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Auger recombination involving dislocations in semiconductors

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Abstract
Auger capture of majority carriers by a charged edge dislocation in n-type semiconductors is considered in the case of weak saturation of the dangling bonds existing on the dislocation core. The dependence of the capture radius on the depth of the one-dimensional dislocation band and on temperature is obtained. Values of temperature and free electron concentration are estimated when Auger capture is the dominant mechanism of nonradiative recombination in crystals with dislocations.

1. Introduction

The recent experimental investigations of luminescence in semiconductors with structural defects revealed that dislocations had a significant effect, resulting in luminescence quenching (Vernon-Parry *et al* 2001). The role of dislocations in recombination processes becomes more apparent in thin-film heterostructures, where a high concentration of dislocations is inevitable. A luminescence study in the quantum wells of gallium-nitride based heterostructures showed that the screw and edge dislocations act as nonradiative recombination centres; the straight edge dislocations decay the luminescence more strongly than do screw and mixed dislocations (Cherns *et al* 2001). This effect may be attributed to the existence of dangling bonds near the edge dislocation core which create a deep and narrow energy band in the semiconductor bandgap.

The carrier statistics in a semiconductor with dislocations can be described by the Shockley–Reed theory using the quantum-mechanical capture radii for different recombination mechanisms (Gulyaev 1961). The probabilities of nonradiative transitions of carriers to the dislocation band due to their interaction with phonons were evaluated in (Vardanian 1977, Vardanian *et al* 1988). The edge dislocation in a semiconductor carries the charge of majority carriers; therefore it is surrounded by an electrostatic field that causes bending of the energy bands. For minority carriers the charged dislocation is an attraction centre and the capture to this centre is described by the Lax cascade mechanism (Vardanian 1977). Meanwhile, for the

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majority carriers the electrostatic field is a barrier and the carrier transition to a dislocation level is accompanied by a single multiphonon process (Vardanian *et al* 1988).

In the case of relatively low temperatures, when the probability of multiphonon transitions decreases, and at high carrier concentrations an impact mechanism of recombination (Auger process) can prevail when the released energy transfers to another carrier (for a review see Landsberg (1970), Robbins (1980)). The study of electron Auger capture by the charged edge dislocation in an n-type semiconductor and the determination of conditions when the impact recombination dominates over multiphonon recombination are the purposes of this paper.

2. Dislocation model; electron wavefunctions

In n-type semiconductors the edge dislocation carries a negative charge due to the saturation of a part of the dangling bonds by electrons, therefore it is surrounded by a cylinder of ionized donor impurities. The positive charge of this cylinder with a radius ρ_{ion} is screened by free carriers at the Debye distance ρ_{D}. The relation of lengths ρ_{ion} and ρ_{D} depends on the degree of filling of the dislocation states, i.e. on the relation of the distances between saturated and dangling bonds, which is determined by the temperature and can be characterized by the parameter $\alpha = e^2/\varepsilon c\kappa T$—the ratio of the interaction energy of the saturating electrons to their thermal energy (here ε is the dielectric constant, κ is the Boltzmann constant and $c = c(T)$ is the temperature-dependent distance between saturated states). Further analysis will be carried out for high enough temperatures when the criterion of weak filling $\alpha \ll 1$ is realized. Note that under this condition the shallow donor levels are completely ionized (i.e. $\kappa T \gg E_{\mathrm{donor}}$), so that in the heavily doped semiconductors the concentrations of free electrons can be sufficiently high to provide efficient impact recombination.

At the considered temperatures the radius ρ_{ion} is related to Debye radius ρ_{D} as follows (Vardanian 1977)

$$\rho_{\mathrm{ion}} = \frac{2\rho_{\mathrm{D}}}{\gamma} \exp\left\{-\frac{1}{2\alpha}\right\},$$

$$\rho_{\mathrm{D}} = \left(\frac{\varepsilon\kappa T}{4\pi n_{\mathrm{d}} e^2}\right)^{1/2}$$

where n_{d} is the donors concentration, and $\ln\gamma = 0.577$ is Euler's constant. At these temperatures a condition $\rho_{\mathrm{ion}} \ll \rho_{\mathrm{D}}$ holds and the electrostatic barrier energy of the straight dislocation at distances ρ from the dislocation less than ρ_{D} is given by the expression (Vardanian 1977)

$$U(\rho) \approx 2\alpha\kappa T \ln\frac{2\rho_{\mathrm{D}}}{\gamma\rho}, \qquad a < \rho < \rho_{\mathrm{D}}. \tag{1}$$

Though the expression (1) is applicable at distances sufficiently in excess of the core size a (here $a \geqslant a_0$, a_0 is the lattice constant), where the influence of the discrete structure of the dislocation core can be neglected, this formula can be extrapolated down to the distance a. At distances $\rho < a$ the dislocation potential is approximated by a square well with the depth providing energy levels for the electron capture. Schematically the dislocation potential is represented in figure 1.

