Cascade Capture of Electrons by Ionized Impurities

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An improved theory of cascade capture by ionized impurities in semiconductors has been developed which retains the basic features of Lax's "giant trap" theory, but which uses a distribution function rather than a trajectory description. Assuming infrequent acoustic-phonon transitions, the classical Boltzmann equation describing the capture process near a single ionized impurity is converted into an integral equation for the distribution function in terms of total energy alone. This equation, which treats transitions between free and bound states identically to transitions between two bound states, is then transformed into a closely related integral equation for the "sticking probability." Numerical solution of the latter yields cross sections which are substantially larger than those previously found and which are in good agreement with recent experimental values for the shallow donors in Ge.

1. INTRODUCTION

THE large capture cross sections associated with ionized impurities in semiconductors have been accounted for by Lax[1] in terms of a cascade capture process. In this model the electron is assumed to be captured initially in an excited state of the impurity by the emission of a phonon, after which it emits and absorbs phonons until it either reaches the ground state or is ejected into the conduction band. In Lax's analysis the cascade process was described completely classically on the hypothesis that only the highly excited states were important. Subsequently, Ascarelli and Rodriguez[2] performed a calculation of the cascade capture for the shallow donors in germanium in which the opposite point of view was taken that only the hydrogenic s states with principal quantum number n from 1 to 4 constributed significantly. Their reasoning was based on the fact that for low values of n the capture cross section falls off considerably for states of higher angular momentum, but since this is no longer true for high values of n, where the multiplicity also becomes large, the *a priori* discard of these higher states would seem to be invalid. In this paper we return to Lax's point of view that it is the higher states which are more important and calculate (for weak acoustic-phonon interaction) the steady-state recombination rate on the basis of classical mechanics, assuming as in previous treatments spherical, parabolic bands. However, by using a distribution function approach rather than a trajectory description, we avoid an additional approximation that Lax introduced, which was based on the virial theorem. In this way we obtain cross sections which are substantially larger than those found either by Lax or by Ascarelli and Rodriguez and which are in good agreement with experimental values for the shallow donors in germanium.[3]

2. THE DISTRIBUTION FUNCTION METHOD

The capture process will be described statistically by the classical Boltzmann equation for an electron interacting with an equilibrium acoustic-phonon field in the presence of a Coulomb potential. The electron density will be assumed sufficiently small that the probability of more than one electron being in the vicinity of the ionized impurity is negligible. For simplicity, the recombination will be treated as a steady-state process. The analysis thus strictly applies only to a situation in which there is some generation mechanism, such as light, which prevents electrons from accumulating in the ground state. Actually the capture cross sections obtained will be applicable to transient problems if the capture rate is fast compared to the rate at which the carrier concentration in the conduction band changes. The previous treatments[1,2] are subject to this same restriction, as has been discussed by Lax.[1]

Also, as in the previous treatments, we shall assume that the mean free path for acoustic-phonon interaction is large compared to the greatest bound-state radius of interest, which is valid for Ge and Si at low temperatures. Under these conditions the distribution function is essentially an equilibrium one (that is, a constant) on each surface of fixed total energy. In fact we shall see that the approximation of treating the electron distribution as a function only of total energy yields a transition rate correct to order $(r_0/l)^2$ for a bound state of radius r_0, where l is the acoustic-phonon mean free path. In order to show this we expand the distribution function $f(\mathbf{r},\mathbf{v})$ in spherical harmonics in velocity space and keep only the first two terms:

$$f(\mathbf{r},\mathbf{v})=f_0(\mathbf{r},v)+\mathbf{f}_1(\mathbf{r},v)\cdot\mathbf{v}/v+\cdots, \qquad (1)$$

where we have written the coefficient of the first harmonic as a vector function of position and scalar velocity, the direction of the vector indicating the axis chosen for expansion at each $\mathbf{r}$. These functions obey the equations[4]

