

## Electric field effects in a two-dimensional Disordered Hubbard-Mott model

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We have studied the effects of disorder, correlation, external electric field, impurity concentration, and impurity location near and at the Si-SiO<sub>2</sub> interface of a metal-oxide-semiconductor field-effect transistor, in the range of experimental interest. We show that the intrainpurity correlation energy and the binding energy have strong dependence with the applied electric field and the impurity location on the interface. Taking into account all the above effects the Hubbard-Mott scenario is presented. As a result we obtain a critical concentration of about 10<sup>11</sup> cm<sup>-2</sup>, which can be discussed in terms of recent experimental findings.

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In contrast to three dimensions, where the occurrence of a metal-nonmetal (MNM) transition is well understood experimental works carried out before 1994 for two dimensions just confirmed the scaling theory of noninteracting electrons.<sup>1,2</sup> According to this theory<sup>2</sup> all two-dimensional (2D) electronic states are localized in the absence of a magnetic field and no metallic phase exists, therefore MNM transition is impossible. Recent experiments on metal-oxide-semiconductor field-effect transistors (MOSFET) structure have provided evidence of a true MNM transition in two dimensions, indicating that electron correlations play an important role in this transition.<sup>3-8</sup> Similar effects have been found in other 2D systems.<sup>9-11</sup> Since then, many other works on MOSFET structure have appeared in the literature.<sup>8,12-15</sup>

The occurrence of impurity band in *n*-type MOSFET structure is well known.<sup>1,6</sup> Such structures are suitable to investigate the 2D MNM transition. In this work, we consider a more detailed investigation using a Hubbard-type Hamiltonian<sup>16,17</sup> to represent the impurity electrons, where the effects of the external electric field, the binding energy variation, the screening, the impurity location near and at semiconductor interface, the disorder,<sup>1,18-20</sup> the correlation, and the impurity concentrations in the range of experimental interest are considered. An attempt to investigate the impurity density of states associated to such structures has already been made for a strictly 2D system<sup>17</sup> and later extended to include the external electric field.<sup>21</sup>

Here we treat the problem in a more realistic way, i.e., taking into account all the above effects on the impurity, which will be present in the ratio between the correlation energy and the bandwidth  $\Delta W$ , leading to the Hubbard-Mott transition.

We consider the problem of impurity band of a disordered 2D system, where the electron-electron correlation is taken into account, by assuming a Hubbard-like Hamiltonian<sup>16,17</sup>

$$H = E_B \sum_{i\sigma} a_{i\sigma}^\dagger a_{i\sigma} + \sum_{i \neq j, \sigma} V_{ij} a_{i\sigma}^\dagger a_{j\sigma} + \frac{U}{2} \sum_{i\sigma} n_{i\sigma} n_{i-\sigma}, \quad (1)$$

where  $E_B$  is the binding energy,  $a_{i\sigma}^\dagger$  and  $a_{j\sigma}$  are the creation and annihilation operators of an electron of spin  $\sigma$  at site  $i$ ,  $n_{i\sigma} = a_{i\sigma}^\dagger a_{i-\sigma}$  is the number operator corresponding to site  $i$

and spin  $\sigma$ ,  $V_{ij}$  is the transfer of an electron from the  $i$ th site to the  $j$ th site, i.e., hopping matrix

$$V_{ij} = \int dz \int d^2r \psi_i(\mathbf{r}, z) V_i(\mathbf{r}, z) \psi_j(\mathbf{r}, z), \quad (2)$$

where  $\psi_i(\mathbf{r}, z) \equiv \psi(\mathbf{r} - \mathbf{R}_i, z)$  is the bound-state wave function of an electron centered at an impurity  $\mathbf{R}_i$  located in the  $z$  Si-SiO<sub>2</sub> region and  $V_i$  is the interaction potential between the electron and an impurity located at site  $\mathbf{R}_i$ . The term  $U$  is the intrainpurity Coulomb interaction (or correlation) energy or Hubbard  $U$ , and is written as

$$U = \int \int d^2r_1 d^2r_2 |\psi_i(\mathbf{r}_1)|^2 V(|\mathbf{r}_1 - \mathbf{r}_2|) |\psi_i(\mathbf{r}_2)|^2, \quad (3)$$

where  $\mathbf{r}_1$  and  $\mathbf{r}_2$  are the coordinators of the electron at the site  $i$  and  $V(|\mathbf{r}_1 - \mathbf{r}_2|)$  is the correlation potential.

