Comprehensive Monte Carlo simulation of the nonradiative carrier capture process by impurities in semiconductors

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The main nonradiative capture mechanisms, cascade and multiphonon emission, have been numerically simulated by the Monte Carlo method. To do so, both mechanisms were included in the frame of a previous numerical procedure to which the nonacoustic-phonon contribution was also added. Different centers were studied. Capture by shallow donors (P, As, and Sb) in n-type silicon were interpreted considering only the cascade process. Capture by acceptors levels of platinum, gold, and titanium in silicon, and one level of Cr, EL2, and EL3 in gallium arsenide, were analyzed considering only multiphonon emission, and calculating the values of Huang–Rhys factor when it is not available. In the study of capture by attractive deep centers, such as single ionized donor centers of sulfur and selenium in silicon, both cascade and multiphonon mechanisms must be combined. In this case the importance of the nonacoustic phonon has been shown in the cascade process. © 1995 American Institute of Physics.

I. INTRODUCTION

The capture of a carrier by an impurity, with phonon emission, has been widely studied since the 1950s.1–4 Several capture models with relative success to explain experimental data have been proposed. Each of these models is applied according to the depth of the impurity level in the gap and its charge state. Basically, there are two well-known models to explain the capture by phonon emission: the cascade process5,6 and the multiphonon mechanism.3,4

The aim of this work is to present the results of a comprehensive study of nonradiative carrier capture by a variety of impurities in several materials and considering different mechanisms of capture. This study has been performed using the Monte Carlo method in which, in addition to the scattering processes of the lattice, the capture mechanisms have been included as one more mechanism in semiconductor transport. We have therefore been able to check the hypotheses made in the former theoretical models proposed for capture and their temperature range of applicability, calculate values of parameters very difficult to obtain experimentally or theoretically, and clarify the values of other parameters used up to now.

A method for studying carrier capture by the cascade process in a Monte Carlo simulation was proposed by Reggiani et al.5 We have applied this method and extended it to other situations. In particular we have included the multiphonon process. This mechanism has been studied using a multiphonon emission rate without arbitrary parameters by a simple assumption set.

In Sec. II a brief review of capture models is made, focusing on unsolved questions and unclear hypothesis; impurities are classified according to the capture process in this section. The details and the main results of our simulation procedures are given in Sec. III. Every model has been checked separately, comparing the thermal behavior of the capture cross-section values (calculated by Monte Carlo simulation and available experimental data) for several centers and semiconductors. We have also simulated the carrier-capture process in an impurity in which both capture mechanisms participate, fitting the numerical results to the experimental data for the thermal dependence of the capture cross sections. Finally, some conclusions are provided.

Despite the simplifying assumptions used in our models, we have verified that they are good approximations of reality due to agreement between the experimental and numerical data. These models have thus provided an easy way to understand the capture process.

II. REVIEW OF CAPTURE MODELS

A. Cascade process

The capture process by one-phonon cascade, proposed by Lax1 in 1960 and widely developed by the Leningrad group,2 has had a certain success in explaining the capture cross sections of charged centers. This model has mainly been applied to interpret the capture by shallow donors and acceptors in Si and Ge. The charged defect is considered as an attractive Coulombic potential and the carrier in the band is considered as a free carrier approaching the defect. The carrier is only captured if there is an adequate mechanism allowing the electron to lose energy. The higher excited states of the hydrogenic series, produced by the Coulombic potential, are assumed to be unaffected by the presence of a short-range term in the impurity potential. Moreover, these states are assumed to be so close to the band edge and so close to each other that the carrier can easily reach one and move among the states of the defect assisted by only one lattice phonon. This means that this set of higher excited discrete states of the defect can be treated as a continuum. Since the probability of one-phonon transition is high, these transitions allow the carrier to leave the band and enter the defect region. The carrier descends through this excited-state series, losing energy by successive emissions of one phonon
until the distance between excited states is so large that one-phonon transition is impossible. Therefore, reaching the fundamental state with one-phonon transition is improbable, even for shallow impurities, unless a multiphonon transition takes place (in the case of nonradiative capture). One-phonon emission in the transition between excited states of an impurity is named the cascade process. At very low temperatures (lower than 50 K), when a carrier is captured by the excited states (so it does not participate in conduction), this charge carrier can be considered captured, since the probability of reemission to the band is negligible.