The wavefunction of the conduction band electron affected by the dislocation potential can be found as the quasiclassical solution of the Schrödinger equation, taking account of the potential energy (1). By matching the quasiclassical functions with an exact solution of the wave equation in the region $\rho < a$, the electron wavefunction with energy E can be found

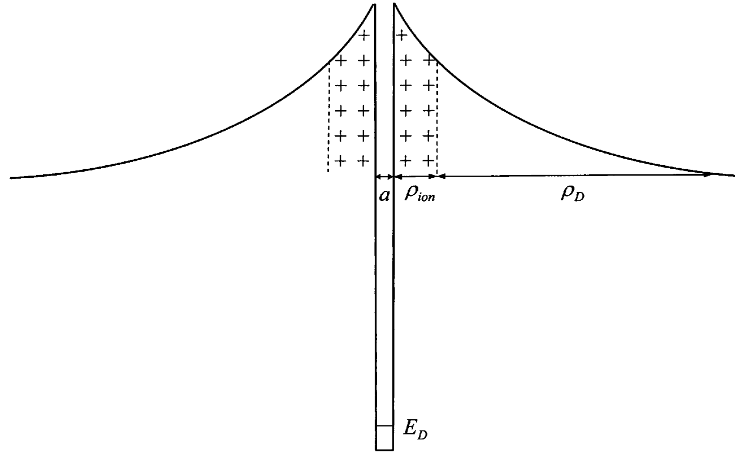

Figure 1. Schematic representation of the electrostatic barrier around the dislocation. The positive charge of ionized donors (depletion region) is indicated by (+). The energy level E_{D} is due to the existence of a 'chemical' well at distances $\sim a$.

(Vardanian 1979). In cylindrical coordinates (ρ, φ, z) with the z-axis along the dislocation line, one has the following view:

$$\Psi_{k,m,k_z} = \left(\frac{k}{4\pi R L_z}\right)^{1/2} R_{km}(\rho) \mathrm{e}^{(\mathrm{i}k_z z + \mathrm{i}m\theta)}, \tag{2}$$

where $k = (2\mu W/\hbar^2)^{1/2}$ is the radial wavenumber of the electron with effective mass μ, $W = E - \hbar^2 k_z^2/2\mu$, k_z is the wavenumber along the z axis and m is the magnetic quantum number. The wavefunction (2) is normalized to a cylinder with radius R and height L_z. The radial component of the wave tunnelling through the barrier is described by the function

$$R_{km}(\rho) = \begin{cases} \dfrac{J_m(\beta\rho)}{J_m(\beta a)} \dfrac{1}{[|k(a)|a]^{1/2}} \exp\left(-\displaystyle\int_a^{\rho_m(k)} |k(\rho)|\,\mathrm{d}\rho\right) & 0 < \rho < a \\ \dfrac{1}{[|k(\rho)|\rho]^{1/2}} \exp\left(-\displaystyle\int_\rho^{\rho_m(k)} |k(\rho)|\,\mathrm{d}\rho\right) & a < \rho < \rho_m(k), \end{cases} \tag{3}$$

where

$$k(\rho) = \left\{\frac{2\mu}{\hbar^2}\left[W - U(\rho) - \frac{\hbar^2 m^2}{2\mu\rho^2}\right]\right\}^{1/2},$$

while the turning point $\rho_m(k)$ is determined by the condition $k(\rho_m) = 0$; $J_m(x)$ is the Bessel function of order m.

The wavefunction of an electron in the dislocation band describes two-dimensional localization at the ground level E_{D} and free motion along the dislocation. This wavefunction was found without taking the influence of the deep dislocation states of the electrostatic field into account (Vardanian 1979), which was justified by the weakness of the dislocation field in comparison with the atomic fields:

$$\Psi_{E_{\mathrm{D}},m,k_z} = \left(\frac{\beta}{\pi\rho L_z}\right)^{1/2} \mathrm{e}^{-\beta\rho} \mathrm{e}^{(\mathrm{i}k_z z + \mathrm{i}m\theta)} \tag{4}$$

where $\beta^{-1} = (\hbar^2/2\mu E_{\mathrm{D}})^{1/2}$ is the electron characteristic localization length.

