Strong excitation of local oscillations of defects in the many-phonon recombination of electrons and holes

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A mechanism for strong excitation of local oscillations of a defect with a deep level in the case of many-phonon recombination and generation on a defect of electron–hole pairs under conditions of a large electron and hole concentration is examined. This mechanism is used to interpret the experimental data on inelastic sputtering of semiconductors and insulators by ion bombardment.

Many-phonon recombination of electrons and holes through the defects with deep levels is linked with the transfer of energy to the local oscillations of the defect on the order of the width of the band gap of the semiconductor, ϵ_g. In the presence of nonequilibrium carriers, the many-phonon recombination therefore leads to a strongly nonequilibrium distribution of defects over the vibration energies. The importance of this result was pointed out for the first time by Wheeks *et al.*[1] in connection with the recombination-stimulated defect reactions.[2]

It is usually assumed that the main factor which prevents a strong heating of the local oscillations is their interaction with the heat sink (for example, with the lattice phonons).[1,3] In the present letter, we will show that in the case of a large concentration of nonequilibrium carriers the heating of the local oscillation is determined by the production and loss of the electron–hole pairs on a strongly excited defect. This can be done if the rate at which the electrons and holes are captured on a strongly excited defect with the vibration energy $E \sim \epsilon_g$ is greater than the rate of the energy relaxation of the local vibrations due to the interaction with the lattice; i.e., the following inequality holds:[1]

$$nc_n(E),\ pc_p(E) \gg \tau_L^{-1}, \tag{1}$$

where n and p are the electron and hole densities, $c_n(E)$ and $c_p(E)$ are the capture

coefficients of electrons and holes which characterize the rate at which the carriers are captured in a unit volume per defect with a vibration energy E, and τ_l is the time scale of the energy relaxation of the local oscillations.

Let us assume that $N_i(E)$ is the number of defects with a vibration energy E in ith charged state: $i=1$ for a defect with a bound electron and $i=2$ for a defect without an electron. Disregarding the kinetic energy of captured and expelled carriers in comparison with the vibration energy, under steady-state conditions the equations for the balance of the defects in states 1 and 2 are

$$\begin{cases} nc_n(E-\epsilon_{TC})N_2(E-\epsilon_{TC}) - [pc_p(E)+e_n(E)]N_1(E) \\ \quad + e_p(E+\epsilon_{TV})N_2(E+\epsilon_{TV}) = 0, & \text{(2a)} \\ pc_p(E-\epsilon_{TV})N_1(E-\epsilon_{TV}) - [nc_n(E)+e_p(E)]N_2(E) \\ \quad + e_n(E+\epsilon_{TC})N_1(E+\epsilon_{TC}) = 0. & \text{(2b)} \end{cases}$$

Here $e_n(E)$ and $e_p(E)$ are the rates of emission of the electrons and holes by a defect with a vibration energy E, and ϵ_{TC} and ϵ_{TV} are the thermal energies of ionization of a defect with an emission of an electron and hole, respectively ($\epsilon_{TC}+\epsilon_{TV}=\epsilon_g$; see Fig. 1).

As was shown in Ref. 4, the emission and capture of carriers by a strongly excited defect (at $E \gtrsim \epsilon_g$) depend only slightly on energy E. For simplicity, we assume below that the emission and capture are constant. In this approximation the continuous solution of system (2), which decreases as $E \to \infty$, is given by

$$N_1(E) = A\left(\frac{nc_n pc_p}{e_n e_p}\right)^{E/\epsilon_g}; \quad N_2(E) = \frac{pc_p}{e_p}N_1(E-\epsilon_{TV}), \qquad (3)$$

where A is a coefficient which does not depend on the local vibration energy. The expressions for the energy distribution "tails" which we found can easily be rewritten

