Gate-Induced Mott Transition

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(May 27, 2003)

For a strongly correlated material, VO$_2$, near a critical on-site Coulomb energy $U/U_c=1$, the abrupt Mott metal-insulator transition (MIT) rather than the continuous Hubbard MIT is observed by inducing internal optical phonon-coupled holes (hole inducing of 0.018%) into conduction band, with a gate field of fabricated transistors. Observed gate effects, change of the MIT drain-source voltage caused by a gate field, are the effect of measurement due to inhomogeneity of channel material and is an average over the measurement region of the true gate effect based on the large conductivity (or effective mass) near the MIT predicted by the Brinkman-Rice picture. A discontinuous gate effect such as digital is observed, which is a characteristic of the transistor and a possible condition of a very high-speed switching transistor.

PACS numbers: 71.27. +a, 71.30.+h

In a strongly correlated system, a metal-insulator transition (MIT) near a critical on-site Coulomb energy, $U/U_c=1$, has long been controversial in terms of whether the transition is Mott’s abrupt (or first-order) MIT or Hubbard’s continuous (or second-order) MIT [1–4]. This is because it is unclear whether experimental observations of the abrupt MIT (Mott transition) follow Mott’s prediction, although a first-order MIT with temperature was observed by McWhan et al. [5]. Rather than the abrupt MIT, Boriskov et al. [6] and Kumai et al. [7] measured the nonconduction-conduction transition (NCT) with an electric field for VO$_2$ and an organic material, respectively. Oka et al. [8] found the NCT with an electric field could be described in terms of a universal Landau-Zener quantum tunnelling through a theoretical consideration based on the Hubbard model. Newn et al. [9] regarded the NCT in a Mott-Hubbard insulator as the Hubbard MIT for a transistor based on the NCT. However, the Mott MIT, which differs from the NCT, has not been observed for a very low doping of charges (hole content of 0.018% for VO$_2$), as predicted by Mott [1]. The very low doping is a decisive key determining an order (first or second) of two kinds of the MIT.

An abrupt MIT breaks down an energy gap between sub-bands in a main band. The energy gap is formed by a strong correlated on-site Coulomb energy. The abrupt MIT in a strongly correlated metal with an electronic structure of one electron per atom was theoretically demonstrated by Brinkman and Rice; this is called the Brinkman-Rice (BR) picture [10]. The abrupt MIT with band filling was also developed through extension of the BR picture by Kim [11, 12]. The extended BR picture was based on a fractional charge justified by means of measurement in an inhomogeneous metallic system [12].

In this letter, we observe the abrupt MIT (or Mott transition), inducing internal optical phonon-coupled hole charges (hole content of 0.018%) into conduction band with a gate field of a fabricated field-effect transistor. This reveals a difference between the abrupt MIT and the continuous MIT. Note that artificial hole doping of 0.018% is not possible other than the method applying the gate field.

In the extended BR picture [11, 12], the effective mass, $m^*$, of a carrier is given by

$$\frac{m^*}{m} = \frac{1}{1 - (U/U_c)^2} \approx \frac{1}{1 - \kappa^2 \rho^2},$$

(1)

where $m$ is the bare electron mass, $U/U_c$ is $\kappa \rho^2 \neq 1$, $\kappa$ is the strength of Coulomb energy between carriers when $\rho=1$, and $0 < \rho \leq 1$ is band filling. When $\rho \neq 1$, Eq. (1) is well fitted in a real metallic system and the effect of measurement (or average) for an inhomogeneous system [12]. An electric conductivity, $\sigma \propto (m^*/m)^2$ [1].

The material at $\kappa \rho^2=1$ in Eq. (1) can be assumed as a paramagnetic insulator (or Mott insulator). The metal at a critical $\rho$ value ($\approx \rho'$) of just below $\rho=1$ shows the best metallic characteristics [13]. The MIT from a metal at both $\rho'$ and $\kappa=1 (\kappa \rho^2 \neq 1)$ to the insulator at both $\rho=1$ and $\kappa=1 (\kappa \rho^2=1)$ is abrupt (or a jump); this is an idea for observing the Mott transition near $U/U_c=1$.

