

The Field Effect and Mott Transistor Based on Vanadium Dioxide

M.A. Belyaev, A.A. Velichko, P.P. Boriskov, N.A. Kuldin, V. V. Putrolaynen and G.B. Stefanovitch

Abstract— The paper presents simulation results of the field control of phase metal-insulator transition in transistor structures based on vanadium dioxide. The calculations of the field and the electron density in the space charge region in the metallic (M) and semiconducting (S) phases are given. It is shown that the field control of the phase transition at room temperature in the forward direction (from S- to M-phase) inefficiency due to the strong screening of the space charge on the Debye length does not exceed two unit cell of VO₂.

Index Terms— metal-insulator transition, vanadium dioxide, field effect transistor, space charge region

I. INTRODUCTION

METAL-OXIDE-SEMICONDUCTOR field-effect transistors (MOSFET) have been for a long time the key elements of modern electronics industry. For the purpose of a permanent integration enhancement, the size of MOSFET has been decreasing exponentially for over decades in compliance with Moore's Law, but nowadays, owing to the intrinsic restrictions, the further scaling of MOSFET devices either encounters fundamental limits or demands more and more sophisticated and expensive engineering solutions. Alternative approaches and device concepts are currently designed both in order to sustain an increase of the integration degree, and to improve the functionality and performance of electronic devices. Oxide electronics is one of such promising approaches which could enable and accelerate the development of information and computing technology. The behavior of d-electrons in transition metal oxides is responsible for the unique properties of these materials, causing strong electron-electron correlations, which play an important role in the mechanism of metal-insulator transition. The Mott transition in vanadium dioxide is specifically the phenomenon that researchers consider as a corner stone of

oxide electronics, particularly, in its special direction known as a Mott-transition field-effect transistor (MTFET).

The metal-insulator transition (MIT) in vanadium dioxide can be initiated by the temperature change: the MIT from semiconducting (S) phase to the metal (M) phase occurs at the critical temperature $T_t \sim 340$ K, and the re-entrant (M→S) MIT occurs at $T_t' \sim 320$ -338 K ($T_t' < T_t$ due to hysteresis [1]). According to the Hall effect measurements, VO₂ is a n-type semiconductor [2]. The electric field effect on the MIT in VO₂ has been studied earlier in many works [3-9]. The actuality of such studies is conditioned both by the necessity of investigation of the influence of electronic effects on the MIT, and by a practical interest, i.e. for fabrication of transistor-like devices [10]. In spite of this, fabrication of a MTFET is an unsolved problem yet [11].

In this work we estimate the field effect on the conductivity of VO₂-based planar structures with the Mott mechanism of MIT [1]. This mechanism is concentration-induced, and transition from the S- to M-phase occurs at some critical electron density $n \sim n_{c1}$. On the other hand, the M→S transition occurs at $n \sim n_{c2}$ ($n_{c2} \approx n_m/3$, where n_m is the equilibrium electron density in the M-phase) [12].

II. RESULTS AND DISCUSSION

We consider an experimental scheme (Fig. 1) for observations of the field control by the MIT. The field in the structure is created by applying a voltage bias U_{Si} to Si-substrate with respect to the metal electrodes. Such configuration has been described in [17], though the resistivity change at room temperature has not been convincingly registered in work [17].

A. The transition from S- to M -phase

Initially, the VO₂ film is in the S-phase at room temperature. Under the action of an external field, the space charge region (SCR) appears at the VO₂ boundaries. The total voltage drop on the structure of U is the sum of the voltage drops on SiO₂ and the sum of the voltage drop across the SCR in VO₂. Because of the negative polarity of U_{Si} on the bottom surface potential $\psi_{su} > 0$ appears in the VO₂ SCR. This ψ_{su} forms a layer enriched by electrons (Fig. 1.b).

