DYNAMICS OF PHOTOGENERATED NONEQUILIBRIUM ELECTRONIC STATES IN A DISORDERED ONE-DIMENSIONAL LATTICE

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The dynamics of photogeneration and pair annihilation of nonequilibrium quasi-particles (photon→A+B→0) in a disordered one-dimensional lattice is examined by numerical simulation. To investigate the nature of the nonequilibrium kinetics of polarons in linear chain materials, the calculation is carried out assuming that every lattice point of randomly disordered lattice can accommodate arbitrary number of particles of the same species. We discuss the time evolution of self-formation of domains during optical pumping and of their decay after discontinuation of pumping.

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Nonequilibrium quasi particle states can be photogenerated in a variety of low-dimensional materials.[1-5] In the present study we examine numerically the influence of the lattice disorder on the photogeneration and decay process of polarons, especially on the self-formation process of domains (aggregates).

In the numerical calculation, we treat a long ring of chain lattice whose sites are divided by the energy barriers of mean height 0.40 eV. We assume that each lattice point can accommodate arbitrary number of particles of the same species, which are electron- or hole-polarons. Presuming also that the electron and hole pairs are photocreated in the randomly selected consecutive sites at the rate of C and that only one particle on a lattice point can jump to either of the adjacent points at every hopping. The disorder of the lattice is introduced by a random distribution of the barrier height that complies with the Gaussian distribution of width σ.

Figure 1(a) shows the time evolution of the average particle number N on a lattice point for the case of the completely ordered lattice of σ = 0 eV. After sufficient pumping, the system reaches a steady state N_s which depends on C/W, where W is the intersite hopping probability. N_s increases monotonously with increasing C/W. In the case of disordered lattice, the hopping probability is assumed to obey the Arrhenius law and W is redefined as the probability for the barrier of

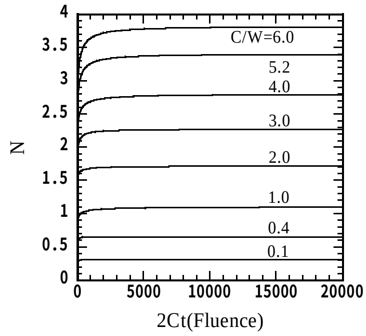

Fig.1(a) Average particle numbers N on a lattice point in photogeneration in an ordered lattice(σ = 0 eV).

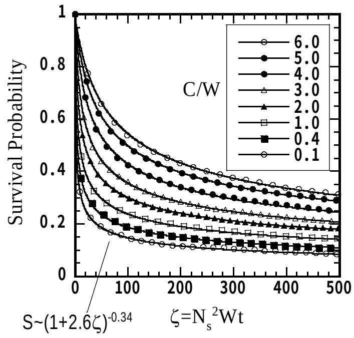

Fig.1(b) Decay of particles after the discontinuation of pumping in an ordered lattice(σ = 0 eV).

mean height. As σ increases the rise of N becomes slower and slower. At the same time N_s for a given C/W increases. The decay after discontinuation of pumping depends strongly on N_s for both cases of σ=0 and σ>0. Fig.1(b) shows the result for σ=0 eV as an example. Using a dimensionless time $\zeta = N_s^2 Wt$, the decay for σ=0 eV is represented well by $(1+\zeta/\tau)^{-\alpha}$, where τ and α are constants. However as σ increases, the decay curve runs off the power law and becomes to obey the Kohlrausch law of $\exp[(-\zeta/\tau')^{\beta}]$, where τ' and β are constants.

We observed the formation of aggregates in both processes of the photo-generation and decay. The aggregate here means a lump of the consecutive lattice points occupied by particles of the same species, whereas the aggregate size is measured by the number of particles included in the lump. Figure 2 shows the growth of aggregates with the fluence $2Ct$ of photogeneration in the disordered lattice of σ=1.0 eV, where the pumping rate is chosen as C/W=6.0. As the fluence increases, the dominant size of the aggregate increases one after another. If the pumping is intensified or the lattice disorder is enhanced, the rate of the larger-size aggregates increases. However, the maximum number of the aggregate having a given size is suppressed by the lattice disorder when the pumping is strong. By weak pumping in an ordered lattice, hardly large-size aggregate grows and the small-size ones monotonously reach a steady state. As far as the growth of aggregate is concerned, no essential difference is seen between the ordered and disordered lattice.

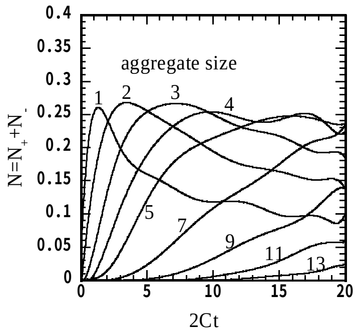

Fig.2 Aggregate growth (C/W=6.0, σ=0.10eV).

The time evolution of the aggregates after discontinuation of pumping is shown in Fig.3. In the strongly disordered lattice[Fig.3(a)], the small-size aggregates such as size-one or -two remain stable or rather grow for a long period. These stability or growth is supported by the supplying particles to small-size aggregates from the larger-size ones that loose particles and reduce themselves with time. The number of vacancies increases in this period.

In the weakly disordered lattice and in an ordered lattice, the density of particles at the discontinuation of pumping is low compared with the disordered lattice. In these cases, the number of aggregates decreases rapidly in the early stage of step and decays slowly after this stage[Fig.3(b)]. The rapid decay may be the reflection of disappearance of the aggregates which are composed of few sites hold a lot of particles and the slow decay may be that of the aggregates consist of many sites with few particles.

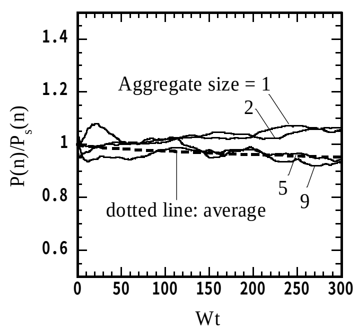

Fig.3(a) Decay of aggregates in the disordered lattice of σ=0.10eV after discontinuation of pumping of *C*/*W* =6.0.

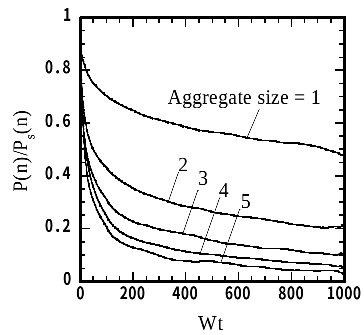

Fig.3(b) Decay of aggregates in the weakly disordered lattice of σ= 0.010eV after discontinuation of pumping of *C*/*W*=2.0.

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