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ELECTRONIC PROPERTIES OF SOLID

Wigner Crystallization of Electrons in Deep Traps in a Two-Dimensional Dielectric

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Abstract—A two-dimensional model is used to examine the spatial distribution of electrons in deep traps in a two-dimensional dielectric. When the trap concentration is much higher than the trapped electron concentration, Coulomb repulsion leads to the formation of a two-dimensional quasi-periodic hexagonal lattice of localized electrons (Wigner glass).

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Coulomb repulsion between free electrons leads to Wigner crystallization, which has been observed on liquid helium surface [1]. In [2–4], it was hypothesized that Wigner crystallization of trapped carriers (electrons and/or holes) could occur in a dielectric with high neutral trap concentration because of Coulomb repulsion, as predicted by the original Wigner model. In [2], holes localized in silicon nitride were assumed to form a quasi-periodic square lattice.

To examine Wigner crystallization of trapped electrons and/or holes, we consider amorphous silicon nitride as a model dielectric. Silicon nitride has memory: it can hold electrons and holes in traps for as long as about 10 years at $T = 450$ K [5]. Practical interest in electron and hole localization in amorphous silicon nitride is motivated by the development of terabit flash memory based on silicon nitride [6]. There are deep electron and hole traps (about 1.5 eV deep) in this compound. According to studies of charge transfer, the neutral trap concentration in Si_3N_4 is $N_e \sim 10^{19}$–10^{20} cm^{-3} [7–11], whereas the concentration of occupied traps is much lower, $n_t \sim (2–6) \times 10^{18}$ cm^{-3} [12, 13]. In [14], electrons were observed to spread in silicon nitride, driven by their own repulsive Coulomb field.

In this study, a two-dimensional model is used to perform numerical simulations of Wigner crystallization in a dielectric with deep traps.

We consider a two-dimensional dielectric with concentration N_s of randomly distributed neutral traps as a model of disordered amorphous structure of a real dielectric. A fraction of the traps are randomly occupied by electrons, with concentration n_s. A trapped electron can be released with probability P by thermal ionization. The ith free electron moves in the plane with the drift velocity $V_i = \mu F_i$ determined by the magnitude and direction of the electric field F_i generated by other (both free and bound) electrons (μ is the electron mobility). An electron that passes by at a distance from a neutral trap shorter than a certain l_s is captured by the trap.

Since only a finite number of traps can be used in numerical simulations, boundary conditions should be set with particular care. In our study, the system was a square with side L, and cyclic boundary conditions were imposed to avoid electric field distortion at its boundaries; i.e., simulations were performed for an infinite number of identical squares.

Traps with concentration N_s were randomly distributed within a square, and n electrons were injected. The electric field strength at the ith electron position is expressed as

$$\mathbf{F}_i = \sum_{j \neq i}^{n_e} \frac{e(\mathbf{r}_i - \mathbf{r}_j)}{[(x_i - x_j)^2 + (y_i - y_j)^3]^{3/2}} + \mathbf{F}_l + \mathbf{F}_k, \qquad (1)$$

where the first term represents the field generated by the electrons within the central square, $\mathbf{r}_i$ and $\mathbf{r}_j$ (x_i and x_j, y_i and y_j) are the respective position vectors (abscissas, ordinates) of the ith and jth electrons (measured from the square's center), $\mathbf{F}_l$ and $\mathbf{F}_k$ are the fields generated by the adjoining squares in the ordinate and abscissa directions, and $\mathbf{l}$ and $\mathbf{k}$ are the corresponding unit vectors:

$$\mathbf{F}_l = \sum_{j=1}^{n_e} \frac{e(\mathbf{r}_i - \mathbf{r}_j) + (L - 2x_j)\mathbf{l}}{[(x_i - L + x_j)^2 + (y_i - y_j)^3]^{3/2}} + \sum_{j=1}^{n_e} \frac{e(\mathbf{r}_i - \mathbf{r}_j) + (L + 2x_j)\mathbf{l}}{[(x_i + L + x_j)^2 + (y_i - y_j)^3]^{3/2}}, \qquad (2)$$