The single-particle Green's function, with the sum of  $G^+$  and  $G^-$ , is defined as<sup>16</sup>

$$G_{ij,\sigma}^\pm(t) = i \theta(t) \langle [a_{i\sigma} n_{i-\sigma}^\pm, a_{j\sigma}^\dagger(t)]_+ \rangle, \quad (4)$$

where  $\langle \rangle$  means the configuration average,  $n_{i\sigma}^+ = a_{i\sigma}^\dagger a_{i\sigma}$  and  $n_{i\sigma}^- = 1 - n_{i\sigma}^+$ .

The equation of motion for  $G^+$  and  $G^-$  is written as

$$(w - E^\pm) G_{ij,\sigma}^\pm(w) = n_{i-\sigma}^\pm \delta_{ij} + \sum_{i \neq l} V_{il} G_{il,\sigma}^\pm(w), \quad (5)$$

where  $E^+ = E_B + U$  and  $E^- = E_B$ . The validity of Eq. (5) is discussed very well in Ref. 16. It is exact in both atomic and band limits, and differs for small  $U/\Delta W$  from the Hartree-Fock theory only by an exponentially small quantity. Also it has a sharp Fermi surface in the metallic region  $U/\Delta W < 1$ . For  $U/\Delta W > 1$ , it gives two separated Hubbard bands.

The average Green function results in

$$\langle G_{ii,\sigma}^\pm(w) \rangle = \frac{n_{i\sigma}^\pm}{w - E^\pm} \xi^\pm(w - E^\pm). \quad (6)$$

The coupled equations derived from this scheme are written as<sup>16,17</sup>

$$\xi^\pm(w) = [1 - \eta^\pm(w)]^{-1}, \quad (7)$$

$$\eta^\pm(w) = \frac{N\xi^\pm(w)}{(2\pi)^2(w-E^\pm)^2} \int \frac{d^2kV^2(\mathbf{k})}{\left\{1 - \left[\frac{N\xi^\pm(w)}{(w-E^\pm)}\right]V(\mathbf{k})\right\}}, \quad (8)$$

where  $N$  is the number of impurity per  $\text{cm}^{-2}$  and  $V(\mathbf{k})$  is the Fourier transform of hopping matrix  $V_{ij}$ , Eq. (2).

Defining

$$\frac{\xi^\pm(w)}{(w-E^\pm)} = \{Na_0^{*2}[u(w) + is(w)]\}^{-1}, \quad (9)$$

where  $a_0^*$  is the effective Bohr radius, we have for the density of states for lower and upper Hubbard bands,  $D^+$  and  $D^-$ , respectively,

$$D^\pm(w) = -\frac{1}{\pi} \text{Im} \left[ \frac{\xi^\pm(w)}{(w-E^\pm)} \right]. \quad (10)$$

Using Eqs. (8)–(10) we get the self-consistent equations

$$w = Na_0^{*2}u(w) + \frac{2}{\pi} \int_0^\infty \frac{v^2(q)[u(w) - v(q)]}{[u(w) - v(q)]^2 + s^2(w)} qdq \quad (11)$$

and

$$Na_0^{*2} = \frac{2}{\pi} \int_0^\infty \frac{v^2(q)}{[u(w) - v(q)]^2 + s^2(w)} dq, \quad (12)$$

where  $\mathbf{q} = \mathbf{k}a_0^*$  and  $v(\mathbf{q}) = a_0^{*2}V(\mathbf{q}/a_0^*)$ . The  $u(w)$  and  $s(w)$  are obtained self-consistently from Eqs. (11) and (12).

For 2D lattice,  $\text{Im}[G_{ii}(w)]$  shows discontinuities at  $w = E_l$  and  $w = E_u$ , where  $E_l$  and  $E_u$  are the lower and upper band edges, respectively, given an impurity bandwidth  $\Delta W$ . The  $\text{Re}[G_{ii}(w)]$  diverge at  $E_l$  and  $E_u$ .

