Effect of FET geometry on charge ordering of transition metal oxides

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We examine the effect of an FET geometry on the charge ordering phase diagram of transition metal oxides using numerical simulations of a semiclassical model including long-range Coulomb fields, resulting in nanoscale pattern formation. We find that the phase diagram is unchanged for insulating layers thicker than approximately twice the magnetic correlation length. For very thin insulating layers, the onset of a charge clump phase is shifted to lower values of the strength of the magnetic dipolar interaction, and intermediate diagonal stripe and geometric phases can be suppressed. Our results indicate that, for sufficiently thick insulating layers, charge injection in an FET geometry can be used to experimentally probe the intrinsic charge ordering phases in these materials.

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Charge ordering in doped transition metal oxides has attracted considerable recent interest, both in theory and experiment. Due to the competing long-range, e.g., Coulomb, repulsion and short range antiferromagnetic interactions in the charge system, a rich variety of phases can occur, including stripes, clumps, and liquid crystalline electron states. Simulation studies of the charge ordering phase diagram showed transitions among four phases depending on the hole density and the strength of a dipolar interaction induced by the holes: a Wigner crystal at low hole densities, a diagonal stripe phase, an intermediate geometric phase, and a clump phase at larger dipole interaction strengths. The behavior of these phases is of interest not only for the charge ordered system, but also for similarities to other pattern forming systems with coexisting short- and long-range interactions, including magnetic films. A natural extension of this model is to consider charges interacting with a distortable charged membrane, which could be relevant to active membrane systems such as ion pumps.

To experimentally probe the charge ordering phase diagram, the hole doping of the material must be controlled. A recently proposed method of controllably varying the hole density is the use of a field effect transistor (FET) geometry to inject holes into the metal oxide plane. The geometry is illustrated in Fig. 1. An insulating layer is deposited on top of the metal oxide, and then a metallic gate is deposited on top of the insulator, forming a capacitive structure. By varying the gate voltage, holes move into or out of the metal oxide layer, allowing the sample to be conveniently tuned to the desired doping level. Source and drain contacts, not shown in the figure, can be used to probe the conductance properties of the structure. A potential drawback of this geometry for mapping the phase diagram is that the holes can interact with the gate layer, in addition to the intrinsic hole-hole interactions within the metal oxide which lead to the charge ordered phases. As a result, the phases could be distorted or disrupted by the presence of the FET geometry.

To assess the effect of an FET geometry on the charge ordering phases, we simulate a model of a single metal oxide layer interacting with a metallic gate layer that is offset by varying thicknesses of insulating material. We find that for a sufficiently thick insulating layer, the charge ordering is unaffected by the presence of the gate. When the insulating layer thickness approaches twice the magnetic correlation length in the metal oxide, however, we find a dramatic downward shift in the onset of the clump phase as a function of dipole interaction strength. The diagonal stripe and geometric phase boundaries do not shift, but these phases may be suppressed by the intrusion of the clump phase as the insulating layer is made thinner. Our results show that, for sufficiently thick insulating layers, the FET geometry provides a reliable probe of the charge ordering phase behavior.

We consider a sample constructed in an FET geometry, illustrated in Fig. 2. The metal oxide plane is parallel to the insulating layer and also to the metallic gate layer deposited on top of the insulator. Experimentally, a gate voltage is used to tune the doping level present in the metal oxide layer. We simulate this effect by directly varying the hole density in our system, which is a rectangular computational box of size $L_x \times L_y$, with $L_x$, $L_y$ up to 100 unit cells in a CuO$_2$ plane. At the beginning of each simulation, we place the holes at random and assign to each hole a magnetic dipole moment of constant size, but random direction. We find the minimum of the total potential in this system using our efficient Monte Carlo method, described in [8].

Our model for the interactions between the charges is based on the spin density wave picture of the transition metal oxides. Full details of the model can be found in [8]. The system is doped with holes with planar...
density $\sigma_s$ in the lower Mott-Hubbard band. The interaction between the holes consists of both a short-range attractive interaction, and a long-range dipolar interaction. These interactions arise from the AF bond breaking and the (dipolar in range) spiral distortions of the AF background. The system is magnetically disordered at finite temperature, and is characterized by the AF background. The system is magnetically breaking and the (dipolar in range) spiral distortions of the form $\phi \propto r^{-1}$, where $r$ is the interparticle distance, $a$ is the distance between the holes to be unscreened, as appropriate at low doping where $r_s = r_0/a_0$ is very large: $r_0$ is the mean interparticle distance, $a_0$ is the Bohr radius, and $r_s \approx 8$. In our model, the effective interaction between two holes a distance $r$ apart in a single metal oxide plane is then of the form

$$V(r) = \frac{q^2}{r} - B \cos(2\theta - \phi_1 - \phi_2)e^{-r/\xi},$$

where $q$ is the hole charge, $\theta$ is the angle between $r$ and a fixed axis, and $\phi_1, \phi_2$ are the angles of the magnetic dipoles relative to the same fixed axis, which we assume can take an arbitrary value. $B$ is the strength of the magnetic dipolar interaction [$B \approx U/(2\pi\xi^2)$], which, in real materials, should be of order $\sim 1\text{eV}$. We have introduced $B \sim B_{xy}/l^2$, where $l$ is some appropriate average length, $a < l < \xi$, in order to avoid the unphysical divergence of the dipolar part of the interaction, while keeping the necessary symmetry of the interaction. We have assumed that $r$ can be relaxed from a crystal lattice position to an arbitrary (continuous) value. The results presented here are for a system with 196 holes with size ranging from $307.15\AA \times 307.15\AA$ (for $n = 3\%$) to $137.4\AA \times 137.4\AA$ (for $n = 15\%$). The value of $\xi$ ranges from $21.9\AA$ for $n = 3\%$ to $9.8\AA$ for $n = 15\%$. The sample is periodic in the x-y plane only.