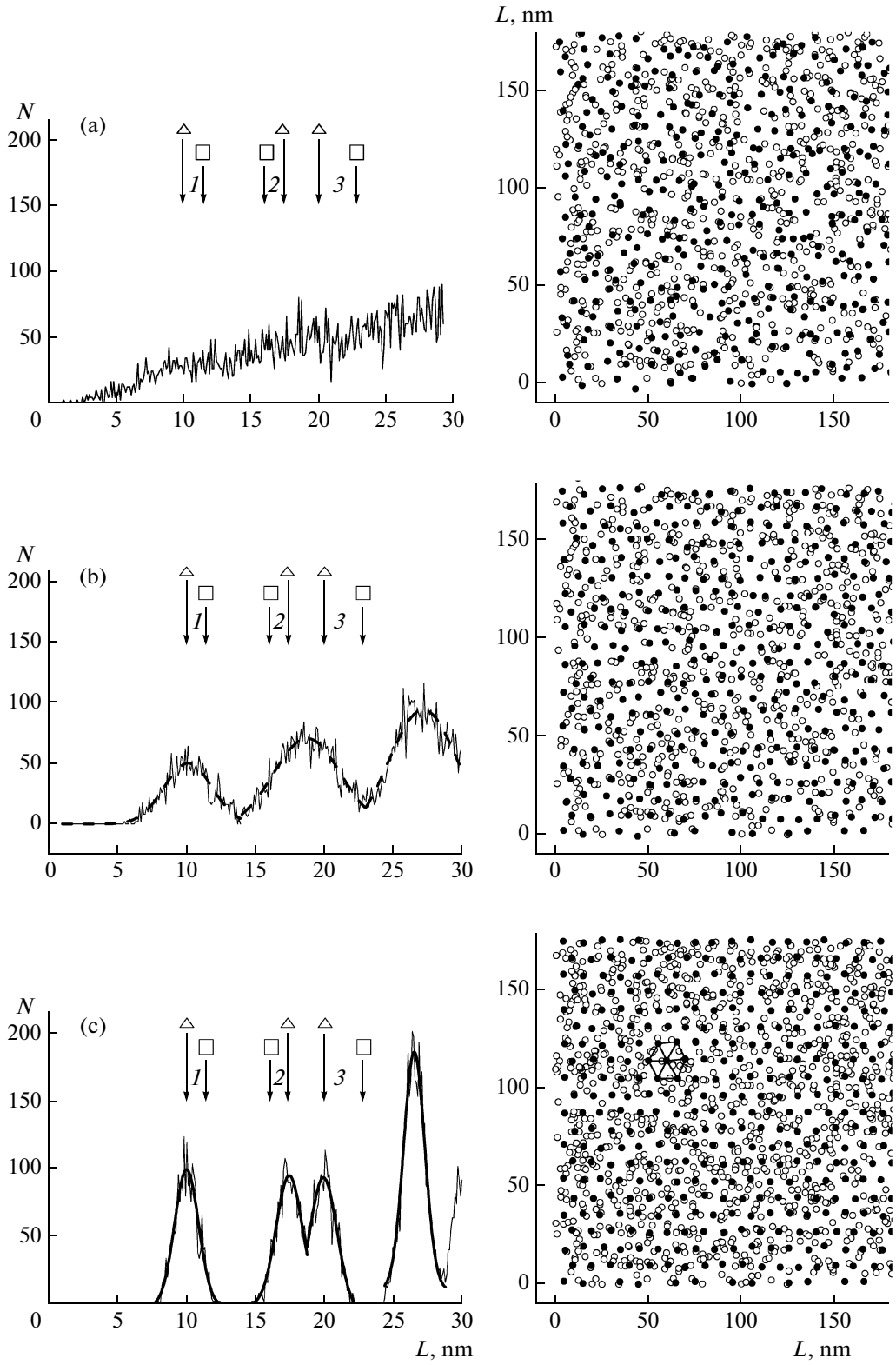

Figure 1. Left column: radial distribution of occupied traps for (a) $n_s/N_s = 0.5$, (b) $n_s/N_s = 0.01$, and (c) $n_s/N_s = 0.001$. Dashed curves are Gaussian approximations of the distribution. Right column: simulated distributions of vacant (○) and occupied (●) traps. Symbols △ and □ represent first, second, and third coordination spheres for triangular and square lattices, respectively.

$$\mathbf{F}_k = \sum_{j=1}^{n_e} \frac{e(\mathbf{r}_i - \mathbf{r}_j) + (L - 2y_j)\mathbf{k}}{[(x_i - x_j)^2 + (y_i - L + y_j)^3]^{3/2}} + \sum_{j=1}^{n_e} \frac{e(\mathbf{r}_i - \mathbf{r}_j) + (L + 2y_j)\mathbf{k}}{[(x_i - x_j)^2 + (y_i + L + y_j)^3]^{3/2}}. \quad (3)$$

The following calculations were performed:

(i) the field strength given by (1) was determined for each electron;

(ii) the drift velocity $V_i = \mu F_i$ was found for each i;

(iii) the displacement $\Delta\mathbf{h} = \mathbf{V}_i\Delta t$ was calculated, where Δt was such that $|\Delta\mathbf{h}| \approx l_s/2$ for the maximum F_i;

(iv) the electron positions were updated, and the distance to the nearest trap was calculated. If it was found that $((x_i - x_g)^2 + (y_i - y_g)^2)^{1/2} < l_s$, then the ith electron was regarded as trapped and the gth trap was charged.

The calculations were repeated until all electrons were trapped (i.e., $n_s = n$ traps were charged), and then the number $n_s(r)$ of charged traps was determined as a function of the distance r between a pair of traps.

