Wigner crystallization due to electrons localized at deep traps in two-dimensional amorphous dielectric

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We calculated the spatial distribution of electrons localized at deep neutral traps in some amorphous dielectric films based on some fundamental physics in order to explain the phenomena such as space ordering of electrons. We showed that when the surface density of traps (N_s) is much larger than that of the trapped electrons (n_s), e.g., $n_s/N_s \leq 0.001$, Wigner crystallization occurs due to the Coulomb repulsion of trapped electrons and a two-dimensional quasiperiodic hexagonal lattice or Wigner glass can be formed. © *2010 American Institute of Physics*. [doi:10.1063/1.3458832]

It was long suggested that Coulomb repulsion of free electrons can lead to some spatial orderings of electrons and give rise to the Wigner crystallization.[1] This phenomenon should also occur in some dielectric films. It was suggested that antiferromagnetic coupling of electrons localized at deep neutral traps should exist in some dielectric films.[2–4] According to this proposal, in a dielectric film with a high density of deep and neutral traps, the local density of charged traps (n_t) would be much smaller than the local total density of traps (N_t) due to the Coulomb repulsion of trapped electrons. In addition, antiferromagnetic coupling of trapped electrons can occur due to the resonant tunneling of trapped electrons via the unoccupied traps. This model explained the experimental observations that no any electron paramagnetic resonance signal due to the trap-localized electrons or holes could be detected in some dielectric films with high amount of traps, such as amorphous silicon nitride (a-Si_3N_4),[2–5] silicon oxynitride,[6] and silicon oxide films with silicon implantation.[7]

Amorphous silicon oxide and amorphous silicon nitride are the two major dielectrics being widely used in silicon microelectronic devices. Unfortunately, high amount of electron and hole traps were often found in these dielectric films.[8] The charge trapping in these materials is the major cause for the instabilities and performance degradations of the microelectronic devices.[8–13] However, the charge trapping in amorphous dielectric also has some practical applications such as it can be used as a charge storage in a flash memory device.[10,14,15] The phenomena of electron and hole trapping in amorphous dielectrics had been the subject of many investigations. It was reported that silicon nitride contains a high amount of deep (≈ 1.5 eV) electron and hole traps. The volume density of these traps can be as high as $N_t \approx 10^{19}-10^{20}$ cm^{-3},[16–18] but the density of filled traps (n_t), in the range of $(2-6)\times 10^{18}$ cm^{-3}, is much lower.[19] By conducting a computer simulation, Maximova *et al.*[20] found that the electron cloud in the silicon nitride spreads out because of the Coulomb repulsion of electrons in their self-field. This result is a preliminary theoretical evidence for supporting the Wigner crystallization theory in amorphous nitride films. This work extends the simulation to present a direct evidence for the Wigner crystallization phenomenon in the amorphous dielectric films.

We consider a two-dimensional dielectric in which the initial sheet density of the randomly distributed neutral traps is N_s. The disordered structure of a real amorphous dielectric was modeled with a random distribution of deep traps. Then, free electrons were randomly introduced into the film until the sheet density reached a value of n_s.

The physical model was based on the following assumptions:

(1) In the two-dimensional plane, neutral traps with amount of N_s are randomly distributed. The energy level of the trap, W, is placed in the forbidden gap of the semiconductor and the averaged electron capture cross-section for the traps is σ.
(2) Free electrons, n_s, are randomly placed in the two-dimensional plane also. The free electrons are then captured by traps according the criteria given later on.
(3) Each ith free electron migrates over the surface under an electric field F_i induced by both the free electrons and the trapped electrons. The drift velocity of a particular electron, V_i, depending on the field F_i, is calculated according to $V_i=\mu F_i$ (here, μ is the electron mobility). For the sake of simplicity, dimensionless unity mobility was used for the calculation. Noting that we need to make such treatment because there are no mobility data for electron in SiO_2 and Si_3N_4 films available. Nevertheless, the mobility value only affect the time for electron to be settle down. It does not affect the final distribution of the trapped electrons and the ordering patterns.
(4) If an electron passes a trap within the region prescribed by the capture cross-section, σ, the electron is considered to be captured on the trap.
(5) An electron captured on a trap may be released according to thermal ionization probability, P.