To determine the possibility of the carrier really being captured or going to the band due to phonon absorption, a “sticking” probability is defined. This probability is used to obtain the averaged capture cross section by integrating to all the allowed energies for the carrier in the excited states, and then averaging the result with the thermal-carrier velocity over the energy-distribution function of the carrier in the band. The main drawbacks and discrepancies to applying this theory come from the sometimes very difficult calculation of the sticking probability.

In addition to this difficulty, another question is the range of bound states having influence in the capture process. Although not universally accepted, some workers have upheld that the excited states whose energy falls into an interval $K_B T$, next to the band edge, are the most important in the capture process and are responsible for the thermal behavior of the capture cross section. Based on this assumption, the Leningrad group calculated a compact expression for the capture cross section by the cascade process.

Another unclear question is what kind of phonon takes part in the cascade process. It has been pointed out that in impurities in Si transitions by nonacoustic phonons are unimportant for the cascade process even at high temperatures. In this article, however, we show that the contribution of optical phonons is not negligible in reproducing the experimental data.

An attractive potential that produces excited states with energies very close to each other is essential for this theory to be applied. There is no experimental evidence of the existence of these states in cases of neutral centers, so this model may not be applied in those circumstances.

### B. Capture by multiphonon emission

In order to explain the nonradiative capture of a carrier by an impurity, there is another theory related to a process in which a simultaneous emission of several phonons takes place. This mechanism is essential when the carrier loses an energy higher than the energy corresponding to a single phonon. This takes place when the transition of the carrier is from the band or from one excited state to the fundamental state of the impurity. The first case (the carrier from the band) occurs in neutral impurities, since there are no excited states. The second case is more probable with deep- or shallow-charged impurities and takes place after a cascade process, as we will see below.

To date, many theoretical works have been published in this area. We have focused our attention on the theory proposed and developed by Ridley, who obtained the multiphonon emission probability $w_{mph}$ using several approximations. He supposed the adiabatic approximation to be valid, and the existence of a weak coupling with a one lattice vibronic mode. Under these conditions, for a carrier energy near the band edge and in the range of low temperatures, the following expression is given:

$$w_{mph} = w_0 (n + 1)^2 e^{-2nS},$$

$$w_0 = \frac{2\sigma \pi \hbar \omega e^{-S}}{(p-1)!} \left[ R_0 + R_1 (p-1) \right] \frac{V_T}{V},$$

where $S$ is the Huang–Rhys factor, $n$ the Bose–Einstein number of the phonon with frequency $\omega$, $R_0$ and $R_1$ can be considered as constants, and $p$ is the number of phonons emitted in the capture process. $V_T$ is the effective impurity volume and $V$ the cavity volume. The mathematical condition of validity of Eq. (1) is $(p + 4)^2 > 4S^2 n (n + 1)$.

In order to obtain physical insight on this hypothesis, a significant problem is the great amount of free parameters left in the final expression. If values are assigned to the parameters and agreement with experimental results is used as a test of validity, different combinations of these parameters are found to fit a same experimental curve. Consequently, there is great dispersion in the values assigned to the parameters in the literature, mainly in the following points.

The phonon frequency used in the multiphonon emission. Whereas Henry and Lang considered that the transition implies a lattice phonon, others have speculated about different local phonons with a frequency similar to the lattice one.

The $S$ factor has been calculated by optic measurements only for a few deep centers; therefore, this free parameter may be used to fit theoretical values and experimental data. A good agreement with different measurements in a same center can be found by simply changing the value of the Huang–Rhys factor in Eq. (1).

The effective impurity volume $V_T$ with the quantum-defect model can be approximated as

$$V_T = 4\pi \frac{r_T^3}{3},$$

$$r_T = a^* \nu_T,$$

where $a^* = m e a_{oH}/m* e_o$, $a_{oH}$ being Bohr’s radius, $m$ and $m*$ the mass and the effective mass of the electron, $e_0$ the vacuum dielectric constant, and $\epsilon$ the semiconductor permittivity. $\nu_T = (R_{HH}/E_T)$ with $R_{HH}$ being the effective Bohr energy and $E_T$ the energy of the deep level associated to the center. However, according to some studies, the electronic wave-function ratio of the bound state is almost independent of the impurity, and is higher than the ratio defined by the quantum-defect model. As may be seen, therefore, this subject is still unclear.