Figure 1 presents the results calculated for $P = 0.01$ and $\mu = 1$. According to these results, when the trap concentration N_s is comparable to the concentration n_s of injected and trapped electrons ($n_s/N_s = 0.5$, see Fig. 1a), the function $n_s(r)$ has no special features and corresponds to a random trap distribution. When $n_s/N_s = 0.01$, a certain structure is clearly seen, with maxima of $n_s(r)$ located between charged traps characteristic of a three-coordinated lattice (see Fig. 1b). As the ratio decreases to $n_s/N_s = 0.001$, the peaks sharpen and the structure becomes more visible (see Fig. 1c). Thus, in a plane containing randomly distributed neutral traps, charged traps organize into a two-dimensional glass with hexagonal lattice. As a criterion for the existence of glass, we can adopt the following condition: the half-width Δr_1 of the first coordination peak is smaller than the distance $r_2 - r_1$ between the first and second spheres:

$$\Delta r_1 < r_2 - r_1. \quad (4)$$

Thus, we have shown that an ordered hexagonal lattice of charged traps can form in a plane containing randomly distributed neutral traps when the ratio n_s/N_s has a certain value. Analogous results were previously obtained for a two-dimensional free-electron gas [1].

A natural question arises about the applicability of the model described above to real systems, in particular about the effect of quantization of electronic states in neutral traps. It is well known that the bulk neutral-trap concentration does not exceed 10^{21} cm^{-3}; i.e., the corresponding surface concentration does not exceed 10^{14} cm^{-2}. As demonstrated in this study, crystallization occurs when $n_s/N_s < 0.01$. Therefore, the surface concentration does not exceed 10^{12} cm^{-2}; i.e., the average separation between electrons must not exceed 10^{-6} cm. It is obvious that the effect of quantization is weak over such separation distances.

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