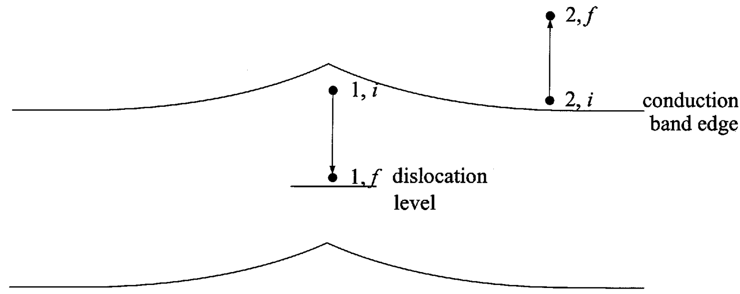

Figure 2. Auger capture of an electron at an energy level in the dislocation band.

3. Capture radius

According to Auger recombination general theory, a band carrier capture at a deep trap with energy transfer to another carrier is described by means of two-particle wavefunctions. In the case of electron capture at a charged dislocation, the initial state of the system is described by the conduction electron tunnelling wavefunction Ψ_1^{i} and a free electron wavefunction Ψ_2^{i}, and the final state is described by the wavefunctions of an electron in the one-dimensional dislocation band Ψ_1^{f} and of a conduction 'hot' electron Ψ_2^{f} (figure 2).

According to the wavefunction (3), the tunnelling probability decreases with an increase in the electron magnetic quantum number m, due to an increase in the centrifugal potential $U_{\mathrm{c}} = \hbar^2 m^2/2\mu\rho^2$. Therefore it is meaningful only to consider electrons with $m = 0$ in the initial state:

$$\Psi_1^{\mathrm{i}} = \left(\frac{k_1^{\mathrm{i}}}{4\pi R L_z}\right)^{1/2} R_{k_1^{\mathrm{i}}0}(\rho)\exp(\mathrm{i}k_{1z}^{\mathrm{i}}z). \tag{5}$$

The free electron wavefunctions in cylindrical coordinates describe subwaves with quantum numbers $(k_2, m_2, k_{2z})^{\mathrm{i}}$ and $(k_2, m_2, k_{2z})^{\mathrm{f}}$ in initial and final states:

$$\begin{aligned}\Psi_2^{\mathrm{i}} &= \left(\frac{k_2^{\mathrm{i}}}{2RL_z}\right)^{1/2} J_{m_2^{\mathrm{i}}}(k_2^{\mathrm{i}}\rho)\mathrm{e}^{\mathrm{i}m_2^{\mathrm{i}}\theta}\mathrm{e}^{\mathrm{i}k_{2z}^{\mathrm{i}}z}\\ \Psi_2^{\mathrm{f}} &= \left(\frac{k_2^{\mathrm{f}}}{2RL_z}\right)^{1/2} J_{m_2^{\mathrm{f}}}(k_2^{\mathrm{f}}\rho)\mathrm{e}^{\mathrm{i}m_2^{\mathrm{f}}\theta}\mathrm{e}^{\mathrm{i}k_{2z}^{\mathrm{f}}z}.\end{aligned} \tag{6}$$

The electron transition in the Auger process is caused by the Coulomb interaction between two electrons. When the exchange interaction between electrons is disregarded, the electron transition from the initial state i of the conduction band to the final state f in the dislocation band is being described by the matrix element (Landsberg 1970)

$$\begin{aligned}M_{\mathrm{if}} = \int &\Psi_1^{\mathrm{f}*}(\rho_1, \theta_1, z_1)\Psi_2^{\mathrm{f}*}(\rho_2, \theta_2, z_2)\frac{e^2}{\varepsilon\sqrt{|\boldsymbol{\rho_1} - \boldsymbol{\rho_2}|^2 + (z_1 - z_2)^2}}\\ &\times \Psi_1^{\mathrm{i}}(\rho_1, \theta_1, z_1)\Psi_1^{\mathrm{i}}(\rho_2, \theta_2, z_2)\,\mathrm{d}\boldsymbol{\rho_1}\,\mathrm{d}z_1\,\mathrm{d}\boldsymbol{\rho_2}\,\mathrm{d}z_2\end{aligned} \tag{7}$$

where $\boldsymbol{\rho}$ is the two-dimensional radius vector. The description of the crystal as a dielectric medium with constant ε down to small distances (most contributing to the matrix element) is assumed in the Auger recombination theory.