The binding energy of the Si-SiO<sub>2</sub> system is obtained from the relation<sup>18,19</sup>

$$E_B = E_0 - E_{\text{imp}}, \quad (13)$$

where

$$E_{\text{imp}} = \left\langle \psi \left| -\nabla_{x,y}^2 - \nu \nabla_z^2 + \frac{\delta}{z} + \zeta \varepsilon z - 2\Phi(\mathbf{r}) \right| \psi \right\rangle \quad (14)$$

and  $E_0$  is the expectation value of the above equation without the impurity term.<sup>18,19</sup> In the Eq. (14),  $\varepsilon$  is the electric field,  $\Phi(\mathbf{r})$  is the screening Coulomb potential,  $\nu$  is the ratio between the transverse and longitudinal masses, and  $\delta$  and  $\zeta$  are related to the dielectric constants of the semiconductor and oxide,  $k_{\text{sc}}$  and  $k_{\text{ox}}$ , respectively. The wave function centered at impurity is given by<sup>18,22</sup>

$$\psi(\mathbf{r}, z) = \phi(\mathbf{r}) \varphi(z) = \left(\frac{a}{2\pi}\right)^{1/2} e^{(-ar/2)} \left(\frac{b^3}{2}\right)^{1/2} z e^{(-bz/2)}, \quad (15)$$

where  $a$  and  $b$  are variational parameters.

The expectation value of  $\Phi(\mathbf{r})$  is given by the expression derived from the momentum transform<sup>23</sup>

$$\langle \Phi \rangle = \int f_1(\mathbf{q}) f_2(\mathbf{q}) d\mathbf{q}, \quad (16)$$

where

$$f_1(\mathbf{q}) = \frac{a^3 q}{(a^2 + q^2)^{3/2}} \quad (17)$$

and

$$f_2(\mathbf{q}) = \frac{b^3}{(b+q)^3} \frac{1}{f_3(\mathbf{q})} e^{-qz_0} \quad (18)$$

with

$$f_3(\mathbf{q}) = q + s \frac{k_{\text{sc}}}{k} F(\mathbf{q}). \quad (19)$$

Here,  $F(\mathbf{q})$  is the screening form factor, given by<sup>1,12</sup>

$$F(\mathbf{q}) = \frac{1}{16} \left(1 + \frac{k_{\text{ox}}}{k_{\text{sc}}}\right) \left(1 + \frac{q}{b}\right)^{-3} \left(8 + \frac{9q}{b} + \frac{3q^2}{b^2}\right) + \frac{1}{2} \left(1 - \frac{k_{\text{ox}}}{k_{\text{sc}}}\right) \left(1 + \frac{q}{b}\right)^{-6}. \quad (20)$$

In the above equations,  $\bar{k}$  is  $[(k_{\text{ox}} + k_{\text{sc}})/2]$ ,  $s$  is the screening parameter,<sup>18</sup> and  $z_0$  is the location of the impurity center within the silicon-dioxide region from the silicon interface.

The parameters left to solve the problem are,  $V(\mathbf{q})$ , which is the Fourier transform of  $V_{ij}$ , and the Hubbard  $U$ .

For  $V(\mathbf{q})$  we obtain

$$V(\mathbf{q}) = -(E_B + q^2) \phi^2(\mathbf{q}) [a_0^{*2} R y^*], \quad (21)$$

where  $\phi(\mathbf{q})$  is the Fourier transform of  $\phi(\mathbf{r})$  in Eq. (15).

The binding energies are evaluated by minimizing Eq. (13) as a function of electric field  $\varepsilon$ , screening  $s$ , and the distance of the impurity from the Si-SiO<sub>2</sub> interface  $z_0$ . In Fig. 1 we show these results. For very high electric field and,  $s = 0.00$  and  $z_0 = 0.00$ ,  $E_B$  goes to the 2D limit of  $4Ry^*$ .<sup>17</sup>

However,  $E_B$  is strongly reduced for  $z_0 = 0.14$ , corresponding to distance of about 4 Å from the interface.  $E_B$  is less dependent on screening as compared to  $z_0$ .

The correlation energy  $U$  is calculated analytically from Eq. (3), with the electron-electron interaction potential  $V(|\mathbf{r}_1 - \mathbf{r}_2|)$  given by Eq. (2.50) of Ref. 1; as a function of the same parameters as for  $E_B$ . The final equation can be derived from the momentum transform.<sup>23</sup> It is written as

$$U = \frac{e^2}{k} \int |f_1(\mathbf{q})|^2 F(\mathbf{q}) d\mathbf{q}. \quad (22)$$

In Fig. 2 we show the correlation energy  $U$ , as a function of the applied field, the screening, and the distance at interface  $z_0$ .  $U$  is strongly dependent on  $z_0$  and it goes to the 2D limit of  $4.71Ry^*$ , for very high electric field, for  $s = 0.00$  and  $z_0 = 0.00$  as well.<sup>17</sup> This limit was not observed in Ref. 21.

