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Switching device based on first-order metal-insulator transition induced by external electric field

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1. Introduction

First-order metal-insulator phase transitions (MIT) in crystalline materials have been known for many years [**1**] and correspond to a transformation between states with a dielectric (semiconductor) and a metallic types of conductivity. These transitions occur under the influence of certain external parameters, such as temperature and pressure, as well as with varying material composition. Materials exhibiting these phenomena include many transition metal oxides of which over 40 are known to possess MIT [**2,3**].

Among the best-known MIT materials are vanadium oxides. Being able to combine with oxygen in 2-, 3-, 4-, and 5-valent states, vanadium forms a series of oxides of which at least 8 exhibit MIT [**4**]. Phase transition in V_2O_3 occurs at a critical temperature $T_c=150K$ and in VO_2 at $T_c=340K$, with the electrical conductivity changing by up to 10 and 5 orders of magnitude, respectively. The MIT in vanadium oxides is also accompanied by a discontinuous variation of other than electrical properties, such as optical, magnetic, etc. Vanadium dioxide, VO_2, is of particular interest for technology because its transition occurs near room temperature and furthermore its T_c is tunable in wide range by doping with impurities such as tungsten.

The nature of MIT in VO_2 and V_2O_3 is not well understood. Possible mechanisms under discussion are of Mott-Hubbard and of Peierls type [**1,5,6**]. A profound difficulty of the theory is the lack of a good explanation for the remarkable fact that the electronic bandgap in the dielectric phase of these materials is much larger than kT_c. This makes the low-temperature phase a good electrical insulator. On the other hand, the electron concentration in the metallic phase of VO_2 and V_2O_3 is typical for a metal ($\cong 10^{21}$ cm^{-3}).

The dramatic difference in the electronic spectrum on the metallic and the dielectric side of the transition opens the possibility for switching applications discussed in this work. Indeed, since an external electric field penetrates very differently into the dielectric and the metallic phase, the field energy in the two

phases is different. As a result, application of an external electric field shifts the critical temperature of the transition [**7-12**].

2. Electric-field induced metal-insulator transition in a thin film

Consider a thin vanadium oxide film sandwiched between two metallic plates insulated from the film by a dielectric layer, Fig. 1.

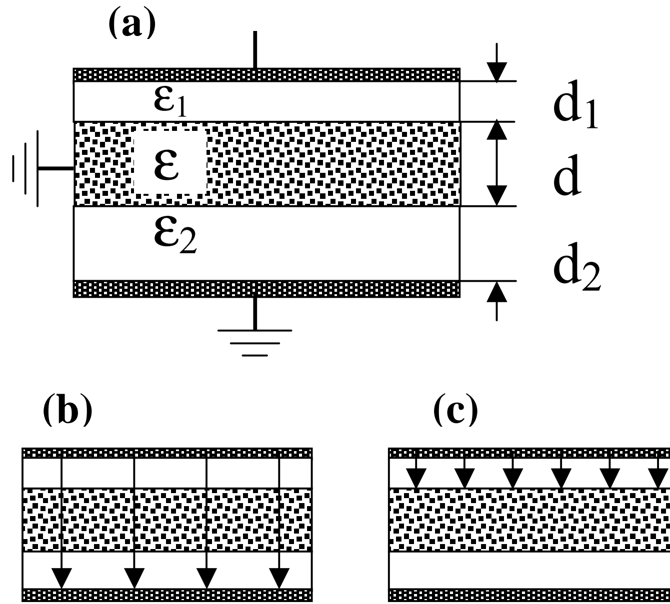

Figure 1. Schematic diagram of an experimental arrangement. Grounded vanadium oxide film (thickness *d* and permittivity ε) is sandwiched between two insulated metallic gates (a). When the film is in dielectric state (b), the electric field lines penetrate through the film and terminate on the bottom metallic plate. When the film is metallic (c), the electric field lines terminate on the film surface.