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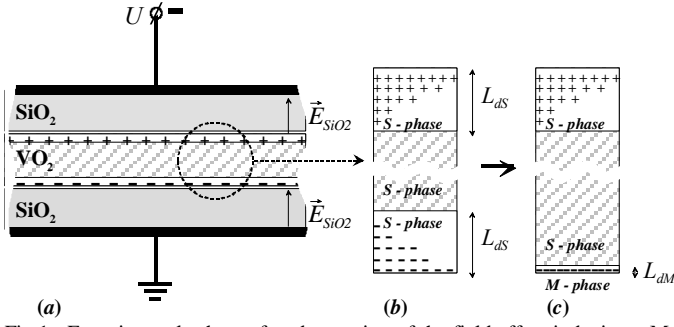


Fig.1. Experimental scheme for observation of the field effect inducing a M-channel (a), SCR in VO₂ at $n < n_{c1}$ (b), SCR in VO₂ at $n > n_{c1}$ (c). U_0 is the voltage determining the measuring current ($U_0 \ll U_{Si}$), R_L – load resistance, U_T – voltage across the structure, L_{dS} and L_{dM} – the Debye length in the S- and M- phases, respectively; E_{SiO_2} is the field in the SiO₂ film.

In order to calculate the electron density distribution in this region, one can use the Poisson equation [14]. As a result, for a n-type semiconductor under the condition ($\frac{d\psi}{dz} \rightarrow 0$, at $\psi \rightarrow 0$), we obtain the expression for the field E :

$$E = \left(\frac{d\psi}{dz} \right) = \frac{\sqrt{2}}{\beta \cdot L_d} (e^{\beta\psi} - \beta\psi - 1)^{1/2} \quad (1)$$

where ψ is the potential, $\beta = \frac{q}{kT}$, q – electron charge, k – the

Boltzman constant, T – temperature, $L_d = L_{dS}$ – the Debye length in the S-phase. The latter is calculated as:

$$L_d = \sqrt{\frac{\varepsilon \cdot \varepsilon_0}{\beta \cdot q \cdot n_0}} \quad (2)$$

with $n_0 = n_s$ being the equilibrium electron density in the VO₂ S-phase, $\varepsilon = \varepsilon_s$ – the dielectric permittivity, and ε_0 – the dielectric constant.

It is impossible to obtain an analytical expression for $\psi(z)$. Therefore Eq. (1) was integrated numerically with the following boundary conditions: $z = 0$, $\psi = \psi_{su}$; $z = z$, $\psi = \psi$. As the result of calculations, the dependences of $E(z)$ and $n(z)$ were obtained (Fig. 2), where

$$n(z) = n_0 \cdot e^{\beta\psi(z)} \quad (3).$$

It should be noted that the surface field $E(0) = E_{SiO_2}$, since $E(z)$ is the external field dependence on the distance from the surface, which drops due to the screening effect.

The ψ_{su} values were chosen so that the critical density was achieved in a 9Å-thick layer (\sim i.e. of the order of two VO₂ unit cell dimension [1]), which can lead to the S→M MIT. The magnitude of the field at the SiO₂-VO₂ boundary at this point is $E_{c1} \sim 1.6 \cdot 10^5$ V·cm⁻¹ (Fig. 2.a).