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[1] M. Lax, Phys. Rev. **119**, 1502 (1960).
[2] G. Ascarelli and S. Rodriguez, Phys. Rev. **124**, 1321 (1961).
[3] A preliminary account of these results has been given previously: D. R. Hamann and A. L. McWhorter, Bull. Am. Phys. Soc. **8**, 219 (1963).
[4] W. P. Allis, in *Handbuch der Physik*, edited by S. Flügge (Springer-Verlag, Berlin, 1956), Vol. 21, p. 404.

$$\frac{v}{3}\nabla\cdot\mathbf{f}_1(\mathbf{r},v)-\frac{1}{3mv^2}\frac{\partial}{\partial v}[v^2\nabla\phi(\mathbf{r})\cdot\mathbf{f}_1(\mathbf{r},v)]=\left(\frac{\partial f_0}{\partial t}\right)_{\text{coll}}, \quad (2)$$

$$v\nabla f_0(\mathbf{r},v)-\frac{1}{m}\nabla\phi(\mathbf{r})\frac{\partial f_0(\mathbf{r},v)}{\partial v}=\left(\frac{\partial \mathbf{f}_1}{\partial t}\right)_{\text{coll}}, \quad (3)$$

where $\phi(\mathbf{r})$ is the potential energy of the electron in the presence of the ionized impurity. Changing the independent variables from $\mathbf{r}$ and v to $\mathbf{r}$ and the total energy $u=\frac{1}{2}mv^2+\phi(\mathbf{r})$, we have

$$\tfrac{1}{3}\nabla\cdot[v^2(\mathbf{r},u)\mathbf{f}_1(\mathbf{r},u)]=v(\mathbf{r},u)\left(\frac{\partial f_0(\mathbf{r},u)}{\partial t}\right)_{\text{coll}}, \quad (4)$$

and

$$v(\mathbf{r},u)\nabla f_0(\mathbf{r},u)=\left(\frac{\partial \mathbf{f}_1(\mathbf{r},u)}{\partial t}\right)_{\text{coll}}. \quad (5)$$

The explicit expressions for the collision terms are[5]

$$\left(\frac{\partial f_0}{\partial t}\right)_{\text{coll}}=\frac{1}{4m^2s^2lkTv}\int_{-2ms(v-s)}^{2ms(v+s)}d(\hbar\omega)\frac{\hbar\omega|\hbar\omega|}{e^{\hbar\omega/kT}-1}\times[e^{\hbar\omega/kT}f_0(\mathbf{r},u+\hbar\omega)-f_0(\mathbf{r},u)], \quad (6)$$

and

$$\left(\frac{\partial \mathbf{f}_1}{\partial t}\right)_{\text{coll}}=\frac{1}{4m^2s^2lkTv}\int_{-2ms(v-s)}^{2ms(v+s)}d(\hbar\omega)\frac{\hbar\omega|\hbar\omega|}{e^{\hbar\omega/kT}-1}\times[\cos\alpha\, e^{\hbar\omega/kT}\,\mathbf{f}_1(\mathbf{r},u+\hbar\omega)-\mathbf{f}_1(\mathbf{r},u)], \quad (7)$$

where

$$\cos\alpha=\frac{v^2(\mathbf{r},u)+v^2(\mathbf{r},u+\hbar\omega)-(\hbar\omega/ms)^2}{2v(\mathbf{r},u)v(\mathbf{r},u+\hbar\omega)},$$

$$l=\pi\hbar^4\rho s^2/E_1^2kTm^2.$$

E_1 is the deformation potential, ρ is the density of the crystal, and s is the speed of sound, assumed isotropic. The lower integrals in (6) and (7) are to be interpreted as zero if $v(\mathbf{r},u)<s$. We have assumed, along with Lax, that the probability per unit time that a collision will take place can be computed at each point by treating the electron as if it were a plane wave with the energy and momentum appropriate to that point. The quantity l is just the "classical" mean free path for acoustic phonons since $(\partial\mathbf{f}_1/\partial t)_{\text{coll}}$ reduces to $-(\mathbf{f}_1v/l)$ when $kT\gg mvs$ and $v\gg s$.