Since only a limited number of traps could be taken in a practical simulation, it is important for the proper selection of the boundary conditions. We assumed that the system under study was in a square shape with a side length of L. To avoid the field distortions near the boundaries of the square,

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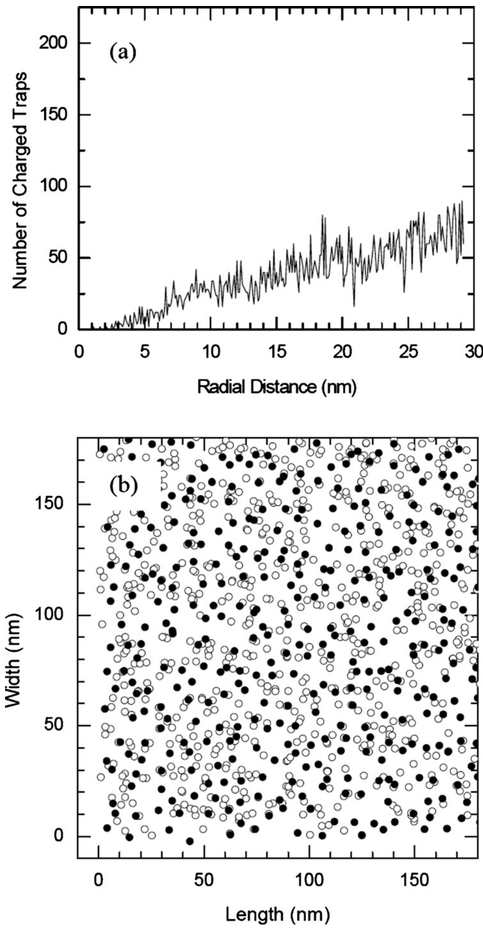

FIG. 1. (a) Radial distribution of charged traps and (b) calculated spatial distribution of neutral traps (open circles) and charged traps (filled circles) for $n_s/N_s=0.5$.

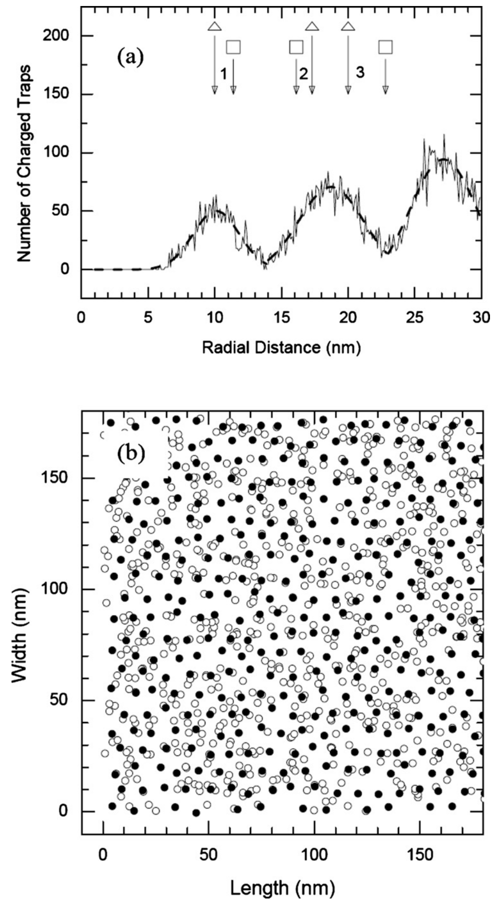

FIG. 2. (a) Calculated radial distribution of charged traps for $n_s/N_s=0.01$ with Gaussian approximation (dashed curve). Three peaks were found and their locations are close to the first, second, and third coordination spheres (marked as 1, 2, and 3, respectively) in a hexagonal (denoted by Δ) or a square crystal lattice ($\square$). (b) Calculated spatial distribution of neutral traps (open circles) and charged traps (filled circles) of the corresponding value of n_s/N_s.

cyclic boundary conditions were used. This treatment in effect makes the calculations being carried out in an infinite plane which is composed by a number of squares mentioned above.

The square region under consideration was first randomly planted with neutral traps to a surface density of N_s. Next, electrons with density of n_s were introduced into the square. Then, the field vectors at the points where the electrons located were calculated. The field vector at the location of the ith electron is given by

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

where the first term is the electric field due to all electrons in the center of the square; $\vec{r}_i$, $\vec{r}_j$ are the radial vectors for the coordinates x_i, x_j and y_i, y_j along the ordinate and abscissa axes, respectively, for ith and jth electrons (the coordinates are reckoned from the center of the square); and $\vec{F}_l$ and $\vec{F}_k$ are the fields produced by squares adjacent to the square under consideration over the ordinate and abscissa axes, with $\vec{l}$ and $\vec{k}$ being unit vectors along $\vec{F}_l$ and $\vec{F}_k$ which are given by following:

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

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

The calculation of the charge distribution involves the iteration of the following process:

(1) for each of the electrons calculate the electric field with Eq. (1);
(2) for each of the electrons calculate its drift velocity with $V_i=\mu F_i$;
(3) for each electron, calculate the incremental displacement with $\Delta\vec{h}=\vec{V}_i\Delta t$. The time step Δt was such chosen that $|\Delta\vec{h}|\cong\sigma/2$ still hold at the highest field F_i;
(4) then, new coordinate values for the electrons are computed and hence the distances to the nearest traps are