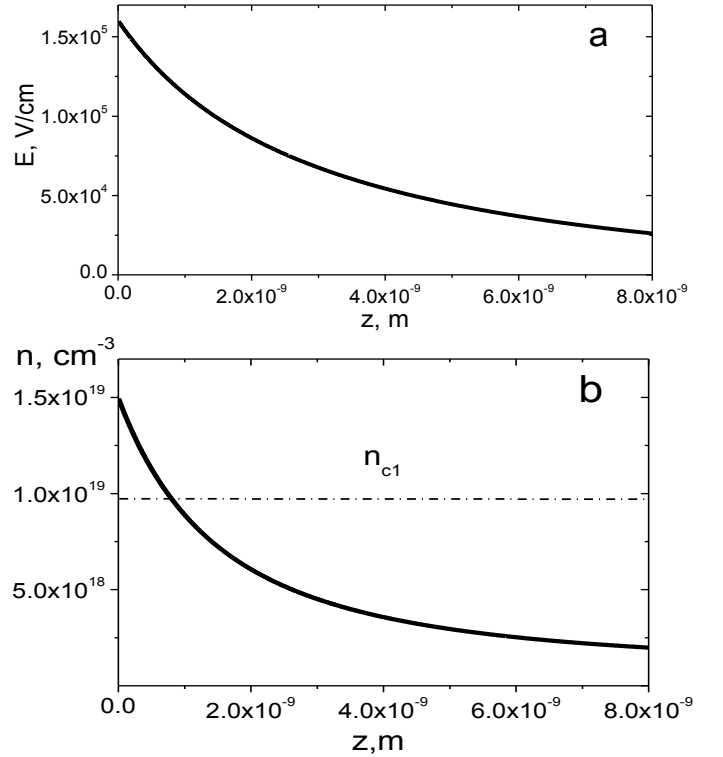


Fig.2. Electric field strength distribution $E(z)$ – (a) and concentration distribution $n(z)$ – (b) in VO₂ SCR; $T = 300$ K, $\varepsilon_s = 41$ [15], $n_s = 10^{18}$ cm⁻³, $\psi_{su} = 0.07$ V, $n_{c1} = 9.7 \cdot 10^{18}$ cm⁻³ [16], $L_{dS} = 7.66 \cdot 10^{-9}$ m.

Now we analyze what happens if a 9 Å - thick layer undergoes the transition into the M-phase. In the formed M-layer, the external field penetrates to a value of $\sim L_{dM}$ (Fig. 1.c). Using Eq. (2) and the values $\varepsilon = \varepsilon_\infty = 9$, $n_0 = n_m = 3.3 \cdot 10^{22}$ cm⁻³ for the M-phase of VO₂ [12] at $T = 300$ K we obtain $L_{dM} \sim 2 \cdot 10^{-11}$ m. Thus, the formed metal layer screens the external field completely. Because of the ohmic contact between the M- and S-phase, there is no electric field behind the metal layer, and hence the SCR in the S-phase eliminates (Fig. 1.b.c). Further increase of the field up to the SiO₂ breakdown ($\sim 1.3 \cdot 10^7$ V·cm⁻¹ [14]), will not result in a significant change of the situation outlined (Fig. 3.a).

As can be seen from the figure 3 the field inside the M-phase falls down to E_{c1} at a distance of ~ 0.8 Å. If we use the value $n_m = 1 \cdot 10^{21}$ cm⁻³ (metallic phase of VO₂ can possess such electron density due to nonstoichiometry [1]), this distance will be ~ 4 Å which again does not exceed one cell parameter.

Theoretically, a transition of a 5 Å-thick layer of VO₂ in the M-phase, in a ~ 1000 Å-thick film, will lead to the decrease of the longitudinal resistance by a factor of six ($\rho_M = 0.001$ Ω·cm, $\rho_S = 1$ Ω·cm are the specific resistivities of the M- and S-phases [1]). In reality, the effect would be much weaker because of roughness of the substrate and defects in the film.

One can offer the scheme (Fig. 4) for observation of this effect, where the field is created by applying a bias voltage to the U_{Si} Si-substrate relative to metallic electrodes. This configuration has been described in [13], however, change in

resistance was relatively low what is apparently explained by the above arguments.

