INTERACTIONS BETWEEN SMALL-POLARONIC PARTICLES IN SOLIDS*

David Emin

Sandia National Laboratories†
Albuquerque, New Mexico 87185

ABSTRACT

When a light particle in a solid composed of relatively heavy atoms is associated with substantial displacements of the equilibrium positions of the atoms immediately surrounding it, the composite entity may be regarded as being small polaronic. Many instances of self-trapping of electronic charge carriers, excitons and light atoms such as hydrogen are known. A significant contribution to the interaction between such particles results from interference between their atomic displacement patterns. As a result oppositely charged small polarons may experience an intermediate-range repulsion, while both like-signed and neutral entities may have a tendency to cluster. These effects can be very important. As examples, the recombination kinetics of electron and hole small polarons and the ordering of defect atoms are discussed.

INTRODUCTION

The introduction of either interstitial atoms, vacancies, electronic charge carriers, or excitons into a solid is generally accompanied by alterations of the equilibrium positions of the atoms of the solid. These atomic displacements become especially significant if they exceed the amplitudes of the zero-point motion of the displaced atoms. This paper is concerned with that interaction between strongly coupled particles (or quasiparticles) which results from their mutual interaction with the atomic displacements of the host material.

APPROACH

A system of static entities which interact with each other and with the lattice containing them is described by a Hamiltonian which presumes a linear interaction between the added particles (or quasiparticles) and the atoms of the lattice, in addition to harmonic interactions between lattice atoms. Specifically, one has

$$H = \sum_i \sum_{\underset{\sim}{g}} \epsilon_{\underset{\sim}{g}} n_{\underset{\sim}{g}} + \tfrac{1}{2} \sum_i \sum_j \sum_{\underset{\sim}{g}} \sum_{\underset{\sim}{g}'} U^{i,j}_{\underset{\sim}{g},\underset{\sim}{g}'} n^i_{\underset{\sim}{g}} n^j_{\underset{\sim}{g}'} + \sum_\lambda \sum_{\underset{\sim}{q}} \hbar\omega_{\underset{\sim}{q},\lambda} \left(b^+_{\underset{\sim}{q},\lambda} b_{\underset{\sim}{q},\lambda} + \tfrac{1}{2}\right)$$

$$+ \sum_\lambda \sum_{\underset{\sim}{q}} \sum_i \sum_{\underset{\sim}{g}} n^i_{\underset{\sim}{g}} \left(V^i_{\underset{\sim}{q},\lambda} e^{i\underset{\sim}{q}\cdot\underset{\sim}{g}} b^+_{\underset{\sim}{q},\lambda} + \text{c.c.}\right) , \qquad (1)$$

where $n^i_{\underset{\sim}{g}}$ and $\epsilon^i_{\underset{\sim}{g}}$ are, respectively, the number and energy of each particle of type i located at a site designated by the position vector $\underset{\sim}{g}$, and $U^{i,j}_{\underset{\sim}{g},\underset{\sim}{g}'}$ is the energy of direct interaction between a pair of static particles. Creation and annihilation operators for phonons of mode λ, wavevector $\underset{\sim}{q}$, and energy $\hbar\omega_{\underset{\sim}{q},\lambda}$ are denoted by $b^+_{\underset{\sim}{q},\lambda}$ and $b_{\underset{\sim}{q},\lambda}$, respectively. The interaction between a particle of species i and a phonon is characterized by $V^i_{\underset{\sim}{q},\lambda}$.

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For any configuration of particles one can find the positions of the lattice atoms which minimize the energy of the system. Then the energy of the system, apart from that due to vibrational motion, is found to be

$$E = E_{\text{isolated}} + E_{\text{direct}} - E_b \quad , \tag{2}$$

where E_{isolated} and E_{direct} represent the first and second terms of Eq. (1), respectively, and E_b is defined by

$$E_b \equiv \sum_{\lambda} \sum_{\underset{\sim}{q}} \sum_{i} \sum_{j} (V^{i*}_{\underset{\sim}{q},\lambda} \; V^{j}_{\underset{\sim}{q},\lambda} / \hbar\omega_{\underset{\sim}{q},\lambda}) \sum_{\underset{\sim}{g}} \sum_{\underset{\sim}{g}'} n_{\underset{\sim}{g}} \; n_{\underset{\sim}{g}'} \; e^{i\underset{\sim}{q}\cdot(\underset{\sim}{g}-\underset{\sim}{g}')} \quad . \tag{3}$$

