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Impact of the current pulse width on the speed of metal-insulator transition in VO_2 nanobeams

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Abstract. VO_2 undergoes an insulator-metal transition at ~ 68 °C, making it an attractive material for the development of tunable metasurfaces, steep-switching transistors, neuristors and other devices. Applications such as wireless communications call for ultrashort transition times, which are believed to be typically limited by heat dissipation. We consider the negative role of heat accumulation in the substrate, which slows down recovery after long heating pulses. Thermal simulations of VO_2 nanobeam gratings show that they can display two different behaviors: single-nanobeam-like in the short-pulse regime and film-like in the long-pulse regime. In the long-pulse regime, the recovery time depends linearly on the pulse duration and approximately quadratically on the hysteresis width, in agreement with analytical expressions. In the short-pulse regime, the dependence is much weaker. To achieve nanosecond recovery times, either the short-pulse regime must be used (pulse duration less than the time constant of heat diffusion between adjacent nanobeams), or hysteresis must be eliminated (e. g., by doping). Our results quantify the impact of the pulse duration and hysteresis on the switching time of VO_2 devices, clarify the conditions under which these factors are important, and therefore can guide the development of fast electronic/optoelectronic devices based on phase-change materials.

Keywords: vanadium dioxide, metal-insulator transition, nanobeams, nanowires, hysteresis, heat transfer

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Влияние длительности импульсов тока на скорость перехода металл-полупроводник в нанопроводах VO_2

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Аннотация. VO_2 претерпевает переход изолятор-металл при температуре ~ 68 °C, что делает его привлекательным материалом для создания управляемых метаповерхностей, транзисторов с высокой крутизной характеристики, нейристоров и других устройств. Такие применения, как беспроводная связь, требуют ультрабыстрых времён переключения, которые обычно ограничены теплоотводом. Мы рассматриваем негативную роль накопления тепла в подложке, которое замедляет восстановление изолирующего состояния после длинных импульсов нагрева. Тепловое моделирование решёток из нанопроводов VO_2 показало, что они могут вести себя двумя способами: как отдельные нанопровода в режиме коротких импульсов и как непрерывные плёнки

в режиме длинных импульсов. В режиме длинных импульсов время восстановления зависит линейно от длительности импульса и примерно квадратично от ширины гистерезиса, в согласии с аналитическими выражениями. В режиме коротких импульсов эти зависимости гораздо слабее. Для достижения наносекундных времён восстановления необходимо либо использовать режим коротких импульсов (длительность импульса меньше характерного времени диффузии тепла между соседними нанопроводами), либо устранить гистерезис (например, легированием). Таким образом, количественно охарактеризовано влияние длительности импульсов и ширины гистерезиса на время переключения устройств из VO_2; прояснены условия, при которых эти факторы важны. Эти результаты могут быть использованы для создания быстрых электронных/оптоэлектронных устройств на фазовых переходах.

Ключевые слова: диоксид ванадия, переход металл-полупроводник, нанопровода, гистерезис, теплопередача

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Introduction

VO_2 undergoes a first-order insulator-metal transition (IMT) at $T_c \sim 68$ °C, accompanied by an abrupt increase in conductivity and reflectivity. This makes it attractive for a range of applications in electronics and optoelectronics [1], including electrically and/or optically controlled metasurfaces [2], steep-switching transistors [3], and neuromorphic devices [4]. Previous theoretical and experimental work has shown that the switching speed of electrically controlled VO_2 devices is typically limited by the rate of heat dissipation [5, 6], while the "intrinsic" characteristic time of the IMT lies in the subpicosecond range [7]. (For completeness, we also mention reports on nonthermal electrically induced IMT in VO_2, which requires a large defect concentration [8].)

Therefore, the most obvious ways of improving the transition speed in VO_2 are (i) downscaling (nanobeams, nanocrystals) and (ii) using substrates with good thermal conductivity (such as Al_2O_3). Both approaches have been successfully tested experimentally [9, 10].

But there remains another possibility, related to the nonstationary nature of heat flow in fast-switching devices. If the device remains in the metallic (high-temperature) phase long enough, heat will accumulate in the substrate and prevent efficient cooling of the device when heating current is switched off, thereby slowing down the reverse, metal-insulator transition (MIT). On the other hand, if VO_2 is heated by short current pulses and stays hot (metallic) only for short periods of time, the substrate will absorb less heat during the pulse, and the reverse switching will be faster. This is especially relevant for the combined optical/electrical control of VO_2 metasurfaces, when electric current is used to reduce the optical switching threshold and does not necessarily have to be pulsed [11].

