Metal-insulator Transition (MIT) Materials for Biomedical Applications

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Abstract
Transitional metal oxides get considerable interest in electronics and other engineering applications over few decades. These materials show several orders of magnitude metal-insulator transition (MIT) triggered by external stimuli. Bio-sensing using Vanadium dioxide (VO$_2$), a MIT material is largely unexplored. In this short article, we investigate the VO$_2$ based thermal sensor performance for measuring the biomolecule concentration. Active sensing layer is chromium and niobium co-doped VO$_2$ as it shows 11.9%/°C temperature coefficient of resistance (TCR) with practically no thermal hysteresis. Our study demonstrated that VO$_2$ based microsensors can be used to measure the biomolecule concentrations, which produce temperature changes in the mK range. For 1mK change in temperature, the maximum detection voltage is near 0.4V.

Keywords: vanadium dioxide, metal-insulator transition, temperature coefficient of resistance, biosensor

Abbreviations: VO$_2$, Vanadium dioxide; TCR, temperature coefficient of resistance; VO$_x$O$_{2-x}$, vanadium oxide mixture; MIT, metal-insulator transition; mK, milli-Kelvin

Introduction
Metal oxide semiconductor materials are widely used in sensing applications. Vanadium dioxide (VO$_2$) shows temperature induced metal insulator transition with several orders of magnitude change in resistivity above room temperature (transition temperature near 68°C). Among many other applications, it has been studied as uncooled bolometer for several decades, because of its large temperature coefficient of resistance (TCR). The temperature coefficient of resistance (TCR) reported for vanadium oxide mixture (VO$_x$O$_{2-x}$) is more than 5% per °C and 25% per °C in a vanadium oxide dioxide. For pure vanadium dioxide (VO$_2$), TCR value can reach more than 70% near the transition temperature. But this material suffers from thermal hysteresis, which results in poor measurement reproducibility.

By chromium and niobium co-doping, TCR can be increased to 11.9%/°C with practically no thermal hysteresis. Strelcov et al., proposed and tested a novel gas sensor using single crystal VO$_2$ nanowire. Single crystal VO$_2$ nanowire (VO$_2$) has sharp and superior transition properties. In addition, small size, low thermal capacitance, and high surface to bulk ratio of VO$_2$ nanostructure, make them potential candidate to be researched as a high sensitivity gas sensor. A shift in MIT transition voltage is used as the indicator for a change in environments (e.g., molecular composition, pressure, and temperatures etc.). Maximum sensitivity of VO$_2$ nanowire sensor is $\pm 10^4$ V/Pa for light gases at low pressure range. Functionalizing the NW surface with catalysts, which promotes exothermic reactions, VO$_2$ based sensor can be used for various chemical and gas sensing with increase in sensitivity and selectivity. Byon et al., demonstrated a highly responsive and selective H$_2$ sensor, based on electro thermo induced MIT of Pd-nanoparticles decorated VO$_2$ nanowire. Simo et al., reported a room temperature H$_2$ sensor using VO$_2$(A phase) nanobelt pellet with concentration limit about 0.17ppm. To the best of our knowledge, biosensing using VO$_2$ material is largely unexplored. Many biological process and biochemical reaction in living cell generates or absorbs heat. These temperature changes are usually in milli-Kelvin (mK).

Inomata et al., demonstrated that a VO$_2$ thermal sensor can detect cholesterol and glucose with minimum 30 and 15μM detection limit respectively. However, poor thermal isolation associated with their diaphragm structure results in high power consumptions. A cantilever based suspended structure could give better thermal isolation and consequently high signal to noise ratio with low power consumptions. In this article, we perform a simulative study on VO$_2$ cantilever based thermal sensor for biosensing applications.

Device description
In this article, we investigate the VO$_2$ based thermal sensor performance for measuring the biomolecule concentration. Cr and Nb co-doped VO$_2$ will be used for the active sensing material for its large TCR and no thermal hysteresis behavior as mentioned above. Our sensor’s schematic is shown in Figure 1. There are two VO$_2$ layers, the first will act as the sensing layer and other will be the reference layer. The reference sensor is primarily used to cancel out the background and measurement noise. The sensing VO$_2$ layer is deposited on top of a silicon cantilever. This suspended structure will provide isolation to external signal and thermal noise. For more thermal isolation a Si$_3$N$_4$/TiO$_2$ layer can be used on top of the silicon cantilever before depositing the VO$_2$ layer.

The semiconductor material’s resistance change with temperature is expressed using the following Arrhenius relationship:

$$R(T) = R_0 * e^{k.T}$$

Where, $k$ is Boltzmann’s constant, $R_0$ is a constant, and $\Delta E$ is the activation energy. From this equation, we can solve for the TCR as

$$TCR = \frac{1}{R} \frac{dR}{dT} = \frac{-\Delta E}{k.T^2}$$

Device temperature response can be expressed as

$$V_{Detect} = G * V_{Supply} * TCR * \Delta T$$

Where, $V_{Detect}$ is the detection voltage, $G$ is the amplifier gain, TCR is the VO$_2$ temperature coefficient of resistance, and $V_{Supply}$ In our
study $V_{\text{Supply}}$ is kept constant at 5V, $\Delta T$ is assumed in the range 1-10mK. The sensor sensitivity can be expressed as

$$S = \frac{V_{\text{Det}}}{\Delta T} = G \cdot V_{\text{Supply}} \cdot TCR$$  \hspace{1cm} (4)

![Figure 1 VO₂ sensor schematic for bio-molecule concentration detection.](image1)

**Result and discussion**

It is evident from Figure 2 that for 1mK change in temperature, the maximum detection voltage is near 0.4V, which is above the noise base. With Tungsten doping or interfacial strain engineering, the transition temperature can be tuned to the biological system’s ambient temperature. At this temperature, TCR value is in the range of 10-70%, and the maximum detection voltage is about 3.73V for 1mK change in temperature. For a gain value of 1000 and TCR=5.0%, we can achieve 0.25V/mK sensitivity using our device. Still, an intensive investigation is required for design optimization to reduce the power consumption. High latent heat (over ~51kJ/kg) of MIT transition can achieve 0.25V/mK sensitivity using our device. Still, an intensive investigation is required for design optimization to reduce the power consumption and increase sensitivity with improved response time.

![Figure 2 VO₂ sensor detection voltage as a function of temperature change in a biochemical process A) For different amplifier gain at TCR=5.0%. B) For different TCR values at gain=1000.](image2)

**Conclusion**

In this study, we demonstrate that VO₂ based microsensors can be used to measure the biomolecule concentrations based on their mK temperature sensitivity. In future work, we will address other technical issues, required when designing robust sensors, such as:

I. Response time.
II. Sensitivity.
III. Reliability.

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**Conflicts of interests**

Authors declare that there is no conflict of interest.

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