If, for example, there were but a solitary particle of type i located in the solid, E_b simply reduces to the small-polaron binding energy of such a particle:

$$E_b = \epsilon^{i}_{b} = \sum_{\lambda} \sum_{\underset{\sim}{q}} |V_{\underset{\sim}{q},\lambda}|^2 / \hbar\omega_{\underset{\sim}{q},\lambda} \quad . \tag{4}$$

However with two particles of the same type (species i) located at sites g_o and g_1 one has that

$$E_b = \sum_{\lambda} \sum_{\underset{\sim}{q}} \left[|V_{\underset{\sim}{q},\lambda}|^2 / \hbar\omega_{\underset{\sim}{q},\lambda} \right] \left\{ 2 + 2 \cos[\underset{\sim}{q}\cdot(\underset{\sim}{g}_o - \underset{\sim}{g}_1)] \right\}$$

$$\equiv 2 \, \epsilon^{i}_{b} + U^{i,i}_{\underset{\sim}{g},\underset{\sim}{g}'}(\text{indirect}) \quad . \tag{5}$$

Here the second term represents that portion of the interaction between the two particles which results from their mutual interaction with the displacements of the atoms of the lattice. Finally, if the particle at sites g_o and g_1 are of different types (i and j, respectively) the energy of their indirect interaction is given by

$$U_{g,g'} = 2 \sum_{\lambda} \sum_{\underset{\sim}{q}} \text{Re} \left[V^{i*}_{\underset{\sim}{q},\lambda} \; V_{\underset{\sim}{q},\lambda} \; e^{i\underset{\sim}{q}\cdot(\underset{\sim}{g}_o - \underset{\sim}{g}_1)} \right] / \hbar\omega_{\underset{\sim}{q}}, \quad . \tag{6}$$

In the present discussion the particle-lattice interaction is taken to be of short range. That is, the energy of a charge carrier on an atomic site depends on the proximity of the nearest-neighbor atoms, while the energy of an interstitial is a function of its distance from the atoms immediately adjacent to it. In these cases $V^{i}_{\underset{\sim}{q},\lambda}$ has a rather weak nonmonotonic dependence on $\underset{\sim}{q}$ with maxima occurring far from the center of the Brillouin zone. Concomitantly, one finds that the indirect interparticle interaction falls off with separation as the oscillatory terms of Eqs. (5) and (6) give rise to increasingly efficient cancellations in the $\underset{\sim}{q}$-summation.

EQUIVALENT INTERSTITIALS

In solids one is often concerned with the strain fields surrounding defects. Here the displacements about neutral interstitials are considered. Presuming a negligible direct interaction between these interstitials, the net interaction energy is simply $-E_b$. As the simplest example consider interstitials placed in a monatomic linear chain. Minimimizing the energy, Eq. (1), yields the displacement patterns depicted in Fig. 1. Namely, each interstitial occupies a space (in this case, a linear dimension) equal to A/k, where A is the (constant) repulsive force exerted