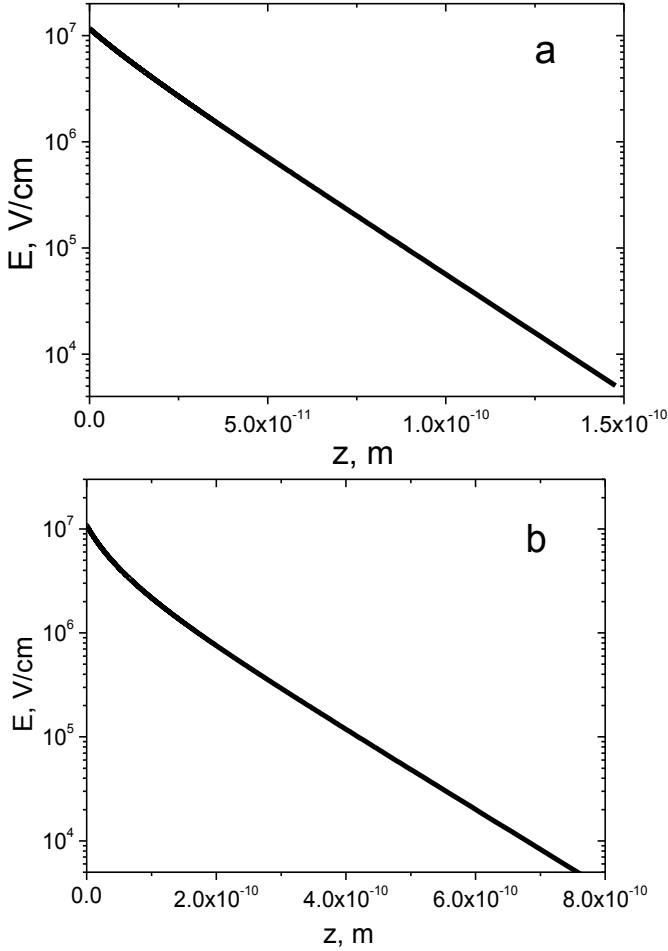


Fig.3. Electric field strength distribution in M-phase (enrichment case): $n_m = 3.3 \cdot 10^{22} \text{ cm}^{-3}$ – (a), $n_m = 1 \cdot 10^{21} \text{ cm}^{-3}$ – (b), $T = 300 \text{ K}$, $E_{ext} \sim 1 \cdot 10^7 \text{ V} \cdot \text{cm}^{-1}$.

Even if the contribution of the formed M-layer to the total resistance could be fixed experimentally, the transistor effect would be absent, because as the field is further increased, as it was said above, it penetrates on a depth not larger than the size of a unit cell, which would not alter the total resistance too much.

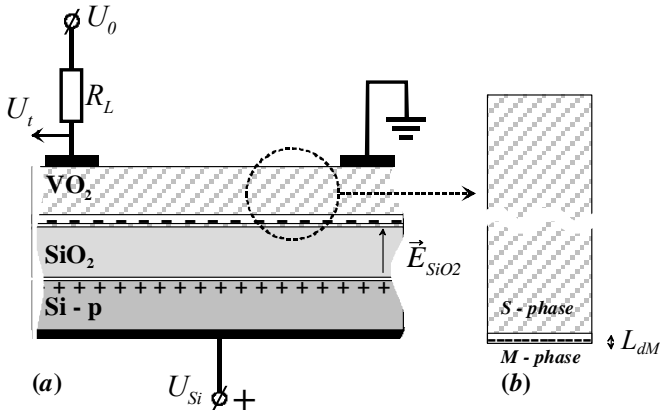


Fig.4. Experimental scheme for observation of the field effect inducing a M-channel. U_0 is the voltage determining the measuring current ($U_0 \ll U_{Si}$), R_L – load resistance, U_t – voltage across the structure, L_{dM} – the Debye length in the M- phase, E_{SiO2} is the field in the SiO_2 film.

The structure would therefore operate as an electronic key or switch. It is to be noted that the above-described results are valid in a static regime, $U_{Si} = \text{const}$. A pulse regime can lead to the appearance of shift currents resulting in new effects influenced upon the MIT. For example, the boundary temperature change due to either the Joule heat or the Peltier effect at the M – S boundary in VO_2 [1] could contribute in this case.

B. The transition from M- to S-phase

Next we analyze a possible field effect on the re-entrant (M→S) MIT. A scheme similar to that shown in Fig. 1.a, was considered, but the ambient temperature was maintained above T_i ($\sim 345 \text{ K}$), and n-type Si with the bias voltage $U_{Si} < 0$ was used.

In this structure, VO_2 is initially in M-phase. Under the field on the border of $\text{VO}_2 - \text{SiO}_2$ SCR forms depleted layer (Fig. 5) and accumulates positive charge of ionized cores of lattice. In this case, the field distribution has a somewhat different character, as high fields can penetrate a greater distance than in the case of enrichment. We prove this by bringing the concentration distribution $n(z)$ and field $E(z)$. Formulae for calculation similar to formulas (1) and (2) except that $\psi_{su} < 0$ and (1) shows the "minus" to the whole expression for the change of the field direction, and $T = 345 \text{ K}$.

