

# Gas Sensor Based on Metal-Insulator Transition in VO<sub>2</sub> Nanowire Thermistor

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## Supplemental materials

### 1. Device fabrication details:

The nanowires, mesoscopic / microscopic ribbons of VO<sub>2</sub> were grown on SiO<sub>2</sub> /Si or Si<sub>3</sub>N<sub>4</sub>/Si wafers. The nanowires imbedded on to the substrate were mechanically extracted using fine glass needles and were placed on to pristine wafer which has pre-deposited Au/Cr electrodes covered

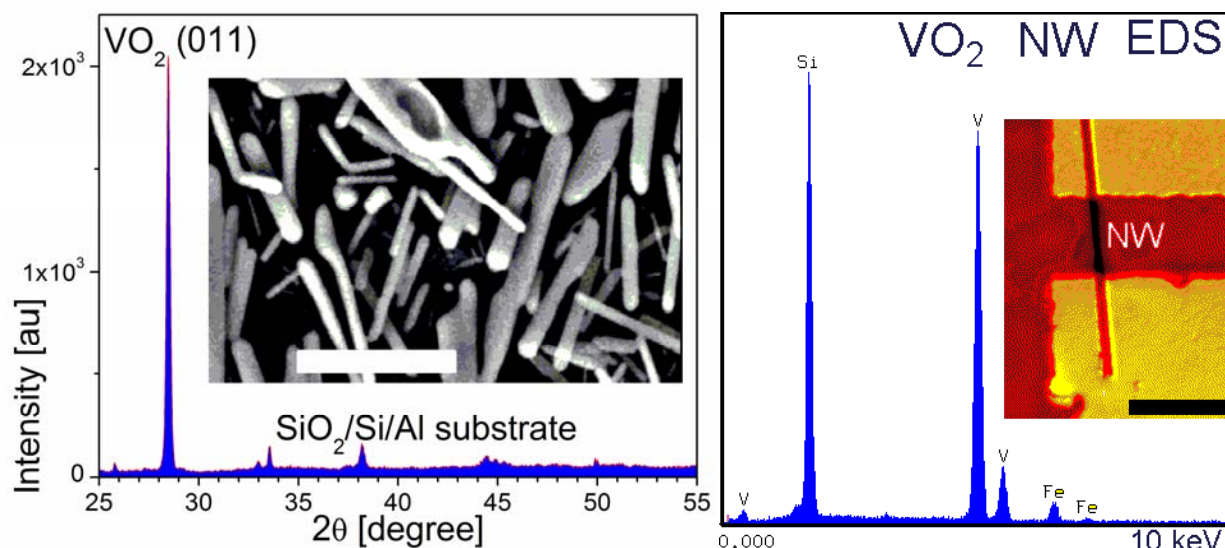


Figure S1 Left: VO<sub>2</sub> nanobeams grown on SiO<sub>2</sub>/Si wafer. XRD of the sample is dominated by monoclinic (011) reflection. The rest of the peaks originate from the support; right panel: EDS made on individual nanobeam. Si, Fe peaks originate from the substrate.

with Ga-In-Sn liquid microdroplets.

### 2. Factors influencing the sensitivity of the device

The sensitivity of the TES-like VO<sub>2</sub> nano-thermistor can be improved in two ways:

