freecarrier energy. Using the theoretical framework developed, it is now possible to describe hot electron effects on the capture cross section even for strong coupling where, in accordance with the configuration coordinate diagram, an enhanced capture of hot electrons is expected.

In Fig. 2, the multiphonon capture probability given by Eq. (5) is shown as a function of the reduced carrier energy  $\varepsilon/E_T$  in the case of a high lattice temperature. The energy depth of the deep level  $E_T$  has been arbitrarily chosen as 0.3 eV. The dimensionless parameter  $\eta$  is defined as  $\eta$  $:=S\hbar \omega/E_T$  and specifies the strength of the electron-lattice coupling of the defect. Obviously, in the case of weak coupling, a monotonic decrease of the capture probability is obtained when the carrier energy is increased. For strong coupling the capture probability first increases, reaches a maximum, and decreases for sufficiently high energies. It is important to recognize that in the case of strong coupling, the



FIG. 3. Free-carrier energy dependence of the multiphonon capture probability for different coupling strengths  $\eta$  and different phonon energies  $\xi := \hbar \omega / E_T$  at T = 77 K. The dotted line depicts the low temperature approximation.

capture probability can increase at room temperature over several orders of magnitude. At low temperatures, this behavior is even more pronounced, as is shown in Fig. 3.

Additionally, the high and low temperature approximations of the capture probability are shown in Figs. 2 and 3 for a specific coupling strength (dotted line). For high temperatures ( $k_B T \gg \hbar \omega/2$ ) the energy dependent capture probability can be approximated by

$$P_{cap}(\varepsilon) \propto \exp\left[-\frac{(E_T - S\hbar\omega + \varepsilon)^2}{4 S\hbar\omega k_B T}\right],\tag{6}$$

or, written in reduced quantities,

$$P_{cap}(\varepsilon) \propto \exp\left[-\frac{(\varepsilon/E_T - \eta + 1)^2}{4 \eta k_B T/E_T}\right].$$
 (7)

This relationship can also be recognized in the general result in Fig. 2 which approximately shows a parabolic energy dependence in the depicted logarithmic scale. Moreover, the high temperature approximation describes the thermally activated behavior of the capture cross section  $\sigma \propto \exp(-E_B/k_BT)$ , where the capture barrier  $E_B$  is given by  $(E_T - S\hbar\omega)^2/4S\hbar\omega$  in the case of low energetic carriers. Furthermore, it explains the resonant energy dependence for strong coupling  $(S\hbar\omega \ge E_T)$ , where the capture probability takes a maximum value at  $\varepsilon_{res} = S\hbar\omega - E_T$ . This is in agreement with Fig. 1(b): the capture barrier vanishes if carriers with this energy are considered.

In the low temperature limit  $(k_B T \ll \hbar \omega/2)$ , the capture probability can be approximated by

$$P_{cap}(\varepsilon) \propto \exp\left\{-\frac{1}{\xi}\left(1+\frac{\varepsilon}{E_T}\right)\left[\ln\frac{1}{\eta}\left(1+\frac{\varepsilon}{E_T}\right)-1\right]\right\},\quad(8)$$

where  $\xi := \hbar \omega / E_T$  specifies the frequency of the coupling phonon mode. The phonon frequency determines the temperature ( $k_B T = \hbar \omega / 2$ ) that separates the low temperature saturation regime and the high temperature thermally activated regime of the capture probability and the capture cross section.

So far, the influence of temperature, coupling strength, and phonon frequency on the energy dependence of the capture probability has been pointed out. Now we extend our investigation of carrier capture by incorporating the analytical expression of Eq. (5) into a Monte Carlo transport simulation.