Later in this work the capture process without transfer of magnetic momentum at the interaction of electrons will be considered. This approximation corresponds to preserving in the Coulomb interaction energy the monopole term only, since already in the dipole approximation

(i.e. when the terms of order ρ_1/ρ_2 are preserved) momentum transfer is possible. The order of magnitude of the dipole term can be estimated by taking into account that the first electron distance from the dislocation is $\rho_1 \sim a$, while the characteristic interaction distance $\rho_2 - \rho_1$ must be of the order of the localization length β^{-1}. Hence the terms containing the ratio ρ_1/ρ_2 are of order $\beta a \sim \sqrt{E_D/E_g}$, where E_g is the bandgap. Even in the case of the considered deep levels, these terms can be neglected when estimating the contribution of Auger processes to the carrier recombination rate.

Thus, taking account of the wavefunctions (4)–(6), the matrix element (7) is equal to

$$M_{if} = D \int \frac{e^{-\beta\rho_1}}{\sqrt{\rho_1}} R_{k_1^i 0}(\rho_1) J_{m_2^i}(k_2^i\rho_2) J_{m_2^f}(k_2^f\rho_2) \frac{\exp(ik_{1z}^i z_1 + ik_{2z}^i z_2 - ik_{1z}^f z_1 - ik_{2z}^f z_2)}{\varepsilon\sqrt{\rho_2^2 + (z_1 - z_2)^2}} \times e^{-im_1^f\theta_1} e^{i(m_2^i - m_2^f)\theta_2} \rho_1 \, d\rho_1 \, d\theta_1 \, dz_1 \, \rho_2 \, d\rho_2 \, d\theta_2 \, dz_2 \quad (8)$$

where $D = \left(\frac{k_1^i k_2^i k_2^f \beta}{16\pi^2 R^3 L_z^4}\right)^{1/2} \frac{e^2}{\varepsilon}$. The angle integration gives Kronecker symbols $\delta_{m_1^i 0}$ and $\delta_{m_2^i m_2^f}$, denoting the transitions without a transfer of the turning momentum. At z integration the δ-function arises corresponding to conservation of momentum of the z-components:

$$M_{if} = 16\pi^3 D\delta(k_{1z}^i + k_{2z}^i - k_{1z}^f - k_{2z}^f) \int_0^{\rho_0(k_1^i)} \sqrt{\rho_1} e^{-\beta\rho_1} R_{k_1^i 0}(\rho_1) \, d\rho_1 \times \int_0^\infty \rho_2 J_{m_2^i}(k_2^i\rho_2) J_{m_2^i}(k_2^f\rho_2) K_0(|k_{2z}^f - k_{2z}^i|\rho_2) \, d\rho_2. \quad (9)$$

Thus, in the approximation $\rho_2 \gg \rho_1$ the matrix element represents the product of two independent integrals over ρ_1 andρ_2.

The upper limit of the integral over ρ_1 can be taken as the turning point

$$\rho_0(k_1^i) = \frac{2\rho_D}{\gamma} \exp\left[-\frac{\hbar^2 k_1^{i2}}{4\mu\alpha\kappa T}\right],$$

since the electron localization length in the final state is $\beta^{-1} \ll \rho_0(k_1^i)$ (at k_1^i values determined by the thermal energy). According to wavefunctions (3) this integral represents a sum of two integrals: over the square well region $0 < \rho_1 < a$ and the region under the barrier $a < \rho_1 < \rho_0(k_1^i)$. Due to two-dimensional localization of the captured electron, the main contribution to the latest integral is made by the initial state wavefunction value at point a. Noting that $\beta a < 1$, we obtain

$$\int_a^{\rho_0(k_1^i)} \sqrt{\rho_1} \exp(-\beta\rho_1) R_{k_1^i,0}(a) \, d\rho_1 = \frac{1}{[|k_1^i(a)|a]^{1/2}} \frac{1}{\beta^{3/2}} \sqrt{\frac{\pi}{2}} \exp\left(-\int_a^{\rho_0(k_1^i)} |k_1^i(\rho)| \, d\rho\right). \quad (10)$$