One of the aims of this work was to determine the values of these parameters by fitting the results of our numerical simulation with experimental data available in the literature. Nevertheless, for this purpose we needed a model with very few free parameters.
C. Two-step capture model

As mentioned above (and as referred to by some reviews), the cascade process and multiphonon emission can be simultaneously present in the capture process of a free carrier by an impurity in a semiconductor. In 1977 a capture model in two steps, where both mechanisms were involved, was formally proposed. This model has been applied to explain the thermal dependence of the capture cross sections of deep centers with an attractive state of charge before capturing a carrier, and neutral when the carrier is trapped. Because of the initial attractive state of the impurity, a Coulombic distribution of excited states is expected to occur near the band edge inside the gap. According to this theory, the capture of a carrier occurs in two steps. First, the cascade process through the excited states lets the carrier descend to the lowest-energy state that is accessible \( E_1 \), by the emission of one or two phonons. Second, there is a jump to the fundamental level by multiphonon emission.

The capture cross section proposed was the combination of both mechanisms,

\[
\sigma_T = \frac{\sigma_c \nu}{\nu + \sigma_{\nu, th} N e^{-E_1/K_B T}},
\]

where \( \sigma_c \) is the capture cross section by cascade to the lowest accessible state (with an energy of \( E_1 \) related to the band edge), \( \nu \) the multiphonon emission probability, \( \nu, th \) the carrier thermal velocity, and \( N \) the effective-state density of the band. Depending on the temperature, one mechanism or the other will be dominant and decide the behavior of the total cross section; however, if the multiphonon-emission probability is temperature independent, the thermal behavior of the total cross section is governed by the cascade process. In particular, at low temperatures, when \( \sigma_c \nu, th N \exp(-E_1/K_B T) \ll \nu \), then \( \sigma_T = \sigma_c \).

This model has been successful in reproducing the thermal dependence of the capture cross sections of the element group of sulfur (S and Se) in Si, using \( E_1 \) as a fitting parameter, however, the assumption that the multiphonon transition is only possible from the lowest accessible state by cascade is not clear. We show that, with a normal range of values of the Huang–Rhys factor, and allowing multiphonon transition to be possible from any of the excited states, our simulation results agree with experimental data.

Once information about the capture mechanisms by phonon emission was amassed, we were able to establish a center classification according to the capture mechanisms that take place in the capture of free carriers from the bands, as follows.

(a) The first are repulsive and neutral centers, which do not create excited states close to each other when next to the band. The most probable capture mechanism in these kind of centers is only a multiphonon transition in which case the trapped carrier comes from the band.

(b) The second are attractive centers, both deep and shallow, in which we can admit the two-step-capture model. The difference between the shallow and the deep centers is the phonons involved in the last step by multiphonon transition, the phonons in the first case being of lower energy than in the second. However, for charged deep levels in GaAs, where the region of the excited Coulombic states is almost negligible, the contribution of the cascade process is not important and we have only considered multiphonon emission from the conduction band, with good results.

III. MONTE CARLO SIMULATION OF NONRADIATIVE CAPTURE PROCESSES

The aim of this work was to determine which mechanisms were involved in the capture process for different kinds of centers, trying to answer the unclear questions mentioned above. To do so we have considered the capture of an electron from the conduction band by deep and shallow impurities in silicon and deep centers in GaAs.

Due to the possibility of combining the scattering events in the semiconductor with the capture mechanism, the Monte Carlo method has demonstrated itself to be an ideal procedure for studying the nonradiative capture mechanism at a microscopic level. We have used it to obtain a complete dependence on temperature of the capture cross sections for different mechanisms, as shown in this section. Comparison with experimental data taken from the literature has allowed us to propose the type of phonon and the mechanism that cause a capture process.