### **III. MONTE CARLO MODELING OF HOT ELECTRON** CAPTURE BY MULTIPHONON EMISSION

To investigate the electric field influence on the nonradiative capture cross section, the multiphonon capture probability is considered self-consistently with the energy distribution of free carriers for a given electric field. With knowledge of the mean capture probability  $\langle P_{cap}(\varepsilon) \rangle$  and the average carrier velocity  $\langle v \rangle$ , the electron capture cross section can be calculated from  $\sigma_n = \langle P_{cap}(\varepsilon) \rangle / \langle v \rangle$ . The mean capture probability  $\langle P_{cap}(\varepsilon) \rangle$  is by definition

$$\langle P_{cap}(\varepsilon) \rangle = \frac{\int P_{cap}(\varepsilon) f(\varepsilon) D(\varepsilon) d\varepsilon}{\int f(\varepsilon) D(\varepsilon) d\varepsilon},$$
 (9)

where  $f(\varepsilon)$  denotes the electron distribution function in energy space and  $D(\varepsilon)$  the density of states in the conduction band.

Incorporating the energy dependent multiphonon capture probability in addition to the usual scattering mechanisms<sup>13</sup> into a Monte Carlo transport simulation allows calculation of  $\langle P_{cap}(\varepsilon) \rangle$  by means of a time and/or ensemble average. Then  $\sigma_n$  in the presence of an electric field is obtained. In general, this leads to a long computation time due to the large difference in time scales of the capture events and the scattering processes.

To overcome this difficulty, we propose to calculate first the distribution function  $f(\varepsilon)$  for each considered electric field strength before Eq. (9) is used. The distribution function  $f(\varepsilon)$  is by definition the distribution that evolves selfconsistently in the presence of capture, emission, and scattering processes. Due to the higher rate of scattering processes, the capture and emission events modify in general only the integrated distribution, i.e., the electron density, whereas the functional shape of the energy (or wave vector) distribution remains unaltered. This reasoning is restricted to nondegenerate materials. In the case of a degenerate material, the variation of density due to capture or emission events is accompanied by a shift of the Fermi level, resulting in a modified shape of the energy distribution function.

Restricting ourselves to nondegenerate materials, the distribution function in the presence of capture and emission processes is simply proportional to the distribution function in the absence of them. Therefore, the distribution obtained by ignoring these events in the Monte Carlo simulation can be used to calculate the mean capture probability with Eq. (9). In this manner, only the usual Monte Carlo simulation on the time scale of the scattering processes has to be performed for each electric field strength considered.

In the Monte Carlo simulation, the band structure of the semiconductor InP is approximated by using a three-valley model which takes into account the nonparabolicity of each PRB 61



FIG. 4. Calculated electric field dependence of the electron capture cross section in InP at T = 300 K for different lattice relaxation energies  $E_R = S\hbar\omega$  specifying different values of the coupling strength. The energy depth  $E_T$  has been chosen as 0.3 eV.

valley. The scattering mechanisms in the simulation include intravalley and intervalley phonon scattering as well as ionized impurity scattering. The material parameters, such as, for instance, the coupling constants and the valley separation energies, have been extracted from the literature,<sup>14</sup> yielding a velocity-field characteristic in close agreement with the available experimental data.<sup>15,16</sup>

#### **IV. RESULTS FOR InP:Fe AND DISCUSSION**

Using the procedure described above, the electron capture cross section in InP has been calculated as a function of the electric field strength at room temperature. The results are shown in Fig. 4 for several values of the coupling strength, specified by the lattice relaxation energy  $E_R = S\hbar \omega$ . The high field capture cross section is shown to vary over six orders of magnitude as a function of  $E_R$ . With respect to its thermal value, a significant enhancement of the cross section in the presence of a high electric field is obtained for strong coupling, whereas, in the case of weak coupling, the electric field causes the capture cross section to decrease. Thus, the widely accepted picture of capture occurring mainly from the bottom of the conduction band, which leads to a reduced capture cross section in the presence of a high electric field, is restricted to the case of weak electron-lattice interaction in the framework of multiphonon theory.