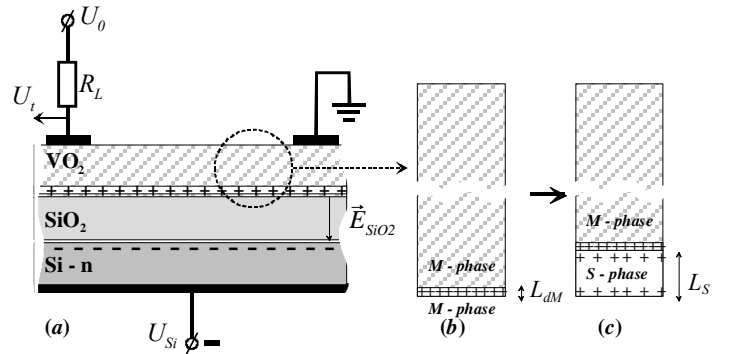


Fig.5. Experimental scheme for observation of the field effect inducing a S-channel, U_0 is the voltage determining the measuring current ($U_0 \ll U_{Si}$), R_L – load resistance, U_t – voltage across the structure, L_{dM} – the Debye length in the M- phase, E_{SiO2} is the field in the SiO_2 film.

As Fig. 6.a shows the critical concentration n_{c2} of reverse MIT can not be achieved even at high field ($\sim 1 \cdot 10^7 \text{ V} \cdot \text{cm}^{-1}$) for value $n_m = 3.3 \cdot 10^{22} \text{ cm}^{-3}$. If we assume, as we did above, that $n_m = 1 \cdot 10^{21} \text{ cm}^{-3}$, then n_{c2} is achieved at distances of about the same size of VO_2 unit cell (Fig. 6.c). Thus, comparing with the Fig. 2.a (the enriched regime), where the field decreases to critical value E_c at distance 9Å instead of 5Å as the case of depletion regime.

We obtain that at $n_m = 1 \cdot 10^{21} \text{ cm}^{-3}$ and $E \sim 1 \cdot 10^7 \text{ V} \cdot \text{cm}^{-1}$ it is feasible to reach the density n_{c2} and thereby to transform a $\sim 5 \text{ Å}$ -thick layer to the S-phase. In this case, the electron density in this layer would fall, and the field is now applied to the S-M boundary; then a next layer will undergo the transition into the S-phase. As the result of this self-spreading wave of the S-

phase (“domino effect”), a significant portion of the metal film might transit into the S-phase.

