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Stretched-exponential law for carrier capture kinetics of a trapping center in compensated amorphous silicon

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The stretched-exponential law is used to describe the optically induced excess conductivity in compensated amorphous silicon. The results support the model of the slow trapping of photogenerated holes in P-B complexes which are in poor communication with the rest of the material, leaving electrons behind to conduct. The capture kinetics of the P-B center is related to the equilibration rate with a characteristic power-law time dependence.

Relaxation of disequilibrated systems towards equilibrium often obeys a time law which is not exponential. The first observation was described by Kohlrausch,[1] who found an empirical formula

$$A(t)=\exp[-(t/\tau)^{\beta}]\,, \tag{1}$$

where $A(T)$ is the normalized transient amplitude as a function of time, τ is a time constant, and β is a stretching factor between 0 and 1. The special case $\beta=1$ represents the conventional Debye relaxation. The $\beta<1$ general case was forgotten in the physics community until its rediscovery in 1970 in the studies of dielectric relaxation in polymetric systems.[2] Since 1970, many relaxation phenomena in disordered systems, including mechanical, dielectric, magnetic, thermal, etc., have been found to be governed by the stretched-exponential (SE) law. Several mechanisms leading to the nonexponential relaxation have been identified including hierarchically constrained dynamics,[3] time-dependent barriers to recombination,[4,5] time-dependent diffusion processes,[6,7] and an exponential distribution of activation energies.[8] Recently, Kakalios, Street, and Jackson[6] demonstrated a microscopic mechanism for SE decay in the electronic properties of hydrogenated amorphous silicon (*a*-Si:H). The relaxation is attributed to the motion of bonded hydrogen which exhibits dispersive diffusion with a characteristic power-law time dependence. In this paper, we demonstrate that the capture characteristics of trapping centers in compensated *a*-Si:H obey the modified SE law.

Recently, other groups[9-11] observed that compensated *a*-Si:H thin films show excess dark conductivity after light exposure. The excess conductivity increases with exposure time nonexponentially. Since the undoped films or those having only one dopant (B or P) do not show the behavior, it has been suggested that this phenomenon results from the slow trapping of photogenerated carriers in P-B complexes which are in poor communication with the rest of the material.[9-11] The energy level $E_{\text{P-B}}$ of P-B complexes can be determined from the peak position of the measurement of excess conductivity as a function of activation energy of dark conductivity in the heat-dried state.[9,10] When the Fermi level is above $E_{\text{P-B}}$, the P-B complexes are filled with electrons. On shining light, they capture holes slowly, leaving electrons behind to conduct, thus the conductivity increases with time. When the Fermi level is below them these complexes are empty, and when it is too close to the conduction band, the dark current is large. Both these situations will give smaller excess conductivity, which can explain the observed peak and give the value of $E_{\text{P-B}}\approx 0.8$ eV below the conduction-band edge.[9] Even though this model can account for the observed phenomena, the mechanism of capture kinetics of P-B center which leads to the nonexponential increase of conductivity with time has not been discussed. It is the purpose here to resolve this problem.

The decay of small departures Δ from equilibrium can be described by the linear relation

$$d\Delta/dt=-\nu\Delta\,, \tag{2}$$

which does not depend on the detailed microscopic mechanism. In order to obtain the SE law, the equilibration rate ν cannot be a single value. In the study of band-tail carriers relaxation in *n*-type *a*-Si:H, Kakalios *et al.*[6] used the fact that the rate of equilibration of band-tail carriers is related to the diffusion of hydrogen. The exponential distribution of diffusion-site energies leads to a power-law time dependence for hydrogen diffusion. If one assumes that the rate constant ν is proportional to the hydrogen hopping rate D_{H}/a^2, where a is a characteristic hopping distance that the hydrogen moves in a single-diffusion step and D_{H} is the diffusion coefficient, the SE relaxation can be obtained.

Our approach to the analysis of the P-B center capture kinetics of holes is similar to that of Kakalios *et al.*[6] The expression for the two charge states of the P-B center can be written as