Throughout this work the following units have been employed,  $Ry^* = 43.6$  meV,  $a_0^* = 21.7$  Å,  $k_{\text{sc}} = 11.5$ , and  $k_{\text{ox}} = 3.9$ .

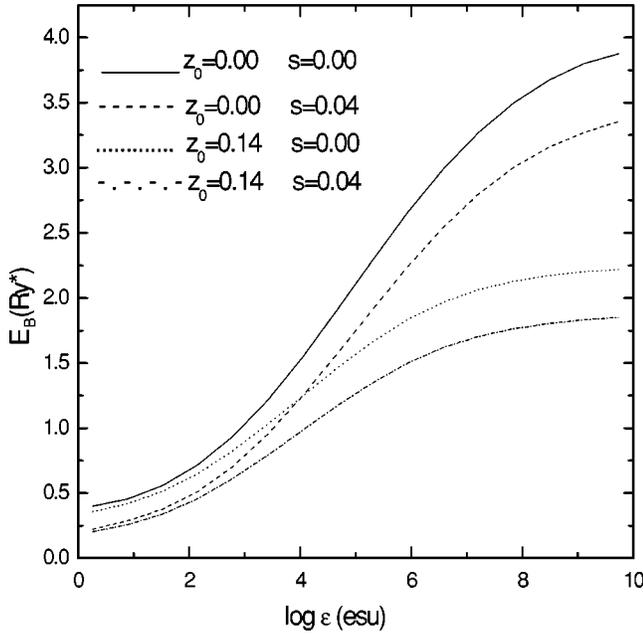


FIG. 1. Binding energies as a function of the applied electric field for different screenings  $s$  and impurity location  $z_0$ .

The impurity density of states for depletion concentration  $N_{\text{dep}} = 0.2 \times 10^{11} \text{ cm}^{-2}$  is shown in Fig. 3, for a concentration just about the bands merging. With increasing impurity concentration the so-called two impurity Hubbard bands will broaden and eventually merge at a ratio of  $\Delta W/U \approx 1$  when the MNM transition occurs, leading to the Hubbard-Mott scenario.<sup>24,25</sup> In our scheme the bands are roughly symmetric, which correspond to a good estimation for this transition.<sup>24,26</sup> The crossing of the bands occurs at  $N_c$

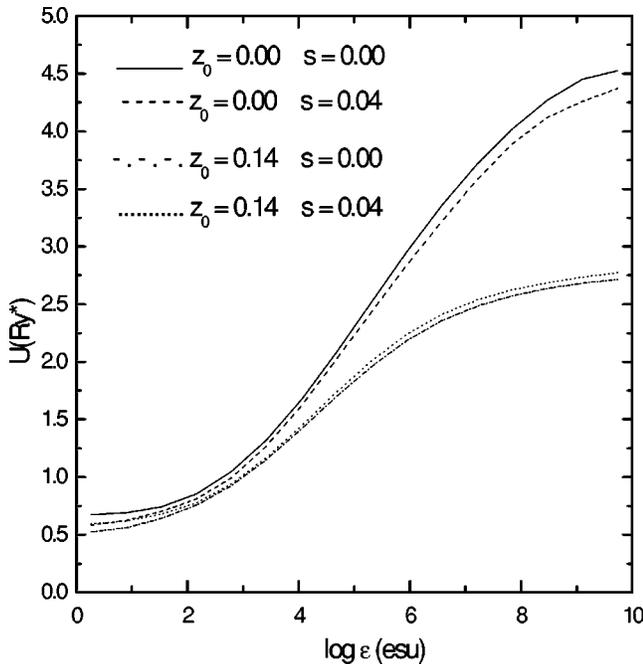


FIG. 2. Correlation energy  $U$  as a function of the applied electric field for different  $s$  and  $z_0$ .

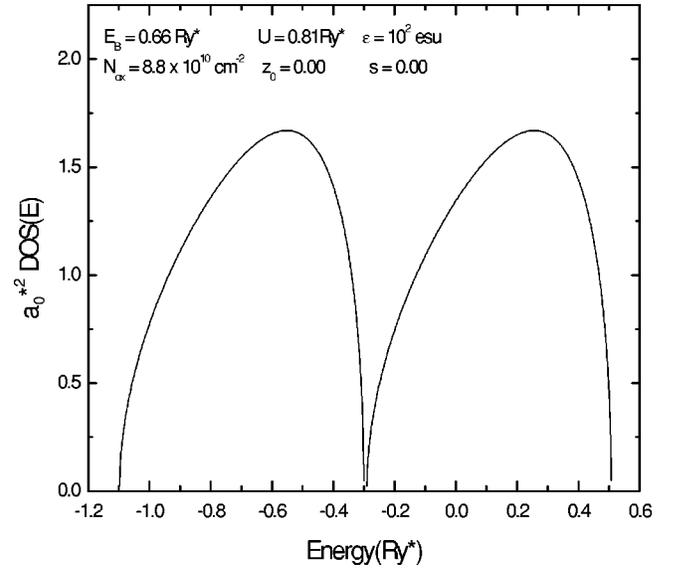


FIG. 3. Density of impurity states for  $N_{\text{ox}} = 8.8 \times 10^{10} \text{ cm}^{-2}$ .