Holes corresponding to the difference (critical hole content, $\Delta \rho' = 1 - \rho'$) between $\rho'$ and $\rho=1$ are induced into a conduction band having electrons by a gate electric field; this is regarded as the decrease of the Coulomb energy [12]. Then, the energy gap breaks down and the metallic system becomes inhomogeneous because of the induced holes [12]. The number of the induced holes can be regarded as $n_c \approx 3 \times 10^{18}$ cm$^{-3}$, predicted by Mott from $n_c^{1/3} a_0 \approx 0.25$ [1]. Here, $a_0$ is the Bohr radius and $n_c$ corresponds to about 0.018% of the number of carriers in the half-filled band, when one electron in the cell volume, $59.22 \times 10^{-24}$ cm$^3$, of VO$_2$ is assumed; $\Delta \rho'=0.018%$. Further, a gate electric field of a transistor induces holes in optical phonon-coupled-hole levels [14, 15] in a Mott insulator, a channel material, into conduction band [16]. The process in which optical phonon-coupled holes change to carriers has been revealed [15]. The hole levels are attributed to impurities such as oxygen deficiency, which indicates that VO$_2$ is inhomogeneous, as proved experimentally by Kumai et al. [7].
We fabricate transistors to observe the Mott transition on the basis of the above theory. The schematic diagram of the transistor is shown in Fig. 1. Thin films of the Mott insulator, VO₂, with a sub-energy gap of about 1 eV in the d-main band [17] have been deposited on Al₂O₃ substrates by laser ablation. The thickness of the VO₂ film is about 900 Å. The resistance of the film decreases with increasing temperature and shows an abrupt MIT at a transition temperature, \( T_{tr} = 340 \) K (68°C) (Fig. 2a). This is the same as that measured by Borek et al. [18]. The decrease of the resistance up to 340 K indicates an increase of hole carriers, and two kinds of electron and hole carriers coexist near \( T_{tr} = 340 \) K (Fig. 2b). From 332 to 340 K, the number of carriers is not clear because of mixing of electrons and holes.

We speculate that the number of hole carriers can be \( n_c \approx 3 \times 10^{18} \text{ cm}^{-3} \) at \( T_{tr} = 340 \) K on the general basis that an exponential decrease of the resistance with temperature in semiconductor physics indicates an exponential increase of carriers. In the metal regime above 340 K, carriers are electrons (Fig. 2).

Gate insulators, amorphous Ba₀.₅Sr₀.₅TiO₃ (BSTO), Si₃N₄ and SiO₂ were used. BSTO and Si₃N₄ were deposited on the VO₂ film at a VO₂ surface temperature, 400°C and 150°C, respectively. The thickness and the dielectric constant of the BSTO and Si₃N₄ films were about 1200 Å, 43 and 2000 Å, 7, respectively. Transistors of channel length, \( L_{ch} = 3 \mu \text{m} \), and gate width, \( L_w = 50 \mu \text{m} \), were fabricated by lithography processes. The gate width of a transistor based on Si substrate is \( L_w = 25 \mu \text{m} \). Au/Cr electrodes were prepared for Ohmic contact. Characteristics of the transistors were measured by a precision semiconductor parameter analyzer (HP4156B). To protect transistors from excess current, the maximum current was limited.

Figure 3a shows the drain-source current, \( I_{DS} \), vs the drain-source voltage, \( V_{DS} \), characteristics of transistor 1 with a gate insulator of BSTO. The measured gate current, \( I_{GS} \), between the gate and the source is an order of \( 10^{-13} \) A at gate voltages of \( V_G = 0 \), -2 and -10 V, which indicates that there is sufficient insulation between the gate and the source. Fig. 3b shows a NCT below the MIT-\( V_{DS} \) of point A measured by an applied electric field between the source and the drain at \( V_G = 0 \). This was observed by using a two-terminal structure by Boriscov et al. [6] and Kumai et al. [7] who used an organic Mott-insulator. The two groups suggested that the NCT occurs due to an applied field [6] and an induced current [7], not an increase of sample temperature due to leakage current. The abrupt MIT of curve 1 has been measured more than 1,500 times without breakdown. \( I_{DS} \) follows the Ohmic behavior up to \( V_{DS} \approx 12 \text{V} \), but shows nonlinear electric conduction in the total regime below the MIT-\( V_{DS} \) of point A (Fig. 3b). The nonlinear conduction behavior is regarded as semiconducting behavior due to the increase of hole carriers by Zener’s impact ionization, as observed by the Hall effect (Fig. 2b). It was revealed through a theoretical consideration that the Ohmic behavior is described in terms of a universal Landau-Zener quantum tunnelling [8]. The NCT is an insulator-semiconductor transition. We suggest that the abrupt MIT at point A occurs when the number of hole carriers produced by impact ionization becomes the number of \( n_c \) predicted by Mott. The semiconduction in Fig. 3a is regarded as the doping process in which \( n_c \) (or \( \Delta \rho' \)) of holes are induced by electric field. Moreover, at the jumped point in curve 1, the current density is about \( J = 3 \times 10^5 \text{ A/cm}^2 \), which is current collective motion observed in metal.