$$\text{PB}^{-}+h^{+}\rightarrow\text{PB}\,, \tag{3}$$

where h^{+} represents a hole with a positive charge. The Fermi level, determined by the free-electron concentration, increases in energy as the recombination process occurs. This has the effect of increasing the activation energy required for hole capture from the Fermi level as a function of time, thereby generating nonexponential capture kinetics. If we assume that the energy of P-B centers is an exponential distribution due to differences in the local atomic configurations of amorphous matrix, the equilibration rate will have a power-law time dependence. To model the P-B center capture process, it is important to note some differences between hydrogen diffusion in *a*-Si:H and the P-B center capture kinetics model as discussed above. The dispersive transport of hydrogen in *a*-Si:H arise from an exponentially weighted distribution of hydrogen release from traps in the sample. As the hydrogen proceeds in its thermally activated motion, it encounters and can be captured and released by a number of defects. In contrast, a hole from the band tail captured by a P-B center has a negligible probability of reemission at the temperature of interest. Therefore, the characteristic capture barrier energy of the particular P-B center that captured a hole is removed from the distributions. Scher and Montroll[7] have examined both regimes of this behavior in their model for transient time dispersion in amorphous solids. While the diffusion of hydrogen in *a*-Si:H would be expected to be of the form of (1), the addition of an adsorbing boundary for carriers, in this case a P-B center, which removes the carriers permanently, causes the sign of β to become negative. The P-B center capture kinetics would then be expected to be of the form[12]

$$B(t)=1-\exp[-(t/\tau)^{-\beta}], \tag{4}$$

where $B(t)$ is the fraction of the number of P-B centers, which did not capture holes, as a function of time.

Figure 1 shows results for compensated *a*-Si:H prepared from pure $\mathrm{SiH_4}$ doped with 1000 ppm $\mathrm{PH_3}$ and 1000 ppm $\mathrm{B_2H_6}$. The data were taken from our previous results.[11] The value of $B(t)$ is defined as

$$B(t)=1-\frac{\sigma(t)-\sigma(0)}{\sigma_{\mathrm{sat}}}, \tag{5}$$

where $\sigma(0)$, $\sigma(t)$, and σ_{sat} represent the dark conductivity of the initial state, after a light exposure of time t, and of the saturated state, respectively. The solid curve is a result of Eq. (4), where known values for τ and β are inserted rather than using these parameters as adjustable. The value of $\beta=0.5$ was taken from the measurements of Kakalios *et al.*,[6] where we have assumed that the exponential distribution of site energies due to the amorphous matrix is the same for hydrogen and the P-B center. The time constant τ defined by Eq. (4) obeys an Arrhenius relationship, with an activation energy E_a, and a preexponential factor τ_0,

$$\tau=\tau_0\exp(E_a/k_BT). \tag{6}$$

We use the value of $\tau_0=10^{-12}$ sec taken from the result of Tiedje, Abeles, and Cebulka,[13] and the value of $E_a=0.9$ eV which is the difference between the energy gap and the energy level of the P-B complex. In this way, we obtain a good fit to the experimental points and the theoretical result. Thus, this result provides an illustrative experimental proof for a novel theoretical approach to interpret the SE law, which causes peculiar phenomena in the time domain in many branches of physics.

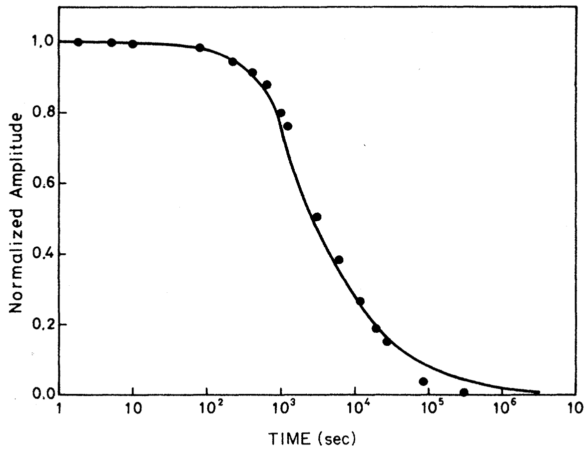

FIG. 1. Time dependence of the fraction of P-B complexes that did not capture holes for compensated *a*-Si:H. The solid line is fitted to the data with use of the capture kinetics law given by Eq. (4).

In conclusion, we have shown that the capture characteristics of the P-B complex in compensated *a*-Si:H can be well modeled by a modified stretched-exponential function. There is quantitative agreement between the SE parameters and the measured values. This result supports the proposed model of the optically induced excess conductivity in compensated *a*-Si:H. Further extensions of this analysis may demonstrate other similarities between the behavior of the P-B center and the diffusion behavior of hydrogen in *n*-type *a*-Si:H. A comprehensive analysis of capture and emission kinetics may also provide greater insight into both the P-B center and the nature of the stretched-exponential law. These results can also help to resolve the microscopic mechanism of the persistent photoconductivity in doping-modulated amorphous silicon superlattices. This paper, for the first time, demonstrates that the capture kinetics of trapping centers in amorphous solids obeys a stretched-exponential law.

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