All phonon-scattering mechanisms were included in the simulation of the electron transport in the conduction band, acoustic phonons, intervalley, and intravalley nonpolar optical phonons. Elastic scattering was omitted since we are interested in scattering that involves a change of energy. The nonparabolic effect was included both in Si and GaAs. We also considered the three lowest minima of the GaAs conduction band. The phonon energies and the coupling constants were taken from Ref. 11 for silicon and Ref. 12 for gallium arsenide. In this work, capture processes were simulated at equilibrium, with zero electric field.

Below is a description of how capture mechanisms were included in the Monte Carlo procedure to simulate total semiconductor transport.

A. Cascade process

To incorporate the cascade process we followed the procedure proposed by Reggiani et al. in p-Si at very low temperatures, studying the motion of an electron that interacts with a Coulombic perturbation. The system is reduced to the energy configuration of an impurity center. In our simulations we considered that first excited level to be located at \( E^{(1)} = -11.5 \text{ meV} \) in Si, where the zero-energy level is at the bottom of the conduction band.

An equilibrium situation is considered and a representation of the total energy (the carrier kinetic energy and the potential energy caused by impurity Coulombic potential) is used. Therefore, the carrier kinetic energy \( E_K \) is equal to the total energy \( E_0 \) minus the potential one \( U(r) \),

\[
E_K = E_0 - U(r),
\]

\[
U(r) = -\frac{e^2}{4\pi \varepsilon r}
\]
where $e$ is the electron charge and $r$ the position related to the impurity. The negative energy was assigned to the bound states. To reduce the simulation to the one-impurity range, spatial averaging of both the energy-state density and the scattering probabilities $A(E_0)$, were done,

$$A(E_0) = \langle A(E_k) \rangle = \frac{\int_{r_0}^{r_{\infty}} A(E_k) r^2 dr}{\int_{r_0}^{r_{\infty}} r^2 dr}, \quad (5)$$

where $r_A = N_T^{-1/3}$ is the average semidistance between impurities in a sample with an impurity concentration of $N_T$, $r_m$ is determined by the carrier energy: $r_m = r_A$ for $E_0 > -E'_0$, and $r_m = -r_B E'/E_0$ for $-E' > E_0 < -E'_0$, with $E_0 = e^2/4\pi\epsilon r_A$.

The averaged capture cross section $\sigma_c$ is calculated from

$$\sigma_c = \frac{1}{\tau_0 N_T(v)} \int_{r_0}^{r_{\infty}} \sigma(A) r^2 dr,$$  \quad (6)

where $N_T$ is the empty-impurity concentration. Equilibrium thermal velocity $\langle v \rangle$ is calculated in the simulation. The averaged capture time, also calculated with our numerical procedure, $\tau_c$, is defined as the time that the carrier spends in the band divided by the number of transitions to the excited-state region. Obviously, it is necessary to define a cutoff energy $E_c$, below which the electron is considered to be captured. In accordance with this definition, two types of transitions can be distinguished: transitions causing an electron go below $E_c$, thus becoming captured, and transitions making an electron go below zero energy and then rise without reaching $E_c$ level. We calculated different cross sections by considering the electron to be captured when its energy falls below zero, and by requiring its energy to fall below $E_c$. These two capture cross-section values are named $\sigma_{1ac}$ and $\sigma_{2ac}$, respectively, where $\sigma_{1ac} \neq \sigma_{2ac}$. In the first case, reemission to the band is not allowed. In this article we have chosen $E_c = -K_B T$, where $K_B$ is the Boltzmann constant and $T$ the absolute temperature.

We have used this procedure to study n-type silicon. As we have mentioned above, among the inelastic mechanisms we included the nonpolar optical-phonon interaction to improve the procedure described in Ref. 5. Although this mechanism is negligible at temperatures lower than 70 K (as we confirmed by simulation), it must be considered at higher temperatures for a total simulation of the two-step-capture process.

The behavior of the average cross sections for the capture of electrons by shallow-donor impurities in n-type Si is shown in Fig. 1. The two curves shown in the figure correspond to $\sigma_{1ac}$ and $\sigma_{2ac}$, respectively (defined above). Experimental data available in the literature referring to shallow donors P, As, and Sb in silicon, have also been plotted for comparison. A good agreement with the results of our simulation can be noted, which can be taken as a validity test of the model and the calculation.