In the same approximation $\beta a < 1$ the integral over the region $(0, a)$ can be neglected. After integration over ρ_2 the matrix element is obtained as

$$M_{if} = \frac{2\sqrt{2}\pi^{5/2}}{R^{3/2} L_z^2} \frac{e^2}{\varepsilon\beta a^{1/2}} \delta(k_{1z}^i + k_{2z}^i - k_{1z}^f - k_{2z}^f) \left(\frac{k_1^i}{|k_1^i(a)|}\right)^{1/2} \exp\left(-\int_a^{\rho_0(k_1^i)} |k_1^i(\rho)| \, d\rho\right) \times \frac{(k_2^i k_2^f)^{1/2}}{[(k_2^f - k_2^i)^2 + (k_{2z}^i - k_{2z}^f)^2]^{1/2} [(k_2^f + k_2^i)^2 + (k_{2z}^i - k_{2z}^f)^2]^{1/2}} \times \left(\frac{[(k_2^f + k_2^i)^2 + (k_{2z}^i - k_{2z}^f)^2]^{1/2} - [(k_2^f - k_2^i)^2 + (k_{2z}^i - k_{2z}^f)^2]^{1/2}}{[(k_2^f + k_2^i)^2 + (k_{2z}^i - k_{2z}^f)^2]^{1/2} + [(k_2^f - k_2^i)^2 + (k_{2z}^i - k_{2z}^f)^2]^{1/2}}\right)^{|m_2^i|}. \quad (11)$$

Due to the one-dimensionality of the dislocation band, only the z-component of the momentum is conserved.

Electron capture by the dislocation is characterized by means of the capture radius

$$r = \frac{W}{L_z n v_T} \tag{12}$$

where n is the electron concentration, $v_T = (3\kappa T/\mu)^{1/2}$—average thermal velocity and W is the capture probability

$$W = \frac{2\pi}{\hbar}\left(\frac{R}{\pi}\right)^3\left(\frac{L_z}{2\pi}\right)^4 L_z \sum_{m_2^{\rm i}} \int {\rm d}k_2^{\rm i}\,{\rm d}k_{2z}^{\rm i} \int {\rm d}k_2^{\rm f}\,{\rm d}k_{2z}^{\rm f} \int {\rm d}k_1^{\rm i}\,{\rm d}k_{1z}^{\rm i} \int {\rm d}k_{1z}^{\rm f}$$
$$\times |M_{\rm if}|^2 P(k_1^{\rm i}, k_{1z}^{\rm i}, k_2^{\rm i}, k_{2z}^{\rm i})\delta(E_1^{\rm i} + E_2^{\rm i} - E_1^{\rm f} - E_2^{\rm f}). \tag{13}$$

Here $P(k_1^{\rm i}, k_{1z}^{\rm i}, k_2^{\rm i}, k_{2z}^{\rm i})$ is the electron distribution function in the initial states; a sufficient number of empty states in the final states is assumed. The densities of states in the integrals over k_1, k_2 are taken as R/π, which correspond to wavefunctions with a certain magnetic momentum. For the non-degenerate semiconductor, the distribution $P(k_1^{\rm i}, k_{1z}^{\rm i}, k_2^{\rm i}, k_{2z}^{\rm i})$ is given by the Boltzmann function:

$$P(k_1^{\rm i}, k_{1z}^{\rm i}, k_2^{\rm i}, k_{2z}^{\rm i}) = \frac{n^2}{N_{\rm c}^2}\exp\left\{-\frac{\hbar^2}{2\mu\kappa T}(k_1^{\rm i2} + k_{1z}^{\rm i2} + k_2^{\rm i2} + k_{2z}^{\rm i2})\right\}$$

where $N_{\rm c}$ is the effective density of states in the conductivity band

$$N_{\rm c} = \frac{1}{4}\left(\frac{2\mu\kappa T}{\pi\hbar^2}\right)^{3/2}.$$

To evaluate the probability of electron capture into the narrow band ($E_1^{\rm f} \sim E_{\rm D} \gg \kappa T$) it is essential that the final state energy for the free conduction electron greatly exceeds the initial state energy, which can be of the order of the thermal energy, i.e. $E_1^{\rm f} \sim E_2^{\rm f} \gg (E_1^{\rm i}, E_2^{\rm i})$. Therefore, assuming a square dispersion law for the conductivity electrons, the condition $k_2^{\rm f2} + k_{2z}^{\rm f2} \gg k_2^{\rm i2} + k_{2z}^{\rm i2}$ is obtained, allowing the use of an approximate relation in the matrix element (11)

$$\frac{1}{[(k_2^{\rm f} - k_2^{\rm i})^2 + (k_{2z}^{\rm i} - k_{2z}^{\rm f})^2]^{1/2}[(k_2^{\rm f} + k_2^{\rm i})^2 + (k_{2z}^{\rm i} - k_{2z}^{\rm f})^2]^{1/2}} \approx \frac{1}{k_2^{\rm f2} + k_{2z}^{\rm f2}},$$

which means that the characteristic interaction length has the order $(k_2^{\rm f2} + k_{2z}^{\rm f2})^{-1/2} \sim \beta^{-1}$.