It is interesting to note that the electron capture cross section varies only slightly for electric fields approximately in the range of 15 kV/cm to 100 kV/cm, especially for strong coupling. This may be surprising, remembering the Gaussian shape of the capture probability as a function of the carrier energy, which suggests a resonant structure for the electric field dependence of the capture cross section. The weak dependence of the capture cross section on the electric field strength in the considered electric field regime can be explained by the almost constant mean total electron energy. This is depicted in Fig. 5, which shows the Monte Carlo result for the mean total energy as a function of the electric field strength in *n*-type InP. It is well known that the stationary drift velocity in InP reaches its maximum value for an electric field of approximately 10 kV/cm due to increasing occupation of the upper valleys. Simultaneously, the carrier heating as a function of the electric field slows down due to



FIG. 5. Calculated mean electron energy as a function of the electric field in *n*-type InP at T=300 K and T=77 K.

the larger effective mass in the upper valleys. A slow increase of the mean electron energy for electric fields between 10 kV/cm and 100 kV/cm is necessary to obtain a broad plateau of the capture cross section.

Similarly, the saturation of the electron capture cross section in Fe-doped GaAs for electric fields between 6 kV/cm and 90 kV/cm, as reported in Ref. 2, can be explained by considering that the maximum drift velocity in GaAs is reached at approximately 5 kV/cm. Moreover, the results in Fig. 4 convince us that the experimentally observed<sup>3</sup> saturation of the electron capture cross section in InP:Fe for electric field strengths of 40 to 140 kV/cm can be described consistently by our theoretical investigation. To show this in more detail, we will now consider the electron capture cross section for the Fe center in InP and the available experimental data.<sup>3</sup> In Ref. 3, a capture barrier of  $E_B = 0.138$  eV was obtained for the thermal electron capture cross section. For a given capture barrier, the energy depth  $E_T$  and the lattice relaxation energy  $E_R = S\hbar \omega$  are related to each other by  $E_R$  $=(E_T-E_R)^2/4E_R$ . This mutual dependence of the trap parameters is illustrated in Fig. 6 where  $E_R$  is plotted as a function of  $E_T$  with  $E_B$  as a parameter. Due to the quadratic relation, there are in general two solutions for the lattice relaxation energy  $E_R$  if  $E_T$  and  $E_B$  are given, one for weak and another one for strong coupling. These two regimes can easily be identified in Fig. 6.

The reported increase of the electron capture cross section for high electric fields<sup>3</sup> leads us to reject the weak coupling solution. In this way, we are restricted to one set of  $E_R(E_T)$ for  $E_B = 0.138$  eV with the energy depth as the only free parameter. Since the electrons can be captured directly by the ground state  $\operatorname{Fe}^{2+}({}^{5}E)$  or by the excited state  $\operatorname{Fe}^{2+}({}^{5}T_{2})$ , followed by an internal relaxation to the ground state, the energy depth concerning capture is unknown a priori. Hence, we have performed calculations by varying the energy depth  $E_T$  and by using the corresponding values of  $E_R$  $=S\hbar\omega$  which yield a capture barrier of 0.138 eV. The results are shown in Fig. 7 together with the experimental values of Ref. 3. As can be seen from this figure, the experimental data are very accurately described if an energy depth of  $E_T = 0.3$  $\pm 0.1$  eV is used. This value of  $E_T$  suggests that the electron capture can be attributed to the excited state  $Fe^{2+}({}^{5}T_{2})$ , the energetic position of which has been determined by optical



FIG. 6. Contour plot of the multiphonon capture barrier  $E_B$  (equi- $E_B$ -lines in eV) as a function of the trap energy depth  $E_T$  and the lattice relaxation energy  $E_R = S\hbar \omega$ .

measurements to be approximately 0.3 eV below the conduction band, whereas the ground state  $\text{Fe}^{2+}({}^{5}E)$  is located deeper in the gap at  $E_{C}$ -0.6 eV.<sup>8</sup>

This interpretation of capture via the excited state is confirmed by the fact that the value of  $\sigma_{\infty} = 1.3 \times 10^{-14} \text{ cm}^2$ , obtained in Ref. 3 from emission experiments in the limit of 1/T=0, differs from the extrapolated value from capture data  $(\sigma_{\infty} = 1.8 \times 10^{-15} \text{ cm}^2)$  by one order of magnitude. This indicates that capture and emission involve two different levels. Assuming that the electrons are emitted from the ground state, it is consistent to attribute the capture to the excited state.