Curves 2 and 3 are \( I_{DS} \) vs \( V_{DS} \) characteristics measured at gate voltages, \( V_G = -2 \) and -10 V, respectively. The abrupt MITs also occur at transition points B and C. The sharp transitions indicate that transistor 1 was well fabricated. The abrupt MIT at point B, which is caused by the induced charges of \( \Delta \rho' \), occurs suddenly at \( V_G = -2 \text{V} \), such as digital, as indicated in Eq. (1). This is the most unique characteristic of this transistor. The gate effect, a change of the MIT-\( V_{DS} \) caused by a gate field, is small, which is that the channel material in the measurement region is inhomogeneous (see, [12]). When only homogeneous region is measured, the true gate effect becomes maximum due to the maximum conductivity (or the maximum effective mass) near the MIT as indicated in the BR picture; MIT-\( V_{DS} \propto (J/\sigma) \rightarrow 0 \). The gate effect increases as homogeneity of the VO₂ film increases. Thus, the observed gate effect is an average of the true gate effect over the measurement region. \( n_c \) (or \( \Delta \rho' \)) may be attained by the gate effect and the impact ionization on the ground of the large transition \( V_{DS} \).

Figure 3c shows current-voltage characteristics of transistor 2 with a gate insulator of an amorphous Si₃N₄. The gate-source current is \( I_{GS} \approx 3.6 \times 10^{-12} \text{A} \) through the Si₃N₄ at \( V_G = -2 \text{V} \) and \( V_{DS} = 0 \). An off-current is \( I_{DS} \approx 1.3 \times 10^{-7} \text{A} \) at point D. The abrupt MITs occur at point F of \( V_{DS} = 13 \text{V} \) (or \( E = 4.3 \text{MV/m} \)) at \( V_G = 0 \) and point G of \( V_{DS} = 9 \text{V} \) (or \( E = 3 \text{MV/m} \)) at \( V_G = -2 \text{V} \). The gate effect at point G at \( V_G = -2 \text{V} \) is similar to that of transistor 1; there is no gate effect at -2V < \( V_G < 0 \). The discontinuous gate effect is a possible condition of a very high-speed transistor. Namely, transconducance related to a switching speed can be regarded as maximum.

Figure 3d shows \( I_{DS} \) vs \( V_{DS} \) near the abrupt MIT of transistor 3 with a gate insulator of SiO₂. Its structure is a VO₂/SiO₂/WSI/Si substrate. Its characteristics are given as follows. First, the gate effect at \( V_{DS} = 14 \text{V} \) and \( V_{gate} = -10 \text{V} \) is due to hole inducing of \( \Delta \rho' = 0.018 \% \); this is the abrupt MIT with band filling near \( U/U_c = 1 \) in Eq. (1) and due to the jump of the gate voltage. Second, the MIT-\( V_{DS} \) increases with an increasing negative gate voltage (or field), which is the decrease of the conductivity (or the effective mass in Eq. (1)); this is due to the continuous change of the gate voltage. Moreover,
the increase of the inducing hole content greater than the critical content, $\Delta \rho > \Delta \rho'$, decreases $\rho$ and the electrical conductivity, $\sigma$, because of $\sigma \propto (m^*/m)^2$; $\sigma$ is maximum at $\Delta \rho'$. From current density of $J=\sigma E$, an electric field, $E$, increases with a decreasing $\sigma$ to constant $I_{DS}(\propto J_{DS})$, as shown at transition points in Figs. 3a, 3c and 3d, vice versa; $E_{x}V_{DS}$. We also observed that the MIT-V$_{DS}$ decreases with an increasing positive gate voltage. Third, $I_{DS}$ in the metal regime over $I_{DS}=2mA$ shows Olnick’s law which differs from the behavior in Fig. 3b. At the jumped point, current density is $j=0.9\times10^{5}$ A/cm$^2$, which is current collective motion measured in metal. Thus, Fig. 3d follows the behavior of Eq. (1) when $\kappa=1$.