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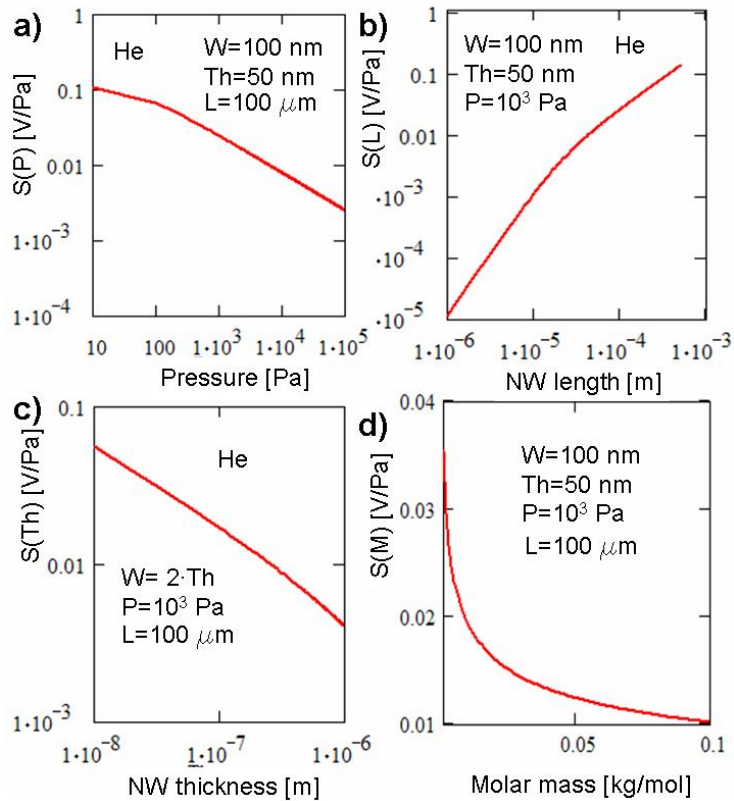


Figure S2. The calculated dependence of the sensitivity  $S$  of the  $\text{VO}_2$  nano-thermistor of a) ambient pressure b) NW length c) NW thickness and c) the type of the gas

a) by optimization of the morphology of the nanowire sensing element and

b) by reducing the scattering of  $V_{MIT}^+$  values.

Figure S2 depicts the calculated dependence of the sensitivity  $S$  [V/Pa] of the  $\text{VO}_2$  nano-thermistor of ambient pressure, NW length, NW thickness and the type of the gas.

The following expressions have been used for estimations:

$$S = \frac{dV}{dp} = \frac{\sqrt{\frac{3\mathcal{R}}{8T_0}} \cdot \rho \cdot \frac{L^2(w+h)\Delta T}{w \cdot h \sqrt{M}}}{\sqrt{4\kappa\rho\Delta T + 2\sqrt{\frac{3\mathcal{R}}{8T_0}} \cdot \rho \cdot \frac{L^2(w+h)\Delta T}{w \cdot h \sqrt{M}} \cdot p}} = \frac{A \cdot L^2(w+h)\Delta T}{w \cdot h \sqrt{M} \sqrt{B\Delta T + 2A \cdot \frac{L^2(w+h)\Delta T}{w \cdot h \sqrt{M}} \cdot p}}; \quad \text{where}$$

$$A = \sqrt{\frac{3\mathcal{R}}{8T_0}} \cdot \rho = 6.3 \cdot 10^{-3} \quad \text{and} \quad B = 4\kappa\rho = 4 \cdot 7 \frac{W}{mK} \cdot 0.1 \Omega m = 2.8; \quad L, w, h \text{ are the NW's length, width}$$

and thickness. As can be seen from the Fig.S2 the sensor has an optimal performance at low pressure range (10-100 Pa), low mass gases ( $\text{H}_2$ , He) and smaller width/thickness of the nanowire (10-100 nm). It is preferable to use ultra long nanowire since the sensitivity improves

drastically with the length (Fig S2 (b)). Figure S3 demonstrates the sensitivity of one of the optimal morphologies of the nanowire to He.