**D. Multiphonon mechanism**

To study the multiphonon mechanism, we introduced the multiphonon-emission probability in the calculus procedure, with a set of assumptions similar to those in the cascade process. We also reduced the simulation to the energy-configuration space of an impurity center.

To do so, we have first replaced volume $V$ in Eq. (1) by the average volume of an impurity in a sample with an impurity concentration of $N_T$, obtaining the following expression for the probability:

$$\langle w_{mph} \rangle_{\text{space}} = w_{mph} V \frac{3N_T}{4\pi} \quad (7)$$

When Eq. (7) was used, we supposed that the impurities were so separated from each other there was no interaction among them (valid for the usual concentrations in semiconductor devices). Because of the proportional dependence of $\langle w_{mph} \rangle_{\text{space}}$ with the center density, the capture cross section is concentration independent [Eq. (6)], as also observed in experimental data. In any case, this point has been confirmed by simulation.

Second, we made the following assumptions about the free parameters mentioned in the previous review of this mechanism. The lattice phonon frequency was used in the multiphonon emission\(^1\) which choice allowed us to simplify the study. We chose the longitudinal optical phonon (LO) for the centers in Si and the polar optical phonon in GaAs.

For the Huang–Rhys factor $S$ we chose experimental data, where available in the literature. We found the values of $S$ for some centers. For the electron capture of the acceptor deep levels of Pt and Au in Si, $S = 0.3$ and $S = 1.3$, respectively, obtained by optical techniques,\(^1\) for the GaAs:Cr system the value $S = 3$ was measured.\(^4\) Although the $S$ factor has been published for few cases, we used them to test the validity of our calculation and model. When we were certain that the results were acceptable we were able to determine the values necessary to achieve a good outcome, providing the $S$ value, for cases where it is unknown. These results are shown below.

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FIG. 1. Average capture cross section of donor impurities in n-type Si at equilibrium as a function of temperature. The donor concentration was $N_D = 10^{13}$ cm$^{-3}$. The dashed and solid lines represent the simulated curves $\sigma_{1ac}$ and $\sigma_{2ac}$. The symbols represent experimental data: (A) from Ref. 14; (+) from Ref. 15; and (L) from Ref. 16 for Si:P; (*) from Ref. 14 for Si:As; and (X) from Ref. 15 for Si:Sb.

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\(^4\)J. Appl. Phys., Vol. 77, No. 5, 1 March 1995

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\(^6\)J. Appl. Phys., Vol. 77, No. 5, 1 March 1995

\(^7\)J. Appl. Phys., Vol. 77, No. 5, 1 March 1995

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According to previous work on the wave function of the bound state, the effective-impurity ratio of the bound-state wave function is assumed to be approximately independent of the impurity, and spreads out several η defined in the quantum-defect model. Therefore, in the case of centers in silicon, a ratio dependent on the lattice only was used in the simulation,

\[ V_r = \frac{4\pi a^*}{3} \]

where \( a^* \) is the effective Bohr ratio. For impurities in GaAs the effective ratio is calculated from Eq. (2).

To sum up, we used the expression of the multiphonon-emission probability with the above assumptions and with only the \( S \) factor as a free parameter when it was unknown, and without any free parameter in the cases in which \( S \) was known. To simulate the multiphonon mechanism, electron capture by acceptor levels in Si and GaAs were studied. At a given temperature, every electron starts with an average energy and undergoes a certain number of scattering events. The capture mechanism is not yet introduced at that point, thus, an electron with a energy according to the energy distribution corresponding to this temperature is obtained. Then, the capture mechanisms (cascade and/or multiphonon) are activated, and the time that an electron spends in the conduction band \( \tau_d \) is recorded. When the multiphonon event occurs, the electron is considered to have been captured by the center. The number of simulated electrons was high enough to obtain a low average deviation of the parameters. Once the simulation was finished, the average thermal velocity in equilibrium (\( \langle V \rangle \)) and the average capture time \( \tau_c \) (mean value of \( \tau_c \)) were obtained. The average capture cross section is determined according to Eq. (6).