For negative values of u we may integrate (4) over the volume bounded by the surface of classical turning points, on which $v(\mathbf{r},u)=0$, and obtain

$$\frac{1}{4m^2s^2lkT}\int d\mathbf{r}\int_{-2ms(v-s)}^{2ms(v+s)}d(\hbar\omega)\frac{\hbar\omega|\hbar\omega|}{e^{\hbar\omega/kT}-1}\times[e^{\hbar\omega/kT}f_0(\mathbf{r},u+\hbar\omega)-f_0(\mathbf{r},u)]=0. \quad (8)$$

Equation (8) is just a statement that the rate of increase of electrons with energy u is zero, and hence is a direct consequence of the original steady-state assumption. However, if f_0 were independent of $\mathbf{r}$, then (8) would become an integral equation for $f_0(u)$, which together with the appropriate boundary conditions would actually be sufficient to determine the capture rate. In order to show that f_0 is in fact independent of $\mathbf{r}$ to a good approximation, we return to Eqs. (4) through (7). Introducing explicitly the Coulomb potential energy $\phi(\mathbf{r})=-e^2/\kappa r$, we transform for negative u to the normalized coordinates $\mathbf{q}=\mathbf{r}/r_0(u)$, where $r_0(u)=-e^2/\kappa u$. Since in the new coordinates $v(\mathbf{r},u)=[(2u/m)(1-1/q)]^{1/2}$, the scale factor $1/r_0(u)$ appears only on the left-hand sides of (4) and (5) through the spatial derivatives, while the factor $1/l$ appears only on the right-hand sides through the collision expressions (6) and (7). Hence, if we assume an isotropic distribution of incident electrons, it is clear from (4) that to lowest order $\mathbf{f}_1$ is proportional to (r_0/l) and from (5) that $\nabla_q f_0$ to lowest order is proportional to $(r_0/l)^2$. Thus for $r_0\ll l$ the term dropped in (8) by assuming f_0 to be a function only of u is proportional to $(r_0/l)^2$. The size of the proportionality factor could, in principle, be determined by inserting the approximate solution of (8) into (6) and using (4), (5), and (7) to obtain the correction term to f_0. However, since this would be quite tedious and involve numerical calculation, a rough approximation to this procedure has been carried out in Appendix A. There it is found that the proportionality factor is of the order of unity, and hence, as previously stated, the approximation of taking f_0 to be independent of $\mathbf{r}$ is correct to order $(r_0/l)^2$. The discussion in Appendix A also shows that for $u>0$ we can take f_0 to be independent of $\mathbf{r}$ to the same degree of approximation with r_0 now being the largest radius at which appreciable capture occurs, at most the interimpurity spacing.

Returning then to (8) with f_0 a function of u only, we note that the integrand is independent of $\mathbf{q}$, but that the limits of the $\hbar\omega$ integration depend on the magnitude of q through $v(q,u)$. These limits arose from the restrictions imposed by energy and crystal momentum conservation on the amount of energy that an electron with a given initial speed may exchange. The order of integration in (8) may be interchanged if these limits are replaced by a restriction on the region of space in which a transition involving given initial and final energies may occur. If we carry out such an interchange and perform the $\mathbf{q}$ integration, we find that (8) becomes

$$\int_{-\infty}^{\infty}du'[f_0(u')K(u',u)-f_0(u)K(u,u')]=0, \quad (9)$$

where

$$K(u,u')=\frac{512\pi s^4e^6}{lkT\kappa^3}\frac{4\pi}{3}\frac{(u'-u)|u'-u|}{[(u'-u)^2-4ms^2(u'+u)+4m^2s^4]^3}\times\frac{1}{e^{(u'-u)/kT}-1}. \quad (10)$$

[5] R. Stratton, Proc. Roy. Soc. (London) **A242**, 355 (1957).

In obtaining (10) we have multiplied (8) by $(4\pi/m)$ in order to make $f_0(u)K(u,u')dudu'$ correspond to the total probability of transition from energy shell $(u, u+du)$ to $(u', u'+du')$. It should be remembered that f_0 is still a density in $(\mathbf{r},\mathbf{v})$ space.