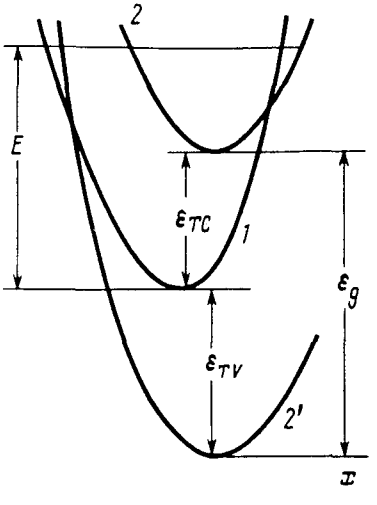

FIG. 1. Schematic representation of adiabatic vibrational potentials of a defect, illustrating many-phonon transitions which are described by Eq. (2a). The potentials 2 and 2' correspond to the presence and absence of a free electron-hole pair. The potential 1 corresponds to a defect with a bound electron; x is the configuration coordinate of the local vibrations. The system of adiabatic potentials for Eq. (2b) can be constructed in a similar manner.

in the form

$$N_{1,2}(E) \sim \exp\left\{-\frac{E}{kT^*}\right\}. \tag{4}$$

The effective "temperature" which we introduced

$$T^* = \frac{\epsilon_g}{k \ln \frac{N_C^* N_V^*}{np}} \tag{5}$$

characterizes the scale of the decay of nonequilibrium distribution at high energies; the effective densities of states are determined from the ratios $N_c^* \equiv e_n/c_n$ and $N_v^* \equiv e_p/c_p$, and in order of magnitude are

$$N_{C,V}^* \sim \left(\frac{m_{C,V}\epsilon_m^{C,V}}{\hbar^2}\right)^{3/2}, \tag{6}$$

where $\epsilon_m^{C,V}$ are the average kinetic energies of electrons and holes emitted by a highly excited defect, and $m_{C,V}$ are their effective masses. It was shown in Ref. 4 that at high vibration energies ($E \gtrsim \epsilon_g$) the energy ϵ_m satisfies the inequalities[2] $kT_{e,h} \ll \epsilon_m \ll E$, where $T_{e,h}$ are the electron and hole temperatures. Let us discuss the limits of applicability of the solution which we found. First, in deriving system (2) we ignored the filling of the band states, which is valid only if $\epsilon_m^{C,V} \gg \epsilon_F^{C,V}$, where $\epsilon_F^{C,V}$ is the Fermi quasilevels for electrons and holes. Secondly, the condition under which the kinetic energy of the ejected carriers is small compared with the vibration energy requires that the inequality $\epsilon_m \ll kT^*$ hold. Using (5) and (6), we thus find the constraints imposed on the electron and hole density, given by

$$\exp\left\{-\frac{\epsilon_g}{\epsilon_m}\right\} \ll \frac{np}{N_C^* N_V^*} \ll 1, \tag{7}$$

which, along with inequality (1), identify the region in which solution (4) is applicable.

The inelastic mechanism for fast-ion sputtering of the surface of solids, at which the energy of bombarding particles is transferred to the surface atoms through excitation of the electron subsystem of the solid, was discussed in Ref. 5. It was established that the energy spectrum of sputtered particles can be approximated by a Maxwellian distribution with a temperature on the order of several thousand degrees which, as a rule, greatly exceeds the melting point of the crystal.

Such an energy distribution can be explained if it is assumed that the inelastic sputtering is caused by the heating of local and surface vibrations of the crystal as a result of many-phonon recombination of nonequilibrium carriers through the defects, which are localized at the surface, or through the surface (Tamm) states. The high-energy defect distribution tail, as was shown above, is characterized by an effective temperature (5). At high nonequilibrium carrier concentrations which are characteristic of inelastic sputtering mechanism, the temperature T for broad-band semiconductors and insulators could easily reach several thousand degrees.

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[1)] It was shown in Ref. 4 that capture coefficient of carriers on a strongly excited defect may reach the values $c \sim 10^{-6}$ cm^3/s. Assuming that $\tau_L \sim 10^{-11}$ s as an estimate, we see that inequality (1) is satisfied even at densities $n,p \sim 10^{18}$ cm^{-3}.

[2)] The energy ϵ_m can be estimated from the relation[4] $\epsilon_m \sim [\beta(\hbar\omega)^2\epsilon_g]^{1/3}$, where ω is the local vibration frequency, and β is a dimensionless coupling constant of the electron–phonon interaction.

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