The good agreement with the experiment obtained in these cases allow us to consider the other parameters as very good approximations. When \( S \) was not known, our procedure allowed us to calculate it by comparing the simulated and experimental capture cross sections as a function of temperature.

Figures 2 and 3 demonstrate the good agreement over a wide range of temperature between the simulated capture cross sections and different experimental data for the acceptor levels of Au and Pt in Si, respectively. The thermal electron velocity has been taken to be \( u_{th}^{*} = 2.07 \times 10^7 (T/300)^{1/2} \) cm/s to unify the experimental data; therefore, some of them have been modified by a scale factor. We have confirmed that the Huang–Rhys parameter values necessary to fit the experimental measurements and the calculated data coincide with the value determined experimentally. The value \( S=1.3 \) had previously been reported for Au (Fig. 2). Due to differences in the experimental data of the capture cross sections, the values of \( S \) needed for our simulations to fit them lay in the interval 1.2–1.35. In Fig. 3, for the system Si:Pt, \( S=0.3 \) was measured\(^{17} \) and all the experimental data were fitted with our numerical results by varying parameter \( S \) in the range 0.35–0.25. The good agreement in these cases, with no free parameters, can be considered as a validation of these values, and of our calculation, allowing us to suppose that our simple assumptions are good approximations to describe the capture process for these kinds of centers. Moreover, in both figures the high sensitivity of the numerical capture cross section with the \( S \) parameter is shown. This fact enhances the accuracy of our procedure for calculating the Huang–Rhys factor when it is not known.

For the acceptor levels of Ti in silicon, in Fig. 4, we have not found information about the values of their \( S \) parameters; therefore, we have used our numerical procedure to calculate the values of \( S \). We determined \( S=1.1 \) and \( S=0.5 \) for centers at 515 and 238 meV from the conduction band, respectively. Another result obtained in this range of temperature is the near independence of these capture cross sections from temperature. In general, this result had not been verified at room temperature, however, it was used as a working hypothesis with metallic neutral centers in Si. It has now been confirmed, with this simulation. An additional conclusion of in-

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**FIG. 2.** Electron capture cross sections of the acceptor deep level of Au in silicon. Lines show the numeric simulations for different Huang–Rhys factors (\( S=1.35, \) dashed line; \( S=1.2, \) solid line), considering only the multiphonon-emission mechanism. Different experimental data are shown with symbols: \((*) \) from Ref. 18; (I) from Ref. 19; and (II) from Ref. 20.

**FIG. 3.** Electron capture cross sections of the acceptor deep level of Pt in silicon. Lines show the numeric simulations for different Huang–Rhys factors (\( S=0.35, \) dashed line; \( S=0.25, \) solid line), considering only the multiphonon-emission mechanism. Different experimental data are shown with symbols: \((+ \) from Ref. 21 and \((\times) \) from Ref. 22.
FIG. 4. Electron capture cross sections of the acceptor deep levels with $E_a - E_F = 0.515 \text{ eV}$ (solid line and circles) and $E_a - E_F = 0.238 \text{ eV}$ (dashed line and squares) of Ti in silicon. Lines show the numeric simulations, considering only the multiphonon-emission mechanism. Symbols represent experimental data from Ref. 23.

FIG. 5. Electron capture cross sections of the Cr level with $E_a - E_F = 0.75 \text{ eV}$ in GaAs. The line shows the numeric simulation, considering only the multiphonon-emission mechanism. Symbols represent experimental data from Ref. 3.

FIG. 6. Electron capture cross sections of EL2 and EL3 levels in GaAs. Lines show the numeric simulation, considering only the multiphonon-emission mechanism. Symbols show the experimental data from Ref. 3.

FIG. 7. Electron capture cross sections of the acceptor deep levels with $E_a - E_F = 0.515 \text{ eV}$ (solid line and circles) and $E_a - E_F = 0.238 \text{ eV}$ (dashed line and squares) of Ti in silicon. Lines show the numeric simulations, considering only the multiphonon-emission mechanism. Symbols represent experimental data from Ref. 23.