Equation (9) holds only for $u<0$. For $u>0$ we may specify $f_0(u)$ arbitrarily since the approximation of neglecting the $\mathbf{r}$ dependence of f_0 means that the positive energy distribution is just that of the incident electron. In particular, if the conduction electrons are in thermal equilibrium at temperature T_e, then

$$f_0(u)=(m/2\pi kT_e)^{3/2}\exp(-u/kT_e).$$

3. STICKING-PROBABILITY FORMULATION OF THE CAPTURE RATE

Since $K(u,u')$ in (10) gives the transition rate from energy u to u', the easiest way to calculate the capture rate would be to shift immediately to Lax's "sticking-probability" formulation,[1] the sticking probability at energy $u<0$ being defined as the probability that an electron of that energy will reach the ground state before escaping into the conduction band. However, we will follow the longer route of setting up the calculation for the capture rate in terms of the integral equation (9) and then transforming to the sticking-probability formulation. This is done partly for the sake of completing the approach already begun, but mainly to show the relation between (9) and Lax's integral equation for the sticking probability.

In the physical problem the capture rate is the rate at which electrons enter the ground state. (As previously discussed, it is assumed in the steady-state analysis that there is some generation mechanism to prevent accumulation of the electrons.) Since the validity of the entire classical-mechanics treatment depends on the fate of the electron being determined before it reaches the ground state, the exact way of mathematically simulating the ground-state sink is not important, as long as it depends only on large negative energies. We will place an absorbing barrier at some finite energy u_0, which will later be allowed to approach negative infinity. The capture rate B_T will then be given by the rate at which electrons cross this barrier:

$$B_T=\int_{-\infty}^{u_0}du\int_{u_0}^{0}du'K(u',u)f_0(u')$$
$$=\int_{u_0}^{0}du'c(u')f_0(u'), \tag{11}$$

where

$$c(u')=\int_{-\infty}^{u_0}K(u',u)du. \tag{12}$$

The upper limit of the u' integration in (11) has been chosen as 0 rather than $+\infty$ because for u_0 sufficiently negative, the rate of direct transitions from the incident distribution to below the barrier will be negligible.

The presence of this barrier must also be reflected in the integral equation for f_0, so (9) will be modified to

$$f_0(u)\int_{-\infty}^{\infty}K(u,u')du'=\int_{u_0}^{0}K(u',u)f_0(u')du'$$
$$+\int_{0}^{\infty}K(u',u)f_0(u')du', \tag{13}$$

where the u' integration on the right-hand side has been divided into two ranges to separate the term

$$s(u)=\int_{0}^{\infty}K(u',u)f_0(u')du', \tag{14}$$

which represents the flux from the incident distribution to the bound states at energy u. If we introduce the normalized kernel

$$\tilde{K}(u',u)=K(u',u)\Big/\int_{-\infty}^{\infty}K(u,u'')du'' \tag{15}$$

and flux

$$\tilde{s}(u)=s(u)\Big/\int_{-\infty}^{\infty}K(u,u'')du'', \tag{16}$$

then (13) may be written in the standard form of an inhomogeneous Fredholm equation of the second kind:

$$f_0(u)=\int_{u_0}^{0}\tilde{K}(u',u)f_0(u')du'+\tilde{s}(u). \tag{17}$$

We now have a complete formulation of the problem, but one which is cumbersome to deal with since for every incident distribution it is necessary to solve (17) and then substitute into (11) to find B_T. In order to transform to the more convenient sticking-probability formulation, let us introduce an abstract vector space whose vectors will represent functions in the interval $u_0\leq u\leq 0$. Then (17) may be written as

$$|f_0\rangle=\tilde{K}|f_0\rangle+|\tilde{s}\rangle. \tag{18}$$

Substituting the formal solution

$$|f_0\rangle=(1-\tilde{K})^{-1}|\tilde{s}\rangle \tag{19}$$

into (11), we find for the capture rate

$$B_T=\langle c|f_0\rangle=\langle c|(1-\tilde{K})^{-1}|\tilde{s}\rangle \equiv\langle p|\tilde{s}\rangle. \tag{20}$$