Let us assume that both the bottom metallic plane and the vanadium oxide film are grounded and that an external voltage V is applied to the top metallic plate. Let us compare the free energies F_M and F_D per unit area of the film in its metallic and insulating states, respectively:

$$
\begin{aligned}
F_M(T) &= F_{M0}(T) + \frac{1}{2} C_M V^2 \\
F_D(T) &= F_{D0}(T) + \frac{1}{2} C_D V^2
\end{aligned}
\qquad (1)
$$

where F_{M0} and F_{D0} are the free energies in the absence of the applied field and C_M and C_D are the electrostatic capacitances of the system per unit area corresponding to the metallic and the dielectric states of the vanadium oxide film, respectively. If the Debye screening length in the dielectric phase is much larger than the film thickness, we can neglect the screening effect and hence the capacitance C_D is given by

$$C_D^{-1} = \left(\frac{d_1}{\varepsilon_1} + \frac{d_2}{\varepsilon_2} + \frac{d}{\varepsilon} \right). \tag{2}$$

In the metallic state, obviously, $C_M = \varepsilon_1/d_1$. The thermodynamic transition temperature T_C is determined by the equation $F_M(T_C) = F_D(T_C)$, see Fig. 2.

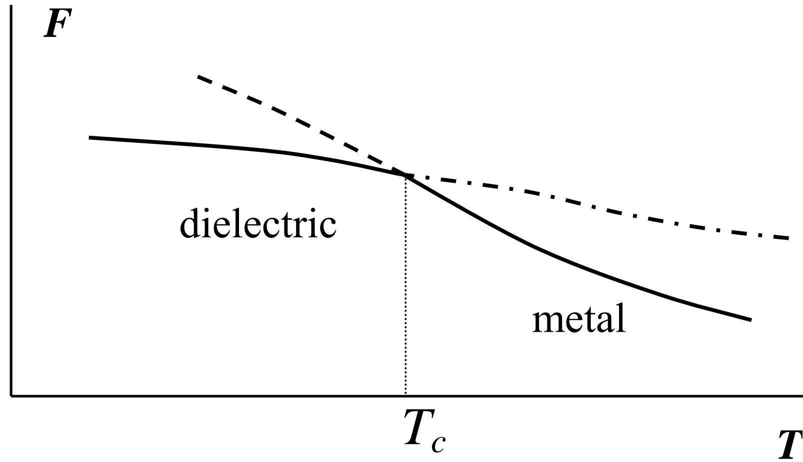

Figure 2. Schematic temperature dependence of the free energy near the metal insulator transition. Dashed line indicates the metastable "overcooled" metal phase and dash-dotted line the "overheated" dielectric. The slope $\partial F/\partial T$ at the transition point suffers a discontinuity ΔS which is interpreted as the entropy of the transition. In terms of the latent heat ΔH of the transition, $\Delta S = \Delta H/T_c$.

Expanding the functions F_{M0} and F_{D0} in powers of $\delta T_C = T_C - T_{C0}$, where T_{C0} is the thermodynamic transition temperature in the absence of an applied field, we find in the first order

$$\delta T_C = \frac{(C_M - C_D)V^2}{2(S_M - S_D)} \ , \tag{3}$$

where S_M and S_D denote the entropy density per unit area of the oxide film in the metallic and the dielectric phase, respectively. Note that we assume that the entire film undergoes the transition. This is undoubtedly true for a thin film, where the formation of an in-plane transition boundary is energetically unfavorable.

The entropy difference can be estimated from the data in ref [**1**], which cites the transition latent heat ΔH=1020 cal/mol for VO_2 at T_c=340 K. This corresponds to the transition entropy ΔS=3 cal/mol·K. For a VO_2 film of thickness $d=100$ Å we find, approximately,

$$S_M - S_D \approx 5 \cdot 10^{-3} \frac{J}{K \cdot m^2} , \tag{4}$$

where we have used for VO_2 the mass density 4.34 g/cm^3. Taking $C_M \approx 10^{-2} F/m^2$ (assuming a conventional SiO_2 gate dielectric, $\varepsilon_I = 3.9$, $d_I = 100$ Å) equation (3) gives $\delta T_C \approx 1K$ for $V=1V$ which is a substantial shift. Note that δT_C is a positive quantity, which means that application of an external voltage drives the system toward the dielectric state. The effect is stronger for thinner films, since the capacitance increases with the decreasing d_I and the transition entropy decreases with the decreasing d. Our freedom to decrease d_I is limited only by the dielectric breakdown. Thickness d of the vanadium oxide film can, in principle, be made as thin as 10-20Å, limited only by the electron correlation length near T_c.