FIG. 8. Electron capture cross sections of the acceptor deep levels with $E_a - E_F = 0.515 \text{ eV}$ (solid line and circles) and $E_a - E_F = 0.238 \text{ eV}$ (dashed line and squares) of Ti in silicon. Lines show the numeric simulations, considering only the multiphonon-emission mechanism. Symbols represent experimental data from Ref. 23.

FIG. 6. Electron capture cross sections of EL2 and EL3 levels in GaAs. Lines show the numeric simulation, considering only the multiphonon-emission mechanism. Symbols show the experimental data from Ref. 3.

chosen phonon to be emitted in the multiphonon transition is the polar optical phonon.

Another important fact to note is that, although the validity limit of Eq. (7) is reduced when the capture cross section is derived by theoretical calculus from Eq. (1), our procedure has allowed us to analyze a wide range of temperatures with satisfactory results, as Figs. 2–6 show.

C. Two-step capture

We analyzed deep-charged centers due to the available experimental data, which allowed us to compare them with the capture cross section obtained by our numerical calculation with the Monte Carlo method.

The essential steps necessary to simulate this process are the same as for the cascade mechanism, with the same value of $E^0$. However, the main difference between this case and the cascade method is that in the latter the electron was considered to be captured when its energy lay below a reference level close to the conduction band. In this case, though, at temperatures higher than 70 K the reemission probability to return a carrier back to the band from the excited states is not negligible. Therefore, the mechanism that determines the capture is the multiphonon transition to the fundamental bound state.

The procedure used in the two-step-capture simulation is the following: simulation of the cascade process, but including the multiphonon-transition probability in the whole negative region of energies. The calculation is stopped when the electron undergoes this transition. The average capture cross section is calculated from Eq. (6).

In Figs. 7 and 8, the experimental and calculated cross sections of the acceptor levels are compared for single ionized centers of S and Se in silicon, respectively. As no reported values of $S$ were found, the experimental curves were compared with our calculated ones by varying the values of this parameter until a good agreement was reached, $S=1.1$ being obtained for sulfur and $S=1.4$ for selenium. We checked that the transitions due to optical phonons are important at high temperatures for the cascade process, as
IV. CONCLUSIONS

The different nonradiative carrier-capture mechanisms by impurities have been analyzed. First, characteristics of previous models and theories have been reviewed and different interpretations noted. A classification of the different centers was established according to these mechanisms, with particular attention being paid to their charge state.

The Monte Carlo method was used to develop a complete simulation of the capture processes for various neutral and attractive centers in polar and nonpolar semiconductors. In the simulation of the cascade process, we included the nonacoustic-phonon transitions, which we have shown to play an important role. This procedure was then tested by obtaining numerically the value of the capture cross sections of shallow donors (P, As, and Sb) in silicon, and fitting them with the experimental data. Good agreement was obtained.

In addition, we used the Monte Carlo method to simulate capture process by multiphonon emission. This was possible by making the space average of Ridley’s well-established model for the multiphonon-transition probability. Simultaneously, by a set of simple assumptions, which simplified understanding of the process, we obtained a model in which the undetermined parameters appearing in the probability expression are reduced to zero or one (in the latter case when the Huang–Rhys factor $S$ is not known). Our assumptions suggest an impurity-independent effective volume of the center, in the case of centers in silicon, and lattice phonons are responsible for the multiphonon emission. Due to the good agreement between the experimental and the numerical data in a wide range of temperatures (when there were no free parameters), these assumptions can be considered as adequate approximations of reality. Under these conditions, the values of $S$ that allow our numerical curves to fit the experimental ones are the same as were previously measured for gold and platinum in silicon and chromium in gallium arsenide. We have also used our procedure to calculate parameter $S$ with great sensitivity in cases where we did not find experimental values. $S$ values for the two acceptors levels of Ti in silicon and the EL2 and EL3 levels in GaAs were calculated.

Finally, carrier capture by attractive centers was simulated by combining the calculation for the cascade process the multiphonon probability. Electron capture cross sections by single ionized centers of sulfur and selenium have been perfectly reproduced with our procedure, and we have also shown the importance of the nonacoustic phonon in the cascade process.