The $m_2^{\rm i}$ sum in (13) represents the sum of a decreasing geometrical progression which, allowing for the condition $(\kappa T/E_{\rm D}) \ll 1$, can be accepted as being equal to unity. Such an approximation corresponds to only leaving in the sum a term with $m_2^{\rm i} = 0$, i.e. the free electrons with non-zero magnetic momentum give a small contribution to transitions. It also directly follows from the conduction electron wavefunction (6) described by the Bessel function $J_{m_2^{\rm i}}(k_2^{\rm i}\rho)$: at the characteristic interaction distance $\rho \sim \beta^{-1}$ the function $J_{m_2^{\rm i}}(k_2^{\rm i}\beta^{-1})$ has a maximal value at $m_2^{\rm i} = 0$ with the condition that $k_2^{\rm i}\beta^{-1} \ll 1$. At non-zero magnetic momentum the centrifugal potential suppresses the electron wavefunction at distances of order β^{-1}.

At accepted approximations the capture radius is equal to

$$r = \frac{2\pi^2\hbar^5 n e^4}{(\mu\kappa T)^3\varepsilon^2\beta^2 a v_T} \int {\rm d}k_1^{\rm i}\,{\rm d}k_{1z}^{\rm i} \int k_2^{\rm i}\,{\rm d}k_2^{\rm i}\,{\rm d}k_{2z}^{\rm i} \int k_2^{\rm f}\,{\rm d}k_2^{\rm f}\,{\rm d}k_{2z}^{\rm f}$$
$$\times \frac{\exp\left\{-\frac{\hbar^2}{2\mu\kappa T}(k_1^{\rm i2} + k_{1z}^{\rm i2} + k_2^{\rm i2} + k_{2z}^{\rm i2})\right\}}{k_2^{\rm f2} + k_{2z}^{\rm f2}} \frac{k_1^{\rm i}}{|k_1^{\rm i}(a)|} \exp\left\{-2\int_a^{\rho_0(k_1^{\rm i})} |k_1^{\rm i}(\rho)|\,{\rm d}\rho\right\}$$
$$\times \delta(k_{1z}^{\rm i} + k_{2z}^{\rm i} - k_{1z}^{\rm f} - k_{2z}^{\rm f})\delta\left(\frac{\hbar^2 k_2^{\rm f2}}{2\mu} + \frac{\hbar^2 k_{2z}^{\rm f2}}{2\mu} - E_{\rm D} - E(k_{1z}^{\rm f})\right). \tag{14}$$

The distinction between an Auger transition of a conduction electron to the one-dimensional dislocation band and transitions to a valence band can be specified at this point. In the latter case for the direct-gap semiconductors the preservation of the total momentum and energy prevents electron transition into the valence band ceiling (Ridley 1982). Consequently, the minimal released energy, which is the threshold energy for the inverse process (i.e. impact ionization), exceeds the bandgap. Meanwhile, in the case of transition to a dislocation, transitions to a level with $k_z = 0$ are allowed. Then the second electron is 'thrown out' with the momentum vector normal to the dislocation. In this respect the capture by a dislocation in an Auger transition is similar to what happens in heterostructure quantum wells (Andreev and Zegrya 1997).

The electron dispersion $E(k_{1z}^{\mathrm{f}})$ in the narrow dislocation band differs from a simple square law. Basically, the dispersion law can be found using a model of a chain of zero-dimensional wells disposed in three-dimensional space (Demkov and Subramanian 1970) for the dislocation description. In this model the dispersion law, as well as the effective mass of an electron moving along the chain, is determined by an interaction of wells. In the case of a strong interaction, the dispersion can be described by a strong coupling approximation. The more complicated dispersion law arises in the case of the chain with a weak interaction between wells—the more suitable model for a dislocation description. However, in this case the exponential reduction of bandwidth is essential. As a result the dislocation bandwidth is less than its depth $\Delta E_{\mathrm{D}} \ll E_{\mathrm{D}}$ and the definition of $E(k_{1z}^{\mathrm{f}})$ is not required; even neglecting the value of $E(k_{1z}^{\mathrm{f}})$ in comparison with E_{D} in the δ-function argument in (14), energy conservation is still fulfilled with enough accuracy.