In the FET geometry, a metal oxide channel is created, then an insulating layer of thickness $d$ is deposited on top of the channel, and finally a layer of metal is deposited to serve as a gate. The interactions between holes in the metal oxide layer is altered by the presence of image charges in the gate layer,

$$\nabla \cdot \mathbf{D} = 4\pi \rho = 4\pi e \sum_i [\delta(r - (r_{ij} + d\hat{z})) - \delta(r - (r_{ij} - d\hat{z}))],$$

(2)

giving the Coulomb energy between charges as

$$E = \frac{e^2}{2\varepsilon} \sum_{ij} \left[ \frac{1}{|r_{ij} - r_{ij}|} - \frac{1}{|r_{ij} - r_{ij} + 2d\hat{z}|} \right].$$

(3)

We modify the Coulomb interaction between the holes in our system to this form. This introduces a new length scale $2d$. As a comparison, we also run simulations with the unmodified Coulomb interaction, representing a bare metal oxide plane without the FET gating.

In the absence of the FET interaction, we find a phase diagram consistent with that observed in Ref. [3], as illustrated in Fig. 2(a). For thick insulating layers, when the FET interaction is included, the locations of the phases are not affected and we obtain the same phase diagram, as shown in Fig. 2(a). As we decrease the thickness of the insulating layer, we find a critical thickness $d_c$ below which the phase boundaries begin to shift. Fig. 2(b) illustrates the phase diagram for the same system in Fig. 2(a) but with the FET term added and with an insulating layer of thickness $d < d_c$, $d = 14\AA$. The onset of the diagonal stripe phase “S” is unaffected, but there is a large shift downward in $B$ of the onset of the clump phase “C,” $B_C$. The size of the downward shift $\Delta B$ increases as the

FIG. 1. Schematic of the FET geometry considered here.

FIG. 2. (a) Phase diagram as a function of the hole density $n$ and the strength of the magnetic dipolar interaction $B$, for a sample without the FET interaction term. “W” is the Wigner crystal phase, “S” is the diagonal stripe phase, “G” is the geometric phase, and “C” is the clump phase. (b) Phase diagram for a sample with the same parameters but with the FET interaction added at an insulator thickness of 14Å, showing the downward shift in $B$ of the clump phase “C” and the suppression of the geometric phase “G”.

"C" and the suppression of the geometric phase “G".
hole density $n$ decreases. The geometric phase that was present without the FET term is now suppressed completely.

The interplay of the correlation length and the insulator thickness affects the onset of the clump phase because only the clump phase possesses a characteristic length scale of order $2\xi$. This is illustrated in Fig. 3, which shows the clump structure at $n = 3\%$ and $n = 13\%$. When the length scale of the insulating layer is similar to the length scale of the clump structure, the interaction with the metal gate above the insulating layer becomes comparable with the interaction with neighboring clumps, and the transition to the clump phase is enhanced.

The effectiveness of the FET term extends only to insulator thicknesses $d$ that are approximately twice the magnetic correlation length, $d \lesssim 2\xi$. This is illustrated in Fig. 4 for a sample with $n = 3\%$ and varying insulator thicknesses $d$. The arrow indicates the saturation of the clump phase onset $B_C$ at $d_c$ to the value of $B = B_C^0$ observed in the absence of the FET term. The other phase boundaries, Wigner to stripe and stripe to geometric, do not shift with $d$ but instead the intermediate phases are suppressed when $B_C$ moves below the onsets of these phases. To test whether the magnetic correlation length is responsible for the shift in the phases, we considered a system at $n = 13\%$, which normally has a correlation length of $\xi = 10.54 \text{Å}$, and artificially changed the screening length to $\xi = 20 \text{Å}$ for one series of runs, and to $\xi = 5 \text{Å}$ for a second series. In the inset of Fig. 4, we show the cutoff insulator thickness $d_c$ beyond which the FET term has no effect as a function of correlation length $\xi$, both for the normal screening lengths and for our two artificially changed screening lengths. We find a linear dependence for the cutoff thickness on the correlation length, $d_c \approx 1.7\xi$.

In conclusion, we find that the FET geometry does not affect the clump ordering phases unless the insulating layer is thin enough, namely less than approximately twice the magnetic correlation length. For thin insulating layers the onset of the clump phase is enhanced. This suggests that the FET geometry with a sufficiently thick insulating layer is suitable for studying the effects of hole concentration on the charge ordering phases because the presence of the FET does not alter the phase structure. Alternatively, FET geometries deliberately created with thin insulating layers can be used to probe the clump phase at higher hole densities, where the underlying value of $B$ may preclude reaching the clump state.

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