We suggest conditions of a good transistor fabrication by comparing transistors 1 and 2. The off-current ($I_{DS}$ at a very low $V_{DS}$ and $V_g=0V$) and the MIT-V$_{DS}$ values of transistor 1 are lower and higher, respectively, than those of transistor 2: $V_{DS}=20.8V$ (or $E=7MV/m$) of point A and $V_{DS}=13V$ (or $E=4.3MV/m$) of point F. The smaller $V_{DS}$ results from the higher off-current arising from an oxygen deficiency of VO$_2$ when the gate insulator is deposited. The off-current is caused by the excitation of the optical phonon-coupled holes. When the number of total holes in the hole levels is given by $n_{tot}=n_b+n_{free}$, where $n_b$ is the number of optical phonon-coupled holes and $n_{free}$ is the number of holes freed from the levels, $n_b$ decreases with increased $n_{free}$, because $n_{tot}$ is constant. In oxide materials, $n_{tot}$ is about $5.5\times10^{18}cm^{-3}$ which corresponds to 0.034% to $d$-band charges [14, 15, 19]. The larger off-current is attributed to the increase of $n_{free}$. For the abrupt MIT, $\triangle n\equiv n_{e}-n_{free}=0$ should be satisfied, where $n_e \approx 3\times10^{18}cm^{-3}$, as predicted by Mott. Hence, the decrease of $\triangle n$ contributes to the reduction of the MIT-V$_{DS}$ (Fig. 3e). In Fig. 3c, the smaller MIT-V$_{DS}$ of transistor 2 is due to the smaller $n_{induced}=\triangle n$ induced by the gate electric voltage (field) than that of transistor 1. For a good transistor, off-current can be decreased when the deposition temperature or oxygen content of VO$_2$ film is slightly increased. In addition, when gate length is less than 100nm, $V_{DS}$ is much less than 1V.

Figure 3f shows the magnified part below $V_{DS}=1.5V$ of the curves in Fig. 3a. A current signal such as noise in curve 1 without $V_G$ is measured when the resistance of the VO$_2$ film between the source and the drain is large. When $V_G$ are applied, curves 2 and 3 show a high gain current of about 250 times at $V_{DS}=0.3V$, which is the gate effect observed in a semiconductor transistor. The high gain represents a significant difference between this transistor with the abrupt MIT and the Mott transistor developed with a Mott-Hubbard insulator, Y$_{1-x}$Pr$_x$Ba$_2$Cu$_3$O$_{7-\delta}$, by Hewns’ et al. [9] Although they regard a transition for the Mott transistor as the Hubbard MIT, the transition is the NCT. Their transistor is not the Mott transistor.

In conclusion, the abrupt MOTT MIT near $U/U_e=1$ is first observed by inducing of internal holes of 0.018% with gate fields, while the continuous Hubbard MIT does not exist in Mott and Mott-Hubbard insulators. Generally, the reason that the continuous MIT is observed in strongly correlated systems including high-T$_c$ superconductors is because the continuous behavior in both Eq. (1) and Fig. 3d is observed when a doped content, $\Delta \rho > \Delta \rho'$. The measured gate effects predicted by Eq. (1) due to inhomogeneity of channel material is an average of the true gate effect. Furthermore, the transistor developed here is a true Mott transistor without short channel effects proposed in metal-oxide-semiconductor field-effect transistors and will be very useful for nanodevices.

We thank Dr. Soo-Hyeon Park at KBSI for Hall-effect measurement, Dr. Gyungock Kim for valuable discussions on the Zener transition, and Dr. J. H. Park for fabrication of Si$_3$N$_4$ films by using CVD. HT Kim, the leader of this project, developed the concept, and wrote the paper. BG Chae and DH Youn deposited VO$_2$ and BSTO films, performed the transistor fabrication process, and measured $I-V$ characteristics. KY Kang prepared the laser-ablation and lithography equipment and generated this project with HT Kim. SL Maeng evaluated transistor characteristics, the shielding measurement system, and Si$_3$N$_4$ film fabrication.

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FIG. 1. Schematic diagram of a transistor. A dot line between VO$_2$ and insulator is channel. The gate insulators are an amorphous Ba$_{0.5}$Sr$_{0.5}$TiO$_3$ for transistor 1 and an amorphous Si$_3$N$_4$ for transistor 2.

FIG. 2. a, Temperature dependence of the resistance of a VO$_2$ film. b, The number of carriers measured by Hall effect. A change of carriers from hole to electron is shown at 332 K. The minus sign indicates that carriers are holes.

FIG. 3. a, $I_{DS}$ vs $V_{DS}$ of transistor 1. The abrupt MIT occurs at A, B, and C. At the jumped point in curve 1, the current density is about $J=3\times10^7$ A/cm$^2$, which is current collective motion observed in metal. b, $I_{DS}$ vs $V_{DS}$ below the MIT point A of curve 1. The Ohmic behavior is shown from $V_{DS}=2.5V$ up to 12V. c, $I_{DS}$ vs $V_{DS}$ of transistor 2. d, $I_{DS}$ vs $V_{DS}$ near the abrupt MIT of transistor 3. Above $I_{DS}=2mA$, the Ohmic behavior is exhibited. At the jumped point, current density is $j=0.9\times10^7$ A/cm$^2$. e, Off-current vs MIT-$V_{DS}$. The off-currents are extracted from 5 transistors. f, $I_{DS}$ vs $V_{DS}$, magnified below $V_{DS}=1.5V$ in Fig. 3a. Black diamonds are data measured at $V_{gate}=-2V$.

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