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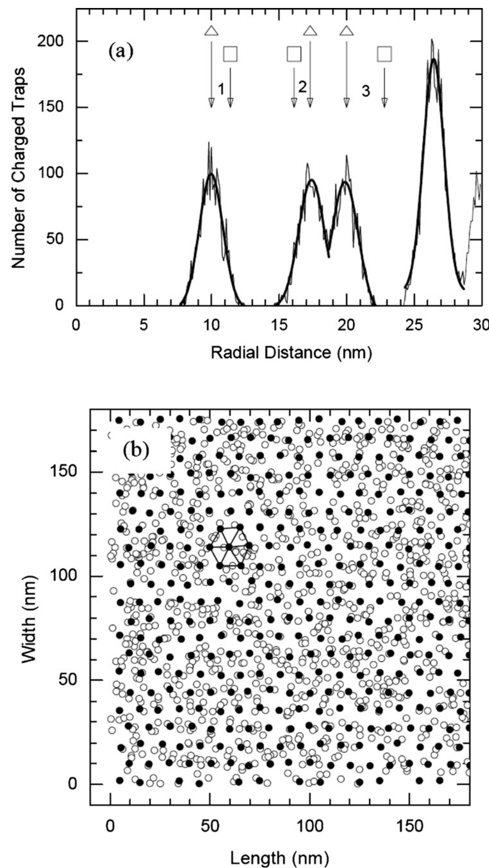

FIG. 3. (a) Radial distribution of charged traps for $n_s/N_s=0.001$ with Gaussian approximation (dashed curve). Numbers denote the first, second, and third coordination spheres positions in the hexagonal (Δ) or square (□) crystal lattice, respectively. (b) Calculated spatial distributions of neutral traps (open circles) and charged traps (filled circles) for $n_s/N_s=0.001$. The charged trap distribution shows some obvious ordering structures. A hexagonal lattice structure is shown in the plot.

determined. If $[(x_i-x_g)^2+(y_i-y_g)^2]^{1/2}<\sigma$, then the ith electron is considered to be trapped and the gth trap be charged.

These procedures were executed repeatedly until all electrons are captured at traps and, as a consequence, traps became negatively charged with electrons. Following the trap charging procedure, we calculated the total number of charged trap, $n_s(r)$, versus the separation r in each trap pair.

The calculated results are shown in Figs. 1–3 for various cases. When the total density of traps, N_s, is comparable with the density of electrons placed in the dielectric, n_s, e.g., $n_s/N_s=0.5$, the calculated electron distribution, $n_s(r)$, increases gradually with radial length [see Fig. 1(a)]. The trapped electrons show a random distribution nature [see Fig. 1(b)]. When $n_s/N_s=0.01$, the calculated spatial distribution of the charged traps starts to exhibit some orderings, with maxima showing up at a distance close to the value of lattice constant of a sixfold coordinated crystal lattice [see Fig. 2]. When the trap density increases further or n_s/N_s decreases further, as depicted in Fig. 3(a), the radial distribution of $n_s(r)$ exhibits even narrower peaks and the quasiperiodic structure of traps becomes more distinct. The splitting of the peak labeled 2 and 3 in the range of 15 and 20 nm is due to the existence of two maxima corresponded to second and third coordination spheres. The magnitude of the forth peak in the range of 25–30 nm corresponds to forth coordination sphere which has larger distance from the central atom and thus has the larger number of localized electrons.

As shown in Fig. 3(b), most of the charged traps distributed in a hexagonal pattern. That is, in a planar dielectric with random neutral traps distribution, the charge trapping can lead to the formation of a two-dimensional imperfect crystal or, more exactly, a glass with hexagonal lattice. This quasiordered lattice is due to the Coulomb repulsion effect of tapped charges or Wigner crystallization. The criterion for short-range ordering of the crystal can be defined as when the half-width at half-maximum, Δr_1, of the first coordination peak is less than the separation between the first and second coordination spheres, r_2-r_1, i.e.,

$$\Delta r_1 < r_2 - r_1. \tag{4}$$

In summary, we have showed with theoretical calculation that the high amount of electronic trapping in a dielectric can lead to the formation of a hexagonal quasiordered lattice or Wigner glass as a result of Coulomb repulsion of trapped charges. This effect takes place in dielectric with a certain value of electron/trap ratio (n_s/N_s). An ordered hexagonal structure is formed when $n_s/N_s \leq 0.001$. Similar results were obtained for two-dimensional electron gas.[1] This present theoretical results also support the proposal for explaining the Coulomb blockade regularities in silicon nitride that a crystal lattice is form due to the localized charge carriers but the structure of Wigner lattice should be a hexagonal rather than a square lattice according to the present simulation.

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