$= 0.95 \times 10^{11} \text{ cm}^{-2}$ , which corresponds to the experimental finding.<sup>4,8</sup> At this value the density of states at the Fermi energy  $D(E_F)$  starts to have a finite value. As the concentration increases  $E_F$  shifts to higher energies and the second band starts to play the role in the thermal and transport properties. We found that  $\Delta W \approx U = D_{\text{max}}^{\text{pd}}(E) = 0.81 \text{ Ry}^*$ , where  $D_{\text{max}}^{\text{pd}}(E)$  is the distance between the peaks of the impurity bands. For concentrations higher than  $1.0 \times 10^{12} \text{ cm}^{-2}$  the lower impurity band is observed to be merged with the inversion layer unperturbed subband.

Table I shows some calculated values just around the merging value of the two bands in comparison to the experimental findings. For concentrations higher than  $2.0 \times 10^{12} \text{ cm}^{-2}$  a strong mixing of the bands occurs, which makes it difficult to compare with the observed values. A rough agreement is found between the theory and experiment.

Besides the conduction activation energy  $E_1$  and the nearest-neighbor hopping activation energy  $E_3$ , presented in previous MOSFET experiment,<sup>1</sup> we may expect another activation energy.<sup>27</sup> In the intermediate-concentration region of impurity conduction, i.e., the transition region from insulating to metallic behavior, where the electron correlation plays

TABLE I. Values of the activation energy  $E_1$ , half-width at half maximum of the impurity band  $\Gamma$  and the maximum of the lower impurity band  $D_{\text{max}}(E)$  as a function of  $N_{\text{ox}}$ . The values are obtained for a depletion charge about  $3.6 \times 10^{11} \text{ cm}^{-2}$  corresponding to  $\epsilon = 10^2 \text{ esu}$  and  $z_0$  about  $4 \text{ \AA}$ . Two upper rows are the calculated values.

$N_{\text{ox}} (10^{11} \text{ cm}^{-2})$	$E_1 (\text{meV})$	$\Gamma (\text{meV})$	$D_{\text{max}}(E) (10^{13} \text{ cm}^{-2} \text{ eV}^{-1})$
1.0	22 <sup>a</sup>	3.5	3.2
2.0	22	4.6	2.4
2.1 <sup>a</sup>	22	4.8 <sup>a</sup>	2.1 <sup>a</sup>

<sup>a</sup>Experimental, Ref. 1.

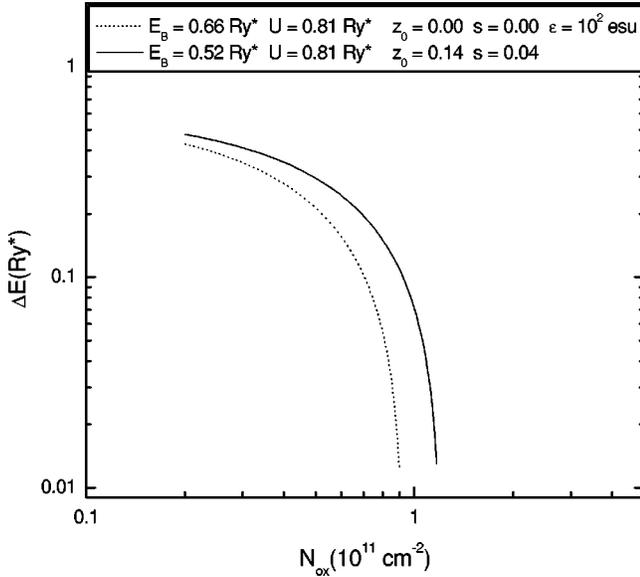


FIG. 4. Energy gap between the two Hubbard bands for  $\varepsilon = 10^2$  esu.

an essential role, a characteristic activation energy  $E_2$ , dependent on the temperature and concentration of the electrical conductivity,<sup>27,28</sup> has been observed for 3D systems. It is worth mentioning that a similar way to evaluate the critical concentration through this electrical conductivity dependence, for the MNM transition in 2D (Refs. 6 and 8) was also done in 3D systems.<sup>27–29</sup>

For comparison, calculations for different computational methods in 3D systems, namely, generalized Drude approach, Hubbard-Mott model, and total energy of the metallic and nonmetallic phase have recently been performed,<sup>27–31</sup> which show good agreement between measurements and calculations.