In this work, we simulate heat transfer in periodic arrays of VO_2 nanobeams (nanobeam gratings) grown on single-crystal Al_2O_3 and study the dependence of the recovery time on the duration of current pulses passing through the nanobeams. The role of hysteresis is also discussed.

Model

We consider infinitely long VO_2 nanobeams of width w = 200 nm and thickness h = 30 nm grown on a single-crystal Al_2O_3 substrate. The nanobeams form a periodic array with a period of 1 μm. They are heated by square current pulses (0.1 mA) to the IMT temperature and then cool down to the temperature of reverse, metal-insulator transition (MIT), switching back into the semiconducting phase. We calculate the switching time by numerically solving the heat equation, taking into account the latent heat of MIT and hysteresis. The switching time is defined as the interval between the end of a pulse and the moment when the whole nanobeam cools down below the MIT temperature. The ambient temperature is T_{env} = 25 °C.

Material parameters used in the simulations: Al_2O_3 heat capacity $c_{Al_2O_3} = 3.5 \cdot 10^6$ J/(m·K), Al_2O_3 thermal conductivity $k_{Al_2O_3} = 30$ W/(m·K), VO_2 heat capacity $c_{VO_2} = 3 \cdot 10^6$ J/(m^3·K), VO_2 thermal conductivity in the metallic phase $k_{VO_2,M} = 6$ W/(m·K), VO_2 thermal conductivity in the semiconducting phase $k_{VO_2,I} = 3.5$ W/(m·K), VO_2 resistivity $\rho_{VO_2,M} = 2 \cdot 10^{-2}$ Ω·m, $\rho_{VO_2,I} = 2 \cdot 10^{-6}$ Ω·m, latent heat of the IMT $\Delta H_{IMT} = 2.7 \cdot 10^8$ J/m^3, transition temperatures $(T_{IMT} + T_{MIT})/2 = 68$ °C, $T_{IMT} - T_{MIT} = \Delta T$. The hysteresis width ΔT was set to either 0, 10 or 20 °C. We assume that both VO_2 phases coexist at T_{IMT} (during heating) or T_{MIT} (during cooling), and the properties of this mixed state (heat capacity, resistivity, enthalpy) are determined by the properties of each phase weighted by their molar fractions. Interface thermal resistance was neglected.

Numerical simulations

The simulation results for three different hysteresis widths are shown in Fig. 1*a*. Indeed, long current pulses lead to slower switching, which is explained by the heat accumulation in the substrate (Fig. 1*b*, *c*). Two regimes are observed. When the pulse duration t_{pulse} is less than the characteristic timescale of heat diffusion between adjacent nanobeams (~30 ns in our simulations), the grating behaves as independent nanobeams, and the dependence of the recovery time on the pulse duration is rather weak (nanobeams are small and cannot dissipate much heat into the substrate). On the other hand, in the long-pulse limit the grating behaves as a continuous film, and the recovery time depends linearly on the pulse duration.

The effect of hysteresis is also pronounced. Hysteresis width ΔT in VO_2 can be controlled, e. g., by doping [12]. Wide hysteresis delays the reverse transition (MIT), because cooling VO_2 from T_{IMT} to T_{MIT} requires more time than just dissipating the latent heat. (Fig. 1*a*) shows approximately quadratic dependence of the recovery time on the hysteresis width in the long-pulse limit, and a weaker, but still significant dependence in the short-pulse limit.