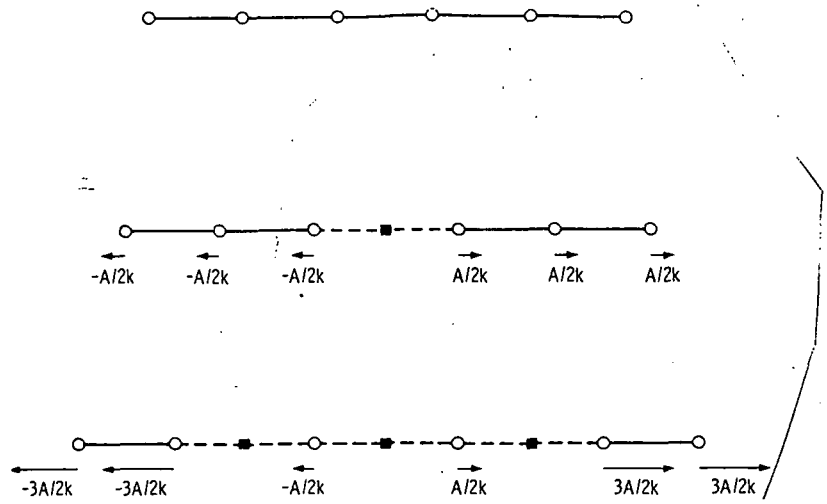

Fig. 1 One and three interstitials added to a monatomic chain. The strained bonds are shown with dashed lines.

between the interstitial and each of the two adjoining atoms, and k is the stiffness constant of the monatomic lattice. This constitutes a one-dimensional microscopic derivation of Vegard's theorem of elasticity theory: an elastic material expands by an amount equal to the extra volume of an inclusion.

In systems in which the added particle interacts with both optical and acoustic modes of the solid the situation becomes more complex.[1] A common situation is that in which light atoms form cages about relatively heavy atoms. A one-dimensional analogue of such a structure is that of a backbone of heavy masses to which light masses are attached. In essence the motions of the heavy atoms are associated with acoustic vibrational modes and the movements of the light masses relative to the heavy masses involve the optical modes. As illustrated in Fig. 2, if the interaction of an interstitial is mainly with the light atoms (optical modes), a local type of deformation pattern is produced which does not extend far from the interstitial. Furthermore, with a collection of three adjacent interstitials the asso-

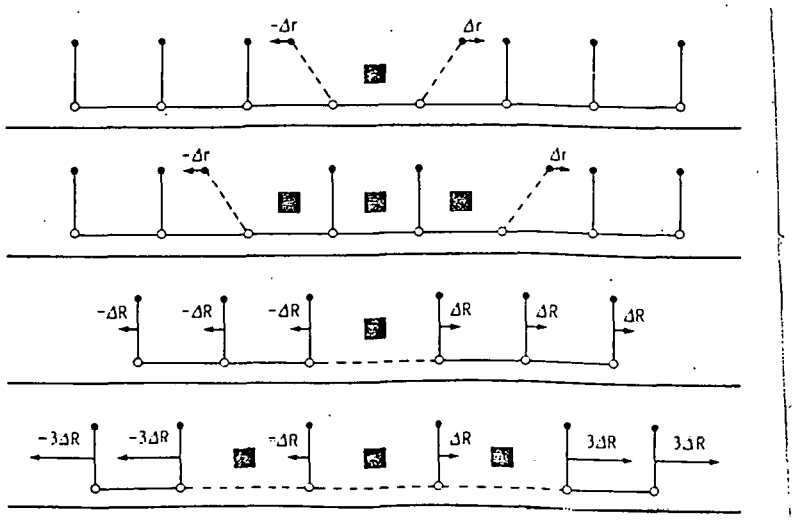

Fig. 2. Interstitials in a diatomic system. The optical-type deformations with one and three interstitials are shown in the top two lines. The respective acoustic-type deformations are shown in the bottom two lines for a diatomic chain. Dashes indicate strained bonds.

ciated deformation patterns tend to cancel. However, if the interaction of the interstitial is mainly with the heavy atoms, acoustic modes predominate and a long-range displacement pattern is established. Here Vegard's theorem may be applied.

Several comments are now in order. First, since Vegard's theorem is an outgrowth of elasticity theory (which involves only long-wavelength acoustic phonons) its inapplicability to some instances where optical-mode displacements play a role does not pose a contradiction for the macroscopic theory. Second, it is both obvious and well known that in systems of higher dimensionality the displacement patterns at long range are altered so as to reduce the magnitude of the displacements of individual atoms at the expense of involving a greater number of atoms. Third, dimensionality plays a major role in the energetics of clustering of added particles. For example, it can be seen from the optical-mode portion of Fig. 2 that it is energetically unfavorable for interstitials to cluster. However in three-dimensional models involving optical-type displacements clustering can be energetically favorable. Similarly, three-dimensional strain fields associated with acoustic-type displacements favor clustering.