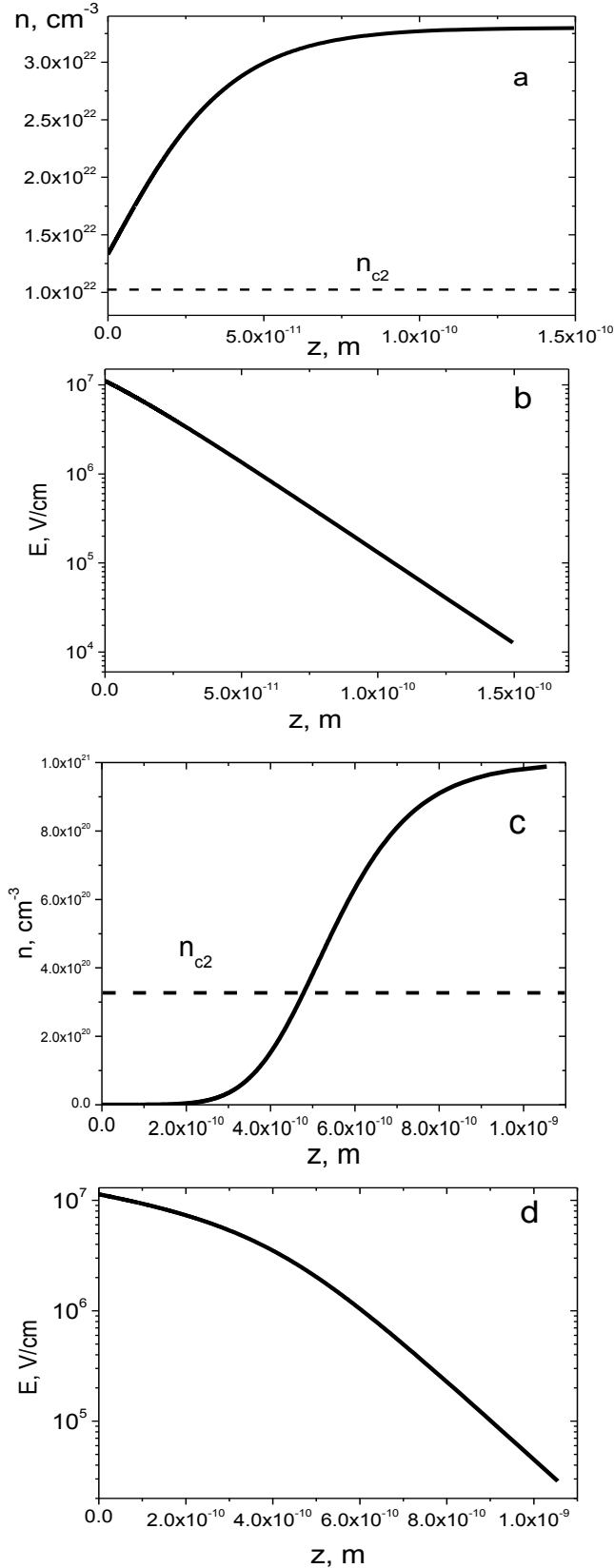


Fig.6. Electric field strength distribution $E(z)$ and concentration distribution $n(z)$ in M-phase (depletion case): $n_m = 3.3 \cdot 10^{22}$ cm⁻³ – (a and b), $n_m = 1 \cdot 10^{21}$ cm⁻³ – (c and d), $T = 345$ K ($n_{c2} \approx n_m/3$); $E_{ext} \sim 1 \cdot 10^7$ V·cm⁻¹.

The thickness of the layer is determined by voltage U_{Si} , which is distributed between SiO₂ and has been converted to S-phase layer of VO₂. Calculate how the field is distributed in the resulting layer of S-phase. If we assume that the equilibrium concentration is $n_0 = n_0(345 \text{ K}) \sim n_{c1}$ and external field is $E_{ext} \sim 1 \cdot 10^7$ V·cm⁻¹, the form $n(z)$ and $E(z)$ is represented in figure 7.ab.

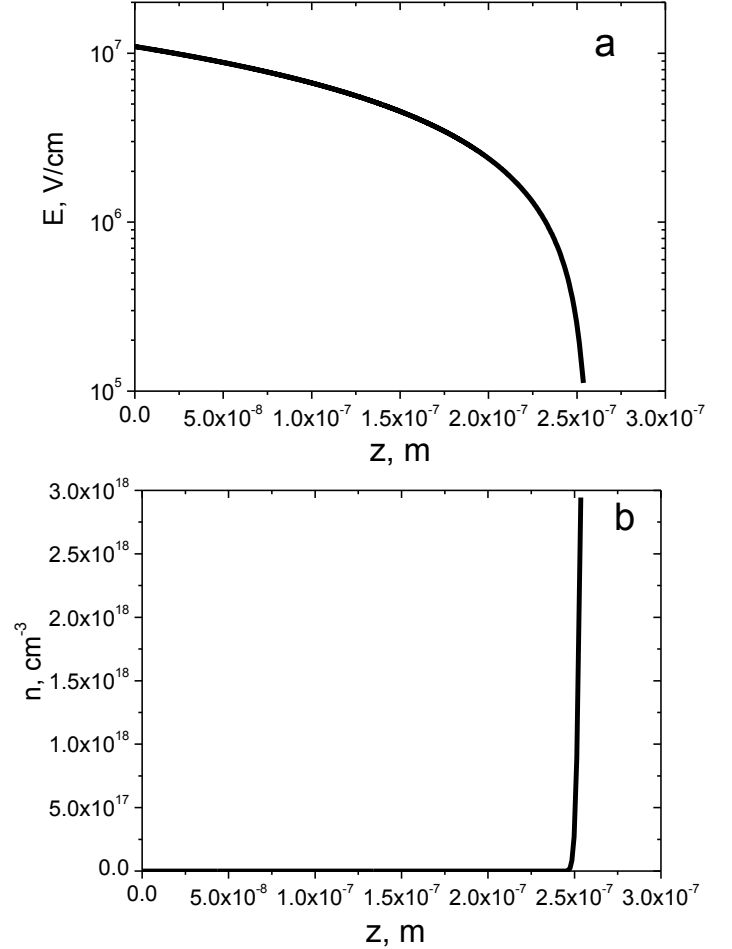


Fig.7. Electric field strength distribution $E(z)$ and concentration distribution $n(z)$ in M-phase (depletion case), $E_{ext} \sim 1 \cdot 10^7$ V·cm⁻¹.