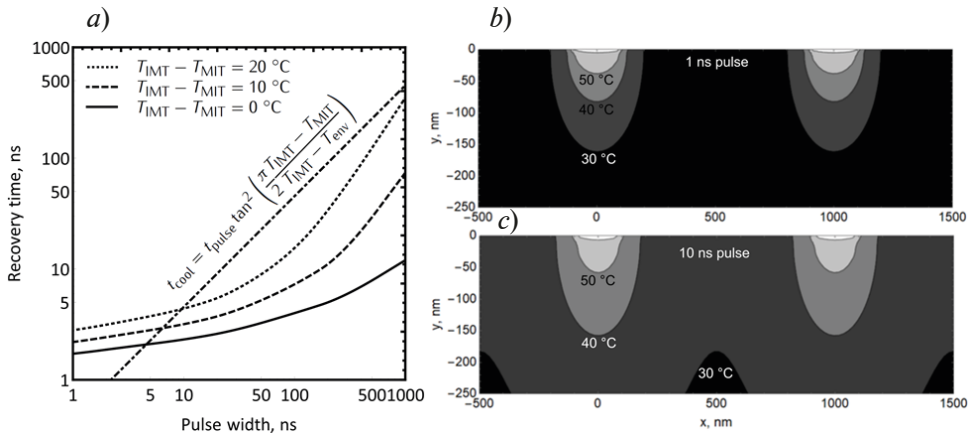

Fig. 1. Transition time in a periodic array of 30 nm × 200 nm VO_2 nanobeams (period 1 μm) on Al_2O_3 substrate vs the duration of current pulses for three different hysteresis widths (*a*). Temperature distribution in the substrate after the end of a 1 ns, 0.1 mA pulse (*b*) or a 10 ns, 0.1 mA pulse (*c*)

Analytical expressions

In the long-pulse limit, a nanobeam grating behaves as a continuous film. Assuming VO_2 heats up to T_{IMT} almost instantaneously and neglecting its heat capacity and finite thickness, we can find the recovery time by solving the one-dimensional heat equation on a half-line with a boundary condition of constant temperature during the pulse, zero heat flux after the pulse, and again constant temperature during the MIT. In the presence of hysteresis, the main contribution to the recovery time is cooling from T_{IMT} to T_{MIT}, with the MIT itself being much faster:

$$t_{recovery} \equiv t_{cool} + t_{MIT} \approx t_{pulse} \tan^2\left(\frac{\pi}{2}\frac{T_{IMT} - T_{MIT}}{T_{IMT} - T_{env}}\right). \quad (1)$$

Without hysteresis, the recovery time is determined by the duration of MIT and has an approximately square-root dependence on the pulse duration:

$$t_{\text{recovery}} = t_{\text{MIT}} = \left(\sqrt{t_{\text{pulse}}} + \sqrt{\frac{\pi}{4\kappa_{Al_2O_3} c_{Al_2O_3}}} \frac{\Delta H_{\text{IMT}} h}{T_{\text{IMT}} - T_{\text{env}}} \right)^2 - t_{\text{pulse}} \approx \sqrt{\frac{\pi t_{\text{pulse}}}{\kappa_{Al_2O_3} c_{Al_2O_3}}} \frac{\Delta H_{\text{IMT}} h}{T_{\text{IMT}} - T_{\text{env}}}. \quad (2)$$

In the short-pulse limit, the grating behaves as independent nanobeams. In this case, analytical expressions become complicated. Qualitatively, the weaker dependence of the recovery time on the pulse duration and hysteresis width can be traced to the fact that the finite width of a nanobeam sets a characteristic timescale of heat diffusion (in contrast to the case of a film, where the only timescale is the pulse duration, leading to a linear behavior of the recovery time).

Conclusion

We have studied quantitatively the dependence of the recovery time in periodic arrays of VO_2 nanobeams on the duration of current pulses applied to VO_2 and hysteresis width (the difference in temperatures of insulator-metal and metal-insulator transitions).

The speed of metal-insulator transition in VO_2 nanobeam gratings depends on the heating protocol because of heat accumulation in the substrate. This dependence is especially pronounced when heat has enough time to diffuse between adjacent nanobeams, effectively blocking heat dissipation in lateral direction. In this case, the recovery time depends linearly on the duration of heating pulses. Hysteresis width has an even stronger influence on the recovery time, because cooling VO_2 to a lower temperature is slower than just dissipating a fixed amount of energy (latent heat).

To keep the recovery time in the nanosecond range, three approaches can be used: (1) using heating pulses shorter than the characteristic time of heat diffusion between adjacent nanobeams; (2) eliminating hysteresis (e. g., by doping [12]); (3) employing nonthermal field-induced transition not associated with significant heat dissipation (e. g., by applying low-fluence laser pulses or introducing a large number of defects into VO_2 [8]).

A significant influence of pulse duration on the recovery time has been observed in VO_2 thin films [13]. However, in two-dimensional films, the picture can be further complicated by filamentary conduction and the kinetics of domain walls. These factors are greatly suppressed in one- and zero-dimensional structures and arrays thereof.

Our results can serve as a guideline for the development of fast electronic/optoelectronic devices based on phase-change materials.

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