Although the preceding discussion considered only neutral interstitials, analogous results apply to the strain fields and clustering of excitons, and (with the addition of the coulomb interaction) excess charges. Indeed, it is the possibility that the atomic-displacement-induced tendency of like charges to cluster may overcome their coulombic repulsion that has led to the consideration of bipolaron formation in both solids and liquids.

ELECTRON-HOLE INTERACTIONS

The lattice-mediated interaction of electron and hole small polarons can be of critical importance in their direct recombination. For the ideal monatomic system illustrated in Fig. 3a the deformation (here a contraction) about an electron has an opposite sense to that about a hole (here an expansion). For illustration the distortions are taken to be local as with light masses harmonically coupled to a rigid frame. The central point is that when the electron-hole separation is reduced sufficiently so that the two distortion patterns overlap substantially the binding energy associated with each small polaron is reduced. In other words, as shown by the curve labeled small polaron in Fig. 3b, the lattice-mediated interaction provides a repulsive component to the interaction between an electron and a hole small polaron. Furthermore, as shown in Fig. 3b, with sufficiently strong polaronic binding the combination of the small-polaron and coulombic terms yields a net energy which contains a repulsive barrier to recombination. This in effect screens out the strong portion of the coulombic attraction.

The luminescence associated with recombination in such a polaronic solid has been described elsewhere.[2] Hence it will only be noted that such a system (potentially) exhibits three luminescence processes: the recombination of excitons prior to lattice deformation, of self-trapped excitons, and of pairs of separated small polarons. These processes are associated with the positions labeled as E, STE, and GS in Fig. 3b.

The photoconductivity of a small polaronic solid is proportional to the average mobility of the photogenerated carriers and their lifetime. Since a finite time is required before an optically generated charge forms a small polaron, each carrier's mobility is an average of its nonpolaronic (precursor) mobility $\tilde{\mu}_e$ or $\tilde{\mu}_h$, and its self-trapped mobility, μ_e or μ_h, weighted by that fraction of the lifetime each exists in the precussor state, f_e and f_h. The average photoconductive mobility is $[\tilde{\mu}_e f_e + \mu_e(1 - f_e)] + [\tilde{\mu}_h f + \mu_h(1 - f_h)]$. Since often $\tilde{\mu} >> \mu$ the obser-