As Fig. 7. shows the screening of the field occurs only at a distance of ~ 2500 Å, at distances ~ 1000 Å field can be considered constant in the absence of free carriers. Thus, the VO₂ films 1000Å thick to form a layer S-phase can be considered a dielectric.

However, taking into account the high-field effects (e.g. Poole-Frenkel effect), the electron density in the S-phase can be estimated:

$$n_0 = n_0(345K) \cdot e^{\frac{bm\sqrt{E}}{2kT}} \quad (4),$$

where $bm = \sqrt{\frac{q^3}{\pi \cdot \epsilon_S \cdot \epsilon_0}}$ – the Poole-Frenkel constant.

Substituting $E \sim 1 \cdot 10^7$ V·cm⁻¹, we obtain $n \sim 5.8 \cdot 10^{21}$ cm⁻³ which gives the distribution $n(z)$ and $E(z)$ (Fig.8.ab). The field seen can be considered constant thickness to ~ 100 Å. Thus,

the channel width of the dielectric can be adjusted to $\sim 100\text{\AA}$. What can be quite appreciable adjustment current passing through the VO_2 channel, with a thickness of up to 1000\AA and above.

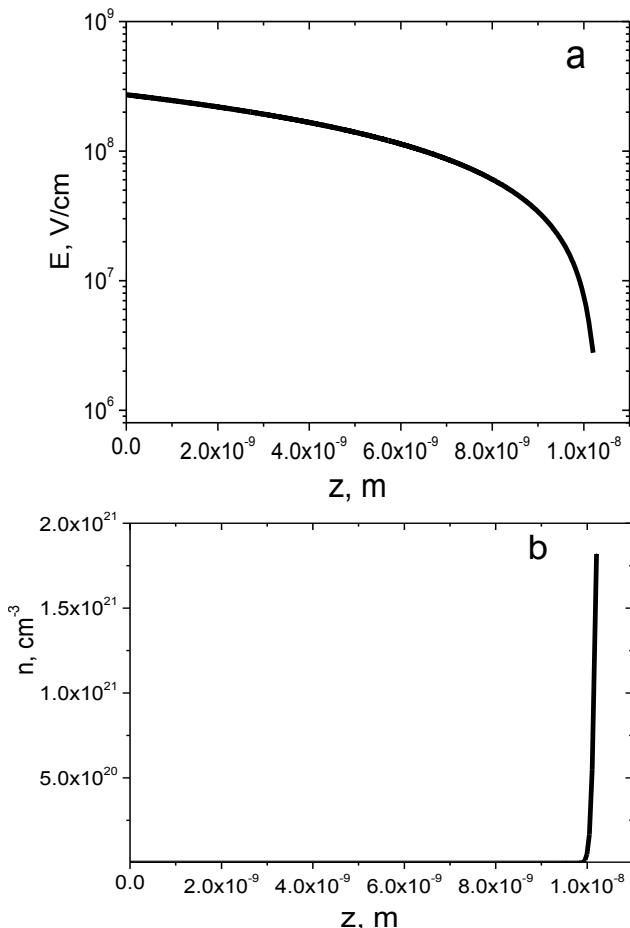


Fig.8. Electric field strength distribution $E(z)$ and concentration distribution $n(z)$ in M-phase considering Poole-Frenkel effect (depletion case), $E_{ext} \sim 1 \cdot 10^7 \text{ V}\cdot\text{cm}^{-1}$.

As the external fields can cause breakdown of SiO_2 , leading simultaneously to the breakdown of the entire structure.

III. CONCLUSION

Thus, the simulation results showed a slight penetration of the field in S- and in M-phase of VO_2 , what greatly reduces the field control efficiency of MIT. This is particularly evident in the case of transition from S- to M-phase, where the strong screening of the space charge gives the Debye length does not exceed two unit cell of VO_2 . An alternative method to enhance the field effect can be a decrease of temperature in the structure, when the relative change of VO_2 channel resistance increases with the growth of the total resistance as shown in [13,18].

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