3. Field-controlled switch

The simplest VO_2 switch is shown in Fig. 3. It contains a gated VO_2 film with two "source/drain" contacts implemented as VO_2 regions that are doped to be metallic in the entire operating temperature regime. We assume that the temperature is above but close to T_c so that in the absence of an applied voltage the entire film is in the metallic state. At some gate voltage $\pm V_G$, such that $|V_G| = U_c$, the film goes into the dielectric state. Conversely, starting from a dielectric state at some $|V_G| > U_c$, we bring the film into the metallic state by lowering the magnitude of gate voltage.

It is important to realize that in our device the switching speed is *not* limited by a transit time of carriers under the gate, as it would be in a field-effect transistor. Indeed, in a FET the transit time delay arises as an *RC* time constant. Let us re-trace the argument that leads to this conclusion [**13**]. Suppose the total amount of charge Q in the channel is traveling with a velocity v between the source and the drain, separated by a distance L. This corresponds to a current $I=Qv/L$. In a field-effect, the magnitude of charge that had to be placed on the gate to induce the channel charge Q must be at least Q, plus charges on parallel parasitic capacitances. Hence, the gate delay, *i.e.* time required for the current I to charge the next gate to the same value of Q, is at least L/v.

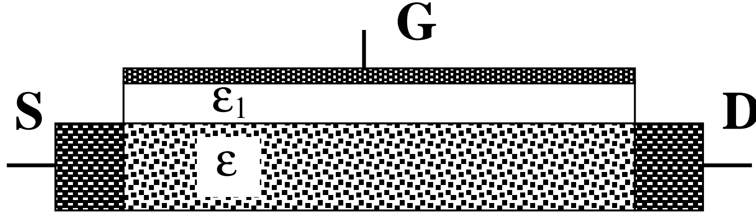

Figure 3. Three-terminal switch with vanadium oxide thin-film channel and a dielectric gate structure of length *L*. At the operating temperature the channel is in the metallic phase in the absence of a voltage applied to the gate. The source/drain contacts are assumed to be implemented of the same material as the channel but brought into metallic phase by doping. Application of a gate field at some voltage $|V_G| = U_c$ brings the channel into the dielectric state.

In contrast, the surface density of mobile charge released in the VO_2 film upon a field induced MIT exceeds the gate charge density by orders of magnitude. There is no *RC* limitation, therefore, analogous to transit time in a FET.

This means that the switching delay is only limited by the kinetics of the inhomogeneous phase transition. While this subject is not well understood theoretically at this time, it appears reasonable that the phase boundary should propagate at a rate determined by the Fermi velocity of electrons in the metallic phase. Due to the natural inhomogeneity of T_c over the film dimensions, one can expect that near T_c both the metallic and the dielectric phases will contain multiple nucleation centers of the opposite phase, so that the typical distances of phase boundary propagation in switching will be substantially shorter than *L.* In this limit, the switching speed should be independent of *L.*

4. Discussion

"Weak" and "strong" mechanisms of field-induced transition. The electrostatic effect discussed in Sect. 2, is based on rigorous thermodynamic considerations and is independent of a physical origin of the metal insulator transition. This mechanism is rather weak, as it allows shifting T_c by at most several degrees K.

Let us now discuss the possibility of a stronger effect, which is based on the assumption that the transition is controlled by the concentration of mobile carriers. Here we assume a model of the transition triggered by the total mobile carrier concentration in the dielectric phase, irrespective of whether it results from doping, thermal excitation, photo excitation – or is induced by electrostatic field effect. We are interested, of course, in the latter case. In an intrinsic insulator in the absence of an applied field, the chemical potential μ is approximately in the middle of the dielectric gap Δ. As the field E is applied, μ moves toward one of the allowed bands and the concentration of electrons (or holes) in the vicinity of the surface increases. At some critical concentration we can expect a transition to the metallic state. Note that in the induced concentration effect the electric field drives the system in the *opposite* direction compared to the electrostatic effect. The application of a large enough gate voltage now drives the system into its metallic state.

Unfortunately, we have no quantitative theory to describe such a transition. Nevertheless, the very existence of induced concentration effect should be

regarded as likely. The critical carrier concentration may be estimated to be of the order of the thermal carrier concentration that arises in the dielectric phase at the transition temperature T_C due to the thermal excitation across the gap. That concentration is about 10^{18} cm^{-3} and should be easily achievable by field-effect. The induced-carrier effect is much “stronger” than the electrostatic effect and should work in a wide range of temperatures. The expected “strong” effect is very attractive for potential applications not only because it relaxes the requirements for temperature control but, more importantly, because it may enable CMOS-like switching circuits where no significant current flows in either state.