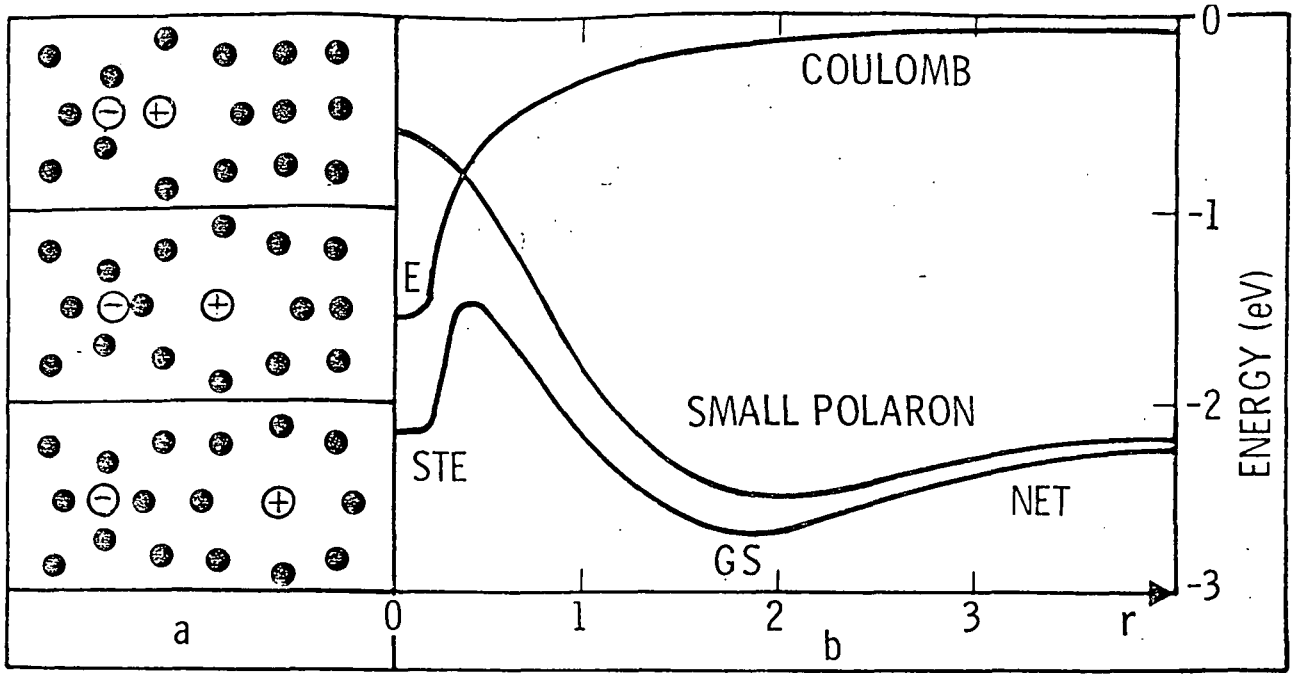

Fig. 3. The deformation patterns for an electron and a hole in a monatomic lattice are shown for three separations in (a). In (b) the net energy of the system as well as the coulombic and distortional (small polaron) components of the energy are plotted against the separation, r, measured in units of the lattice constant.

vation of a low photoconductive mobility requires that $f_e, f_h << 1$.

For direct recombination of low-mobility charge carriers it has generally been assumed that the room-temperature recombination is diffusion limited.[3] That is, electrons and holes hop together spatially and then recombine. Specifically, the probability that, once within their mutual coulomb capture radius, a pair will separate rather than recombine has been assumed to be insignificant. Nonetheless, there are previously unexplained situations in which the photoconducting carriers have very low (hopping) mobilities for which the recombination coefficient does not display the temperature dependence characteristic of diffusion controlled recombination.[4] The presence of a repulsive barrier provides a mechanism to resolve this dilemma. Namely, the barrier keeps the carriers apart and thereby reduces their overlap and recombination rate. In addition, by shielding the carriers from the steepest portion of their attractive coulomb potential, the probability of their separation is enhanced. Thus such a barrier to the recombination of small polarons may be significant in understanding the photoconducting properties of insulating and semiconducting glasses and crystals in which the charges form small polarons.

REFERENCES

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1. David Emin, Sandia Technical Report, SAND78-0165.
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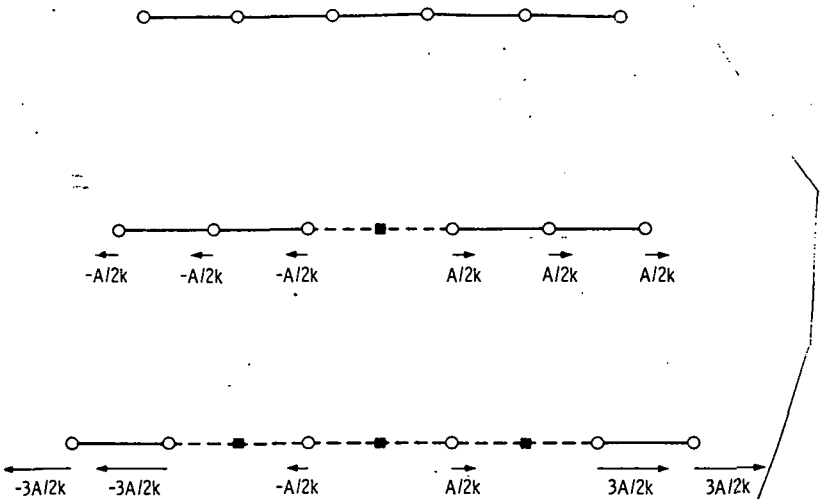