Knowledge of $\langle p|$, which is defined by (20), would enable us to calculate B_T directly for any incident distribution without solving the integral equation for f_0. From its definition we see that $\langle p|$ satisfies the equation

$$\langle p|(1-\tilde{K})=\langle c|, \tag{21}$$

or returning to function notation

$$p(u)-\int_{u_0}^{0} p(u')\tilde{K}(u,u')du'=c(u). \tag{22}$$

The normalized function

$$P(u)=p(u)\Big/\int_{-\infty}^{\infty} K(u,u'')du'' \tag{23}$$

satisfies

$$P(u)\int_{-\infty}^{\infty} K(u,u')du'-\int_{u_0}^{0} P(u')K(u,u')du' =\int_{-\infty}^{u_0} K(u,u')du'. \tag{24}$$

From (20) it is obvious that $P(u_0)$ approaches unity as $u_0\rightarrow-\infty$, although this can also be proved mathematically from (24). Therefore, in the limit $u_0\rightarrow-\infty$ we have for $P(u)$ the homogeneous integral equation

$$P(u)\int_{-\infty}^{\infty} K(u,u')du'=\int_{-\infty}^{0} P(u')K(u,u')du' \tag{25}$$

with the boundary condition $P(-\infty)=1$. If (20) is rewritten, using (14), (16), and (23), the capture rate for an arbitrary incident distribution may be expressed in terms of $P(u)$ as

$$B_T=\int_{-\infty}^{0} duP(u)\int_{0}^{\infty} du'K(u',u)f_0(u'). \tag{26}$$

Examination of (25) and (26) shows that $P(u)$ is just the sticking probability introduced by Lax, who derived similar equations from a direct argument. The key assumption in Lax's derivation is that the cascade is a Markov process in total energy, which is also the case in the present treatment since f_0 has been assumed independent of **r**. Equations (9) for f_0 and (25) for P are, in fact, special forms of the forward-time and backward-time Kolmogorov equations studied in the theory of Markov processes.[6]

One advantage of the distribution-function approach is that the simultaneous treatment of the initial capture and subsequent cascade shows that the same kernel appears in (25) and (26). Lax's expression for the rate of the initial capture is identical to ours, although his result was calculated from a detailed description of the trajectories of incident electrons. The kernel in his sticking-probability equation, however, was found in a much more approximate manner.

If we also define a differential capture rate $b(u)$ by setting

$$B_T=\int_{0}^{\infty} f_0(u)b(u)du, \tag{27}$$

then from (26)

$$b(u)=\int_{-\infty}^{0} K(u,u')P(u')du'. \tag{28}$$

Using the explicit relation (10) for K and letting $x=u/\frac{1}{2}ms^2$, $x'=u'/\frac{1}{2}ms^2$, and $\gamma=kT/\frac{1}{2}ms^2$, we have

$$b(x)=\frac{4\pi s^2\sigma_1}{m}\int_{-\infty}^{0} dx'\frac{(x'-x)\,|x'-x|}{[1-\frac{1}{2}(x'+x)+\frac{1}{16}(x'-x)^2]^3} \times\frac{1}{e^{(x'-x)/\gamma}-1}P(x'), \tag{29}$$

where σ_1 is Lax's[1] temperature-independent unit of cross section and is given by

$$\sigma_1=\frac{\pi}{12}\left(\frac{e^2}{\kappa\frac{1}{2}ms^2}\right)^3\frac{1}{\gamma l}. \tag{30}$$

4. RESULTS

The integral equation for $P(u)$ was solved by numerical methods for several values of the dimensionless lattice temperature $\gamma=kT/\frac{1}{2}ms^2$. These results are shown in Fig. 1 (solid lines) and compared to Lax's results for the same values of γ (broken lines). The present theory yields significantly higher values for P because some transitions between bound states are included which Lax's virial-theorem approximation neglects. The sticking probability goes to zero at zero-binding energy since the volume term in the kernel becomes infinite for upward transitions at this point, while remaining finite for downward transitions. The only boundary condition which the theory imposes on $P(u)$ is that $P(u)$ approach unity as u approaches $-\infty$. If the volume in which each trap can act is limited to