The integration over the final states of the conduction electron k_2^{f} and k_{2z}^{f} can be made using δ-function properties. After integrating over the final state of the captured electron k_{1z}^{f}, we get

$$r = \frac{(2\pi\hbar^3)^2 n e^4}{\mu^2(\kappa T)^3\varepsilon^2\beta^2 a v_T}\frac{1}{(2\mu E_{\mathrm{D}})^{3/2}}\int \mathrm{d}k_1^{\mathrm{i}}\,\mathrm{d}k_{1z}^{\mathrm{i}}\int \mathrm{d}k_2^{\mathrm{i}}\,\mathrm{d}k_{2z}^{\mathrm{i}} \times \exp\left\{-\frac{\hbar^2}{2\mu\kappa T}(k_1^{\mathrm{i}2}+k_{1z}^{\mathrm{i}2}+k_2^{\mathrm{i}2}+k_{2z}^{\mathrm{i}2})\right\}\frac{k_1^{\mathrm{i}}k_2^{\mathrm{i}}}{|k_1^{\mathrm{i}}(a)|}\exp\left\{-2\int_a^{\rho_0(k_1^{\mathrm{i}})}|k_1^{\mathrm{i}}(\rho)|\,\mathrm{d}\rho\right\}. \tag{15}$$

Now the integration over the initial states of the electron remains. Because of the Boltzmann distributions the contribution to integrals on k_2^{i} and k_{2z}^{i} is made by all states up to energy κT and the integral is proportional to $(\kappa T)^{3/2}$, while after k_{1z}^{i} integration the factor $(\kappa T)^{1/2}$ arises. Thus, the capture radius becomes

$$r = \frac{(2\pi)^3\hbar n e^4}{\kappa T\varepsilon^2\beta^2 a v_T}\frac{1}{(2\mu E_{\mathrm{D}})^{3/2}}\int\frac{k_1^{\mathrm{i}}}{|k_1^{\mathrm{i}}(a)|}\exp\left\{-2\int_a^{\rho_0(k_1^{\mathrm{i}})}|k_1^{\mathrm{i}}(\rho)|\,\mathrm{d}\rho\right\}\exp\left\{-\frac{\hbar^2 k_1^{\mathrm{i}2}}{2\mu\kappa T}\right\}\mathrm{d}k_1^{\mathrm{i}}. \tag{16}$$

The subintegral function in (16) contains two exponential functions of k_1^{i}. The first function denotes a small probability of electron capture with large values of k_1^{i} because of the Boltzmann distribution of particles. The second exponential function describes an increase in capture probability with k_1^{i} growth, due to a high tunnelling probability through the dislocation barrier. Notably, the argument of the second function itself depends on energy exponentially, due to the logarithmic dependence of the dislocation field (1) on the distance: at $|k_1^{\mathrm{i}}(\rho)| = (4\mu\alpha\kappa T/\hbar^2)^{1/2}[\ln(\rho_0(k_1^{\mathrm{i}})/\rho)]^{1/2}$ one has

$$\int_a^{\rho_0(k_1^{\mathrm{i}})}|k_1^{\mathrm{i}}(\rho)|\,\mathrm{d}\rho = \frac{2\rho_{\mathrm{D}}}{\gamma}\left(\frac{4\mu\alpha\kappa T}{\hbar^2}\right)^{1/2}\exp\left(-\frac{\hbar^2 k_1^{\mathrm{i}2}}{4\mu\alpha\kappa T}\right)\gamma\left(\frac{3}{2},\ln\left(\frac{\rho_0(k_1^{\mathrm{i}})}{a}\right)\right),$$

where $\gamma(\alpha, x)$ is an incomplete gamma-function.

Thus, because of the presence of two 'competing' mechanisms of dependence on energy, the greatest contribution to integral (16) is made by electrons with an energy $\tilde{W}$ which can be determined by calculating the k_1^{i} integral by the method of steepest descent. Then the 'saddle' energy is obtained as

$$\tilde{W} = \frac{\hbar^2 \tilde{k}_1^{\mathrm{i}2}}{2\mu} = 2\alpha\kappa T \ln\left[\frac{2\rho_{\mathrm{D}}}{\gamma}(\pi\mu\kappa T/\alpha\hbar^2)^{1/2}\right], \tag{17}$$

while the value of the integral is determined by the turning point at energy $\tilde{W}$

$$\rho_0(\tilde{W}) = \frac{2\rho_{\mathrm{D}}}{\gamma}\exp\left[-\frac{\tilde{W}}{2\alpha\kappa T}\right] = \left(\frac{\alpha\hbar^2}{\pi\mu\kappa T}\right)^{1/2}$$

i.e. by the tunnelling distance of the electrons being most effectively captured.