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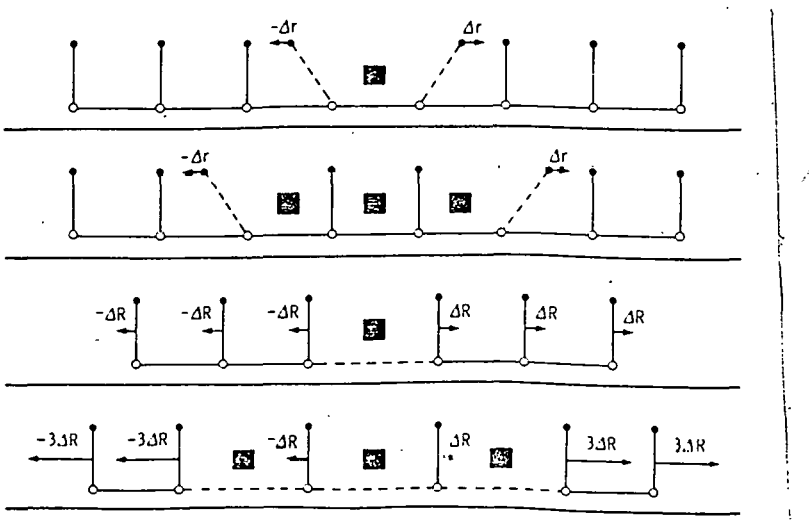

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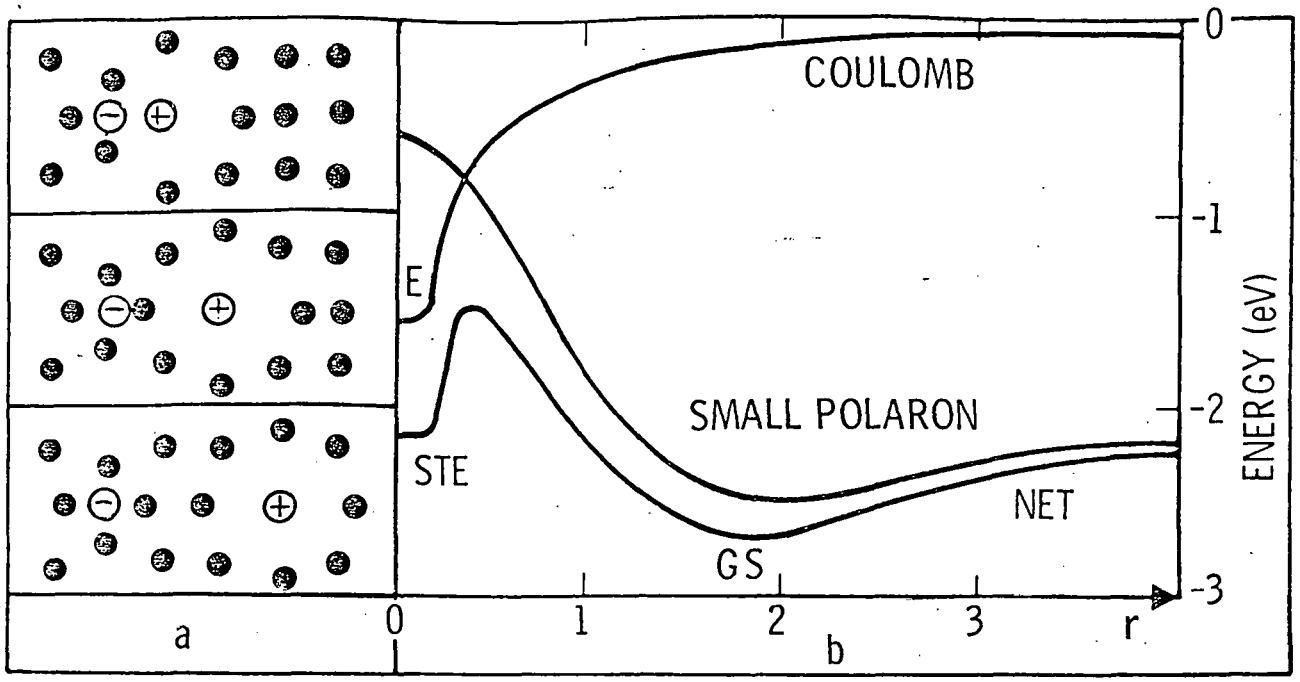

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