Consider the circuit shown in Fig.4 where two MIT switches are designated by FET symbols. The two are connected in series between a high voltage level (*VDD*) and a low level (*GND*). The gates of both switches are connected together and an input voltage V_{in} is applied to both. When V_{in} = *VDD,* the lower switch is in the metallic state. At the same time, the upper switch contains a dielectric region near its drain where the gate-to-channel voltage remains low. The Schottky barrier thus appears in the channel of the upper switch. The output node in this state is low, V_{out} = *GND*. However, when V_{in} = *GND,* the Schottky barrier emerges in the lower switch while the upper switch is fully in the metallic state. In this case, the output node is high, V_{out} = *VDD*. In both configurations the circuit represents a voltage divider with a huge ratio of on/off conductances and dissipates little power in either of its two stable configurations. The circuit thus acts like an inverter similar to that employed in complementary silicon circuits.

We note that if the operating effect were electrostatic, then the circuit of Fig.4 would still be a switching logic circuit but it would *not* be an inverter. Instead, it would be a voltage amplifier in which V_{out} would logically follow V_{in}.

Either way, the circuit operation relies on the symmetry of the field-induced phase transition with respect to the sign of the field. For the electrostatic effect this symmetry is exact, based on the fact that the electric field energy is quadratic in the field. The exact symmetry is not likely in the induced concentration effect but this misbalance can be readily compensated by doping.

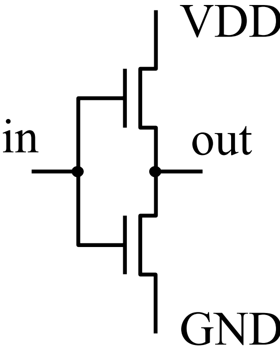

Figure 4. Logic circuit comprising two gate-controlled VO_2 switches. If the mechanism that drives the MIT is such that high $|V_G|$ corresponds to the dielectric phase, then the amplified OUT voltage follows IN. If high $|V_G|$ drives the film into its metallic state, then the circuit is a logic inverter.

Transition speed. As discussed in Sect.2, there is no transit time limitation for a current switch based on field-controlled metal insulator transition. The question arises, what is the real limitation for the switching speed? One possible upper limit may be due to the speed of lattice relaxation. Even if the transition is of Mott type, it is necessarily accompanied by the relaxation of atoms to new equilibrium positions. The characteristic rate of this process is given by Debye frequency and is in the terahertz range. We believe, however, that a more restrictive limitation is related to the kinetics of the first-order phase transition.

In a truly homogeneous sample, the transition speed would be controlled by nucleation of critical droplets [**14**]. In a real situation, however, we can expect a much faster transition. This is because, in a large enough sample, nucleation sites should be present in both phases, due to various inhomogeneities, either natural or built-in by design. In this case, the characteristic delay time should be associated with the propagation of the phase boundary over distances between the phase nuclei and *is independent of the device dimension.*

We estimate the phase boundary velocity to be of the order of the Fermi velocity of electrons in the metallic phase, which is of the order of 10^8 cm/sec. If the typical distance between the nucleation sites is less 1000 Å the switching time is below 1 ps. Experimentally, there have been studies of the semiconductor-metal transition in VO_2 under femtosecond laser illumination [**15**]. These studies have demonstrated a transition time of less than 5 ps.

Possible applications. The ultra-fast switch can find use in electronic as well as optical circuits. Optical applications may be based on the dramatic change in either transmittance or reflectance of light accompanying the metal-insulator transition. Whether or not the range of possible electronic applications may include large-scale integrated circuit applications depends on the transition energetics. The latent heat of transition of 10^3 cal/mol in VO_2 corresponds to about 0.1 eV per electron released. This compares favorably with the power dissipation in a single CMOS switching event.

5. Conclusion

First-order metal insulator phase transitions in thin films can be controlled by an applied electric field. The effect can be employed for the implementation of useful devices such as a three terminal ultra-fast switch. Unlike field-effect transistors, the speed of such a switch is not limited by carrier drift time under the gate. Two field-controlled phase transition switches can be arranged in a CMOS-like inverter circuit in which no significant current flows in either of its steady states.

Acknowledgements

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