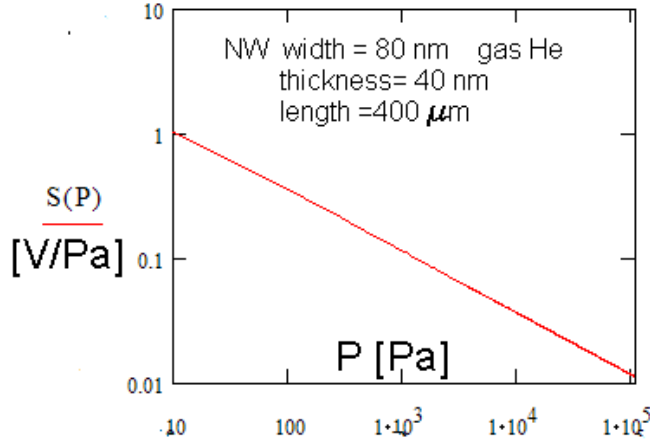


Figure S3. The evaluation of the sensitivity for one of the optimal morphologies of the VO<sub>2</sub> nano-thermistor

The second factor, which influences the ultimate sensitivity of the thermistor is the scatter in the  $V_{MIT}^+$  values from ramp to ramp, which is related to instabilities occurring in the sensor itself rather than in ambient pressure (see Fig. 2 in the article). These scattering is limiting the ultimate sensitivity of the method.

We assume that these scattering of  $V_{MIT}^+$  values is due to either contacts effects and/or stochasticity in nucleation and growth of the metal/insulator domains within the NW. The unstable contact resistance can influence the Joule

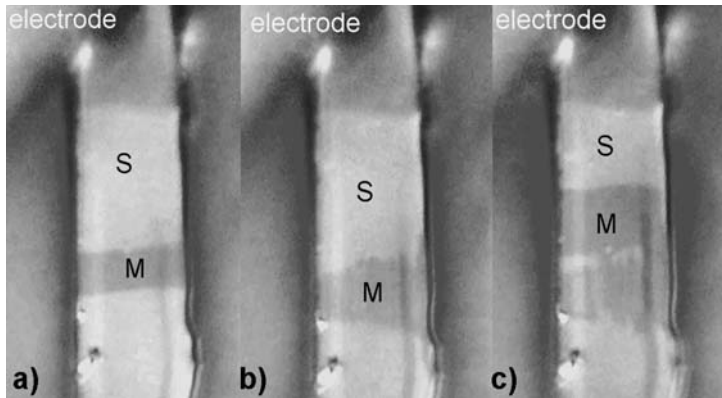


Figure S4. Appearance and enlargement of the metal domains (M) in the preheated micro-ribbon upon increase of the bias voltage a) 1V bias b) 20 V bias c) 20 V bias and longer time. Optical image 1000x

heat distribution in the nanowire resistor device. These contact resistance instabilities can be induced by microscopic movements of the nanowire as a result of the axial stress accompanying the MIT. To eliminate/reduce the latter source

of instabilities, liquid contacts with lower viscosity and smaller surface tension coefficient have

to be used. Alternatively, the instability in the  $V_{SMT}^+$  can originate as a result of irregular nucleation and growth of metal domains along the NW length at the onset of SMT. The formation of these domains under a different set of conditions (mechanical stress, current driven) has been reported earlier [1-3]. We were able observe these domains and their evolution using high-resolution optical imaging of microscopic VO<sub>2</sub> ribbons in polarized light (Fig.S4). The genesis and dynamics of these domains in nanowires appears to be a function of thermal gradients, bias voltage, mechanical stress and nanowire dimensions. A comprehensive analysis of the domains dynamics is given in [3] for a broad frequency range in vacuum. A separate set of thorough optical observations combined with electron transport measurements is currently conducted to elucidate the specific factors, which deteriorate the reproducibility of  $V_{SMT}^+$  in different gas environment.

### 3. Thermal equilibrium:

As can be seen from the estimation of the thermal relaxation time given in [4]:  $\tau \propto \rho c L^2 / k$  (here  $\rho$ ,  $c$ ,  $\kappa$ , are density, specific heat and thermal conductivity of VO<sub>2</sub> nanobelt correspondingly) the thermal equilibrium within the nanobelt establishes within a fraction of microsecond time domain [5].

### References

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