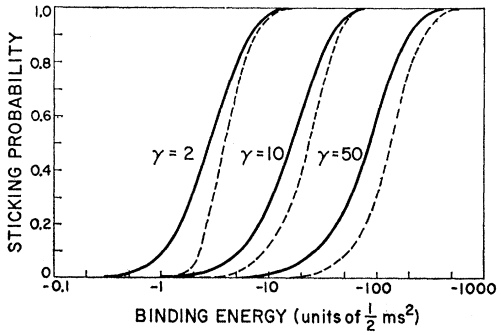

FIG. 1. Sticking probability as a function of binding energy for several values of dimensionless temperature $\gamma=kT/\frac{1}{2}ms^2$. Solid lines are present results; dotted lines are Lax's results (Ref. 1).

[6] W. Feller, *An Introduction to Probability Theory and its Applications* (John Wiley & Sons, Inc., New York, 1957), 2nd ed., Chap. 17.

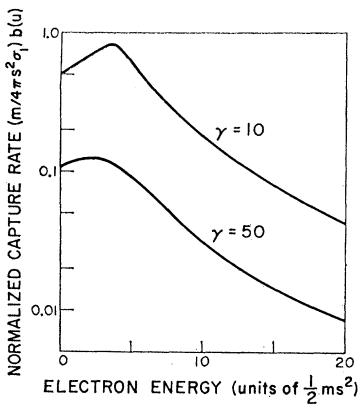

FIG. 2. Normalized capture rate as a function of free-electron energy for two values of dimensionless temperature $\gamma = kT/\frac{1}{2}ms^2$.

take into account the existence of neighboring traps, $P(u)$ need not go to zero at $u=0$.

In Fig. 2 we have plotted for $\gamma=10$ and $\gamma=50$ the normalized differential capture rate $(m/4\pi s^2\sigma_1)b(u)$ as a function of $(u/\frac{1}{2}ms)^2$, using (29) and the numerical values for $P(u)$. Note that $b(u)$ remains finite at $u=0$, so that the cross section is infinite at zero energy. For germanium σ_1 has a value of about 7×10^{-9} cm^2.

We have also computed the total capture cross sections for a thermal distribution of incident electrons using the same parameter values for Ge employed by Lax: $m=\frac{1}{4}m_0$, $s=4\times10^5$ cm/sec, $l=8.0\times10^{-6}$ cm at 300°K, and $\kappa=16$.[7] Our results are shown in Fig. 3, compared to those of Lax's theory and the recent experimental data of Koenig, Brown, and Schillinger.[8] The calculation employed the sticking-probability results of Fig. 1, and an analytic approximation to these curves for interpolation to intermediate temperatures. The upper branch of the solid curves in Fig. 3 was computed using the

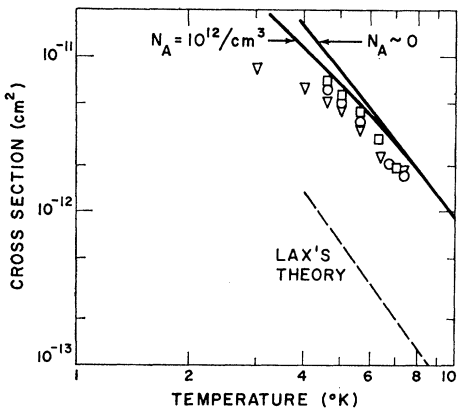

FIG. 3. Computed capture cross section for thermal electrons versus temperature compared with experimental results of Koenig, Brown, and Schillinger (Ref. 8) and theoretical results of Lax (Ref. 1). Following Ref. 8, the cross section was obtained by dividing the capture rate B_T by the rms velocity $(3kT/m^*)^{1/2}$, where m^* is the density-of-states mass.