Note that characteristic energy $\tilde{W}$ in the considered temperature range exceeds the thermal energy κT. One can infer this fact from the quasiclassical approximation requirement that the tunnelling distance must greatly exceed the electron wavelength, i.e. $k\rho_0 \gg 1$, limiting the range of applicable temperatures. Writing down this condition for electrons with energy $\tilde{W}$ and taking into account that in the considered case the inequality $\alpha \ll 1$ holds, we get

$$2\alpha\pi^{-1/2}\left\{\ln\left[\frac{2\rho_{\mathrm{D}}}{\gamma}(\pi\mu\kappa T/\alpha\hbar^2)^{1/2}\right]\right\} \gg 1$$

so that for the energy (17) the condition $\tilde{W} > \kappa T$ is obtained.

Finally the capture radius value follows as:

$$r = r_0 \frac{\exp\left\{-2\alpha\left[1 + \ln\left(\frac{2\rho_{\mathrm{D}}}{\gamma\rho_0(\tilde{W})}\right)\right]\right\}}{\left(\frac{2\mu\kappa T a^2}{\hbar^2}\ln\frac{\rho_0(\tilde{W})}{a}\right)^{1/2}} \tag{18}$$

where

$$r_0 = \frac{2\pi^{7/2}\hbar^2 e^4}{\mu^{3/2}\varepsilon^2 v_T E_{\mathrm{D}}^{5/2}} n.$$

Auger transition to a dislocation differs from transition to a zero-dimensional centre (e.g. an impurity atom creating a single level in the bandgap) by a stronger dependence on the depth of energy levels; the capture radius r (18) depends on $E_{\mathrm{D}}^{5/2}$ compared with a factor of $3/2$ for the cross-section of capture by the dot centre. Besides, the capture radius by the dislocation has a dependence on temperature. This dependence arises from the temperature dependence of the energy at the saddle point, i.e. it is caused by the electrostatic barrier. Therefore the expression r_0 in (18) represents the capture radius by a neutral dislocation. The rest part of the radius (18) describes electron tunnelling through a barrier of the charged dislocation.

4. Conclusions

The obtained radius of electron Auger capture by the edge dislocation is valid in the temperature range restricted by the dangling bonds' weak saturation condition $\alpha = (e^2/\varepsilon c\kappa T) \ll 1$ from below and by the quasiclassical approximation applicability $k\rho_0(k) \gg 1$ from above. For example, for germanium ($\varepsilon = 16$) this is an interval 200–500 K, where a significant mechanism of nonradiative recombination is the multiphonon capture. The probability of the multiphonon transition decreases exponentially with temperature due to the activation character of the process, therefore it is reasonable to compare the capture radii for Auger and multiphonon transitions in the bottom limit of the specified temperature interval. At $T = 200$ K

and for the parameters $\mu \approx 10^{-28}$ g, $E_D = 0.3$ eV, $a \sim 10^{-8}$ cm and $\alpha = 0.5$ the radii of multiphonon (Vardanian 1979) and Auger captures are comparable at electron concentrations $n \approx 5 \times 10^{16}$ cm^{-3} and are of order $\rho_{ph} \sim \rho_{Auger} \sim 10^{-15}$ cm. At higher temperatures the Auger mechanism can prevail only in the case of degenerated semiconductors, while at lower temperatures and higher concentrations this mechanism will prevail even in non-degenerate semiconductors.

More accurate evaluation of Auger capture radii requires an account of the exchange term in the matrix element, as well as a description of band electrons by Bloch wavefunctions. However, it unlikely that these can change the order of magnitude of the capture radii estimated above.

The carrier mobility in a one-dimensional dislocation band is small which allowed us to neglect the bandwidth in comparison with its depth in the calculation of the capture radius. If the electron–phonon coupling in this band is strong enough, electron autolocalization, i.e. creation of 'one-dimensional polaron', can be realized. In this case the Auger transitions will be inevitably accompanied by phonon subsystem disturbance. However, the account of such transitions is the subject of separate research.

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