Photoexcitation of local vibrations in semiconductors

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A new mechanism for the excitation of local vibrations of defects with a deep level is discussed. If the density of free carriers is high, and if the photoexcitation of the defects is intense, the energy of the absorbed light may be transferred to local vibrations as the result of a radiationless multiphonon capture of carriers by photoionized defects.

Several investigators have studied the effect of photoexcitation of defects on defect-induced reactions.[1–3] It has been suggested that in the course of photoionization a defect goes into a metastable state with an antibonding configuration of atomic orbitals, initiating a defect reaction. In the present letter we discuss an alternative mechanism for photostimulated defect reactions.

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We consider a semiconductor with a high electron density in the conduction band, n. We assume that this semiconductor contains defects with a deep level, which is separated from the conduction band by the ionization energy ϵ_T. We assume that the extent to which defects are occupied by electrons is determined by the radiationless capture and ejection of electrons by defects. It has been shown in the classical theory of radiationless multiphonon transitions (Ref. 4, for example) that an electron is captured by a defect only if the energy of the local vibrations of the defect, E, is greater than the energy (ϵ_2) corresponding to the crossing of the adiabatic terms of the vacant and occupied defects (Fig. 1). We assume that the electron density in the conduction band is so high that the rate at which these electrons are captured by a defect with a vibration energy E satisfies $nC_n(E) \gg \tau_E^{-1}$, where τ_E is the relaxation time of the local vibrations. When an electron is captured, the energy of the local vibrations of the defect increases by an amount ϵ_T, becoming $E + \epsilon_T$. The rate at which electrons with this larger vibration energy are ejected, $e_n(E + \epsilon_T)$, is also considerably greater than the energy relaxation rate τ_E^{-1}. The capture and ejection lead to a dynamic equilibrium between the populations of the vibrational states of the vacant defects, $N_2(E)$, and of the defects occupied by electrons, $N_1(E + \epsilon_T)$:

$$nC_n(E)N_2(E) = e_n(E + \epsilon_T)N_1(E + \epsilon_T). \tag{1}$$

It follows from this relation that the extent to which the defects with a vibration energy E are occupied by electrons is determined by the ratio of the electron-capture and electron-ejection rates:

$$f^* \equiv \frac{N_2(E)}{N_2(E) + N_1(E + \epsilon_T)} = \frac{nC_n(E)}{nC_n(E) + e_n(E + \epsilon_T)}. \tag{2}$$

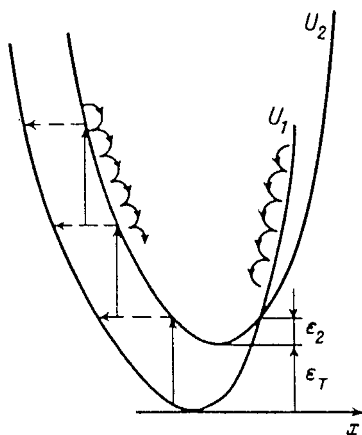

FIG. 1. Transitions of a defect during photoexcitation of local vibrations. U_1—Adiabatic potential of the vibrations of a defect with a bound electron; U_2—the same, without the electron; horizontal arrows—radiationless transitions; vertical arrows—photoionization of a defect; wavy lines—energy relaxation of local vibrations; x—configurational coordinate of the local vibrations.

The coefficients $C_n(E)$ and $e_n(E+\epsilon_T)$ depend only weakly on the energy E at $E>\epsilon_2$ (Ref. 5), so we can assume that f^* is essentially independent of the energy. The dynamic equilibrium in (1) is reached over a time on the order of $(nC_n+e_n)^{-1}$.

We now assume that the semiconductor is illuminated by light with a photon energy in the extrinsic absorption region. We assume that this light is so intense that the inequality $e_{\rm ph} \gg \tau_E^{-1}$ holds, where $e_{\rm ph}$ is the rate of photoionization. Since the cross section for the photoionization of a defect is usually several orders of magnitude smaller than the cross section for the radiationless capture of an electron by a highly excited defect, we have

$$e_{\rm ph} \ll nC_n,\ e_n. \tag{3}$$

We assume that a defect with a local-vibration energy E is initially occupied by electrons. During photoionization, the defect becomes vacant, with essentially no accompanying change in local-vibration energy. Once vacant, the defect quickly recaptures an electron. As a result of a radiationless multiphonon transition, the energy of the local vibrations increases by an amount ϵ_T. Since, by virtue of inequality (3), the photoionization rate is considerably smaller than the rates of radiationless capture or ejection of an electron by a defect, the extent to which the defects are occupied by electrons, f^*, remains essentially constant during illumination in the extrinsic region. It is again given by expression (2). As a result, the energy balance equation for the local vibrations becomes

$$\frac{dE}{dt} = \epsilon_T e_{\rm ph} f^* - I(E). \tag{4}$$

The first term on the right describes the energy input into the system of local vibrations, while the second term describes the energy relaxation of the vibrations. Adopting the model of a damped harmonic oscillator for the interaction of the local vibrations with the lattice vibrations, we can estimate the term $I(E)$ from $I \approx E/\tau_E$. In this case the steady-state value of the energy, corresponding to equal rates of excitation and dissipation of the vibrations $(dE/dt=0)$, is

$$E_{\rm st} = \epsilon_T e_{\rm ph} f^* \tau_E = \epsilon_T \frac{nC_n e_{\rm ph}\tau_E}{nC_n+e_n}. \tag{5}$$

The photoionization rate can be found from $e_{\rm ph} = N_{\rm ph}\sigma c$, where $N_{\rm ph}$ is the concentration of photons in the extrinsic illumination, σ is the photoionization cross section, and c is the velocity of light in the medium. Setting $N_{\rm ph} \sim 10^{18}$ cm^{-3} (this figure corresponds to a radiant power density of 10^7 W/cm^2) and $\sigma \sim 10^{-17}$ cm^2, we find $e_{\rm ph} \sim 10^{11}$ s^{-1}. The energy relaxation time in semiconductors can reach values $\tau_E \sim 200$ ps, according to experimental estimates.[6] Assuming an electron density $n \sim 10^{18}$ cm^3, $C_n \sim 10^{-6}$ cm^3/s, and $e_n \sim 10^{13}$ s^{-1} (Ref. 5), we find $E_{\rm st} \sim \epsilon_T$. Since we would have $\epsilon_T \sim 1$ eV for deep centers, the steady vibrational state of the defect is highly excited. As a result, there is a sharp acceleration of defect reactions, in particular, the annealing of defects. The photoexcitation of local vibrations is shown schematically in Fig. 1.

The mechanism discussed here may be pertinent to the laser annealing of defects in the solid phase. When carriers are excited by light pulses in the intrinsic absorption region of a semiconductor, extrinsic illumination can significantly increase the efficiency at which the defects are annealed out.

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