[7] The correct dielectric constant for Ge was used by Lax, despite the statement to the contrary in the caption to his Fig. 1.

[8] S. H. Koenig, R. D. Brown, and W. Schillinger, Phys. Rev. **128**, 1668 (1962).

kernel (10) directly, and corresponds to the limit of zero ionized-impurity density. To examine the effects of neighboring ionized impurities, the kernel was modified to include a volume cutoff corresponding to a density of approximately 10^{12}/cm^3. Trial calculations of the sticking probability with this modified kernel indicated that a good approximation could be obtained simply by shifting the results from the unmodified kernel along the energy scale (to the left in Fig. 1) by an energy equal to the Coulomb potential at the cutoff radius. When this is done, it should be noted, the sticking probability is no longer zero at zero-binding energy, in accordance with previous discussion. Trapping cross sections computed with the cutoff kernel and the approximate cutoff sticking probabilities are shown as the lower branch of the solid curve in Fig. 3. We see that the slope of this curve seems in good agreement with experiment. The agreement in absolute magnitude must be regarded as somewhat fortuitous, however, since the average values of electron mass, speed of sound, and deformation potential were chosen somewhat arbitrarily. A derivation beginning with an accurate model of the ellipsoidal conduction-band valleys and the phonon-spectrum branches of Ge would have to be carried out to find a systematic method of computing the necessary parameters. In addition, a more rigorous treatment should include an averaging of cutoff kernels over a distribution of interimpurity spacings, rather than the simple cutoff correction used here.

We have not shown the theoretical results of Ascarelli and Rodriguez[2] in Fig. 3 since their introduction of a factor of 4 in their cross section to account for the 4 valleys in Ge is incorrect. They argue that the thermal-excitation rate (and hence the capture rate of thermal electrons) is approximately equal for excitation from a bound state associated with a certain valley to equivalent free states in either the same valley or another valley. However, since the energy of the intervalley phonons is comparable with the binding energy of the donor ground state, intervalley thermal excitations from the states important in cascade capture must proceed at a negligible rate compared to intravalley emission. In addition, these authors used the rather large value of 20 eV for the (effective) deformation potential, which together with their reasonable but slightly higher choice for the value of s makes their cross sections about six times larger than those of Lax or ourselves for the same physical situation, not counting the factor of 4 just mentioned.

As a rough check of the self-consistency of our initial assumption of the importance of the highly excited states, we recomputed the cross sections for thermal electrons for several temperatures, cutting off the integration over the sticking probability—the u integration in (26)—at an energy corresponding to the $5s$ state. The change produced was less than 10% in all cases. This is to be contrasted with the substantial reduction that

occurred in the very low-temperature cross sections when a cutoff of the higher states was introduced to correspond to an impurity density of $10^{12}/\text{cm}^3$.

ACKNOWLEDGMENT

We wish to thank Miss Sylvia Sillers for carrying out the numerical calculations.

APPENDIX A: SPATIAL DEPENDENCE OF f_0

The spatial dependence of f_0 will be estimated by a perturbation calculation, using as an initial approximation a distribution $f_0^0(u)$ which is uniform on each surface of constant energy. Consider first the case where $-(kT)^2/8ms^2<u<-\frac{1}{2}ms^2$. Since we are dealing with a steady-state problem, the total rate at which electrons enter a surface of energy u is the same as the rate at which they leave, and from (8) is given by

$$\frac{f_0^0(u)}{4m^2s^2lkT}\int d\mathbf{r}\int_{-2ms(v-s)}^{2ms(v+s)} d(\hbar\omega)\frac{\hbar\omega|\hbar\omega|}{e^{\hbar\omega/kT}-1} \approx \tfrac{4}{3}\pi r_0^3\frac{|u|}{ml}f_0^0(u), \quad \text{(A1)}$$