Furthermore, it is suggested that the excited state couples strongly to the lattice. The lattice relaxation energy, the socalled Franck-Condon shift, obtained from the calculations is approximately 1.1 eV, which is comparable to the value obtained for the *DX* centers in Si or Sn-doped  $Al_xGa_{1-x}As$ .<sup>9,17</sup> This strong coupling could also be the reason for the persistent currents observed in highly-Fe-doped InP at low temperatures<sup>18</sup>; radiative capture is not possible for a deep center with large lattice relaxation energy  $S\hbar \omega$ . Moreover,



FIG. 7. Comparison between the simulation results using different trap parameters (curves) and experimental data (Ref. 3) (symbols) of the electron capture cross section in InP:Fe as a function of the electric field strength at room temperature. The trap parameters used in the simulation have been chosen to yield a capture barrier of 0.138 eV.



FIG. 8. Calculated temperature dependence of the electron capture cross section in InP:Fe for different electric field strengths Fusing a phonon energy of 0.021 eV. The symbols represent the experimental data of Ref. 3. To illustrate the sensitivity to the phonon energy, which leads to an uncertainty at very low temperatures, the calculated thermal cross section using a phonon energy of 0.043 eV is also shown (broken line).

optical measurements<sup>19</sup> indicate no large Franck-Condon shift of the ground state, which gives further evidence that the level involved in the capture process is the excited state.

Finally, in Fig. 8, the electron capture cross section in InP:Fe is shown as a function of the inverse temperature with the electric field as a parameter. One can easily recognize the lowering of the capture barrier for high electric fields. As there is no information available about the low temperature behavior of the thermal electron capture cross section, the theoretical prediction for a zero electric field is shown for two different values of the phonon frequency (compare the broken line and the lowest continuous line). This illustrates the direct influence of the phonon frequency on the temperature  $k_B T = \hbar \omega/2$  that separates the high temperature thermally activated and the low temperature saturation regime of the thermal capture cross section. Finally, it should be

pointed out that the temperature and the electric field dependence of the capture cross section in Fig. 8 is of striking similarity to the behavior reported in Ref. 2 for several deep levels in GaAs.

In summary, an excellent agreement between the experimental data and our theoretical calculations has been obtained concerning the electric field and the temperature dependence of the electron capture cross section in InP:Fe.

#### V. SUMMARY

It has been shown that hot electron capture can be explained within the framework of a multiphonon theory in the case of a strong electron-lattice interaction of the deep level. This conclusion has been reached by analyzing the multiphonon capture probability with regard to its detailed freecarrier energy dependence. It is pointed out that the expression deduced for the multiphonon capture probability does not show any restrictions on the carrier energy or the coupling strength. By performing a Monte Carlo transport simulation, the enhanced capture of hot electrons, as is observed in  $Al_rGa_{1-r}As$  for *DX* centers,<sup>4</sup> can be explained. In addition, the lowering of the capture barrier in the presence of a high electric field, reported for a variety of deep levels in GaAs (Ref. 2) and InP (Ref. 3), is demonstrated. Moreover, by means of a quantitative comparison, excellent agreement between the calculated and the experimentally measured<sup>3</sup> electron capture cross sections in InP:Fe as a function of the electric field and the lattice temperature has been obtained. The Monte Carlo results reveal that the slow increase of the mean carrier energy for increasing intermediate electric fields leads to a plateau of the capture cross section in the case of strong coupling.

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