In an earlier work by Kikuchi,<sup>32</sup> the energy gap  $\Delta E$  between the two Hubbard bands as a function of impurity concentration from low to high region has a remarkable similarity to the behavior of  $E_2$  for the Ge:Sb system. Such similarity was later confirmed for various materials.<sup>32,33</sup> Energy  $E_2$  sharply decreases and vanishes at a critical concentration  $N_c$  where the MNM transition takes place. In Fig. 4 we show the behavior of  $\Delta E$  for the MOSFET structure. Using a fit to the critical expression<sup>34</sup>

$$\Delta = \Delta_0(N_c - N_{ox})^\lambda \quad (23)$$

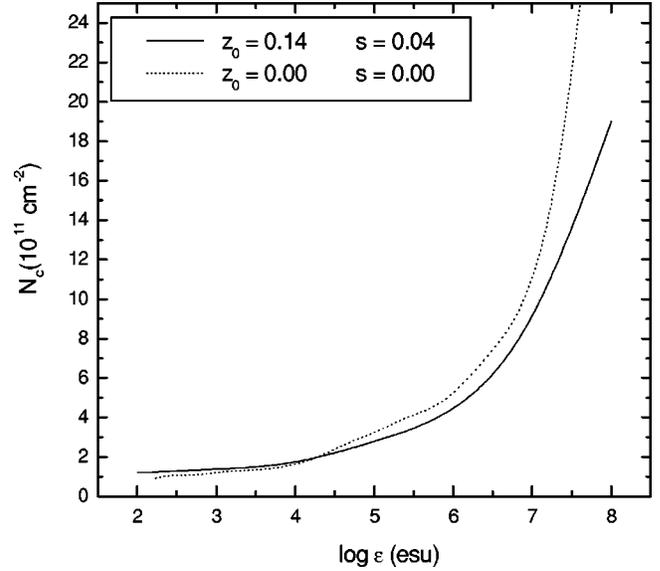


FIG. 5. The Hubbard-Mott critical concentration  $N_c$  as a function of the applied electric field.

yields  $\Delta_0 = 0.55$ ,  $\lambda = 0.50$ , and  $N_c = 0.89 \times 10^{11} \text{ cm}^{-2}$  for  $s = 0.00$ ,  $z_0 = 0.00$ , and  $\varepsilon = 10^2$  esu, as well as  $\Delta_0 = 0.48$ ,  $\lambda = 0.50$ , and  $N_c = 1.16 \times 10^{11} \text{ cm}^{-2}$  for  $s = 0.04$ ,  $z_0 = 0.14$ , and  $\varepsilon = 10^2$  esu. Also  $\Delta_0 = 1.04$ ,  $\lambda = 0.50$ , and  $N_c = 1.3 \times 10^{11} \text{ cm}^{-2}$ , for  $s = 0.04$ ,  $z_0 = 0.14$ , and  $\varepsilon = 10^6$  esu. For this later electric field and  $s = 0.00$  and  $z_0 = 0.00$ ,  $N_c = 2.0 \times 10^{11} \text{ cm}^{-2}$ .

In Fig. 5 we show that with a field up to  $\varepsilon = 10^4$  esu, the critical concentration for the transition is not much sensitive, and remains until  $N_c \approx 1.0 \times 10^{11} \text{ cm}^{-2}$ , for both  $s = 0.00$  and  $z_0 = 0.00$  and  $s = 0.04$  and  $z_0 = 0.14$ .

To summarize, the transition reported here resembles a Hubbard-Mott transition in two dimensions in the presence of both disorder and interacting electrons, as well as, electric field, screening, and impurity location. It is worth mentioning that, despite of no transport property evaluated here, the reliability of the Hubbard-Mott model is very well discussed in Refs. 24–26, 30–33, in terms of two different Hubbard bands touching each other, leading to the MNM transition. The Hubbard-Mott transition is not very much sensitive to an electric field up to  $\varepsilon = 10^4$  esu. The results provide a transition in two dimensions observed in recent experimental findings.

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