where $r_0(u)=-e^2/\kappa u$. Unfortunately, we cannot determine how these entering electrons are spatially distributed over the energy surface without solving (8) for $f_0^0(u)$, and this we wish to avoid because of the complexity involved. However, in order to obtain an upper limit for the correction to f_0, we consider an extreme situation in which all of the electrons leave at a single radius r_1 and all enter at a single radius r_2. Then combining (4) and (5) we have

$$\nabla\cdot\left(\frac{lv^2}{3}\nabla f_0^1\right)=f_0^0\frac{r_0^3|u|}{3ml}\left[\frac{\delta(r-r_1)}{r_1^2}-\frac{\delta(r-r_2)}{r_2^2}\right], \quad \text{(A2)}$$

where f_0^1 is the correction term to f_0, and $(\partial f_1/\partial t)_{\text{coll}}$ has been approximated by $-f_1v/l$, which is valid for $-(kT)^2/8ms^2<u<\frac{1}{2}ms^2$. The first integration of (A2) yields

$$\frac{df_0^1}{dr}=f_0^0\frac{r_0^3}{2l^2r(r_0-r)}\times\begin{cases}1, & r_1<r<r_2\\ 0, & \text{elsewhere}\end{cases} \quad \text{(A3)}$$

and the final integration gives

$$f_0^1\leq f_0^0\left(\frac{r_0}{l}\right)^2\frac{1}{2}\ln\frac{r_2(r_0-r_1)}{r_1(r_0-r_2)}. \quad \text{(A4)}$$

Since the positions of the source and sink enter only logarithmically, we conclude that even in the extreme situation being considered f_0^1 is of order $(r_0/l)^2$ compared to f_0^0.

When $u<-(kT)^2/8ms^2$, the average value of l is reduced by the factor $kT/(ms^2|u|)^{1/2}$, but f_0^1/f_0^0 continues to decrease monotonically with u since r_0 varies as $1/|u|$.

For the case $-\frac{1}{2}ms^2<u<0$ it is important to note that we must have $v>s$ for downward transitions to occur, and hence that there is a maximum radius $r_s=2e^2/\kappa ms^2$ for which such transitions can take place. The total rate at which electrons leave the region $r<r_s$ of energy surface u, either because of upward or downward transitions, is approximately

$$\tfrac{4}{3}\pi r_s^3(5s^2/2l)f_0^0(u). \quad \text{(A5)}$$

Again taking an extreme situation to exaggerate the spatial dependence of f_0, we assume all of these electrons leave at a single radius r_1 and an equal number enter at r_s, the latter amount representing the sum both of electrons making direct transitions into the region $r<r_s$ and of electrons captured into $r>r_s$ which subsequently flow into the region $r<r_s$ before being re-emitted. A calculation similar to the one above yields

$$f_0^1\leq f_0^0\left(\frac{r_s}{l}\right)^2\frac{5}{4}\ln\frac{r_s(r_0-r_1)}{r_1(r_0-r_s)}, \quad \text{(A6)}$$

and hence f_0^1/f_0^0 is of order $(r_s/l)^2$. Actually since $r_s\sim10^{-3}$ cm in Ge, the cutoff due to interimpurity spacing will generally come sooner than that due to r_s.

For the free electrons we have a similar situation. Let r_m be the maximum radius which is effective in the capture process, at most the interimpurity spacing. It can easily be shown that the worst situation occurs for the low-energy electrons with $u<(8ms^2e^2/\kappa r_m)^{1/2}$, their total capture rate being approximately

$$\tfrac{4}{3}\pi r_m^3\frac{e^2}{\kappa r_m}\frac{1}{ml}f_0^0(u). \quad \text{(A7)}$$

If we again assume all of these electrons are removed at a single radius r_1 and that an equal number, representing both re-emitted electrons and incident electrons, are added at radius r_m, then

$$f_0^1<f_0^0\left(\frac{r_m}{l}\right)^2\frac{1}{2}\ln\frac{r_m(r_0+r_1)}{r_1(r_0+r_m)}, \quad \text{(A8)}$$

where $r_0=e^2/\kappa u$. Hence f_0^1/f_0^0 is of order of $(r_m/l)^2$.