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VO₂薄膜の相転移温度における基板熱膨張率効果

Impact of thermal expansion of substrates on phase transition temperature of VO₂ films

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1. Introduction

VO₂ shows thermally- induced structural phase transition from MoO₂- type monoclinic (M1) to rutile- type tetragonal (R) structures at 341 K under no strain. It is known that elongation (shrinkage) of its $c_{\rm R}$ axis length results in higher (lower) transition temperature, $T_{\rm tr}^{1,2}$ For (010)_{M1}-[or (100)_R-] oriented VO₂ films, one can expect that a larger thermal expansion coefficient (α) of the substrates, $\alpha_{\rm sub}$, would result in shorter $c_{\rm R}$, and thus lower $T_{\rm tr}$. In the present study we demonstrate the $\alpha_{\rm sub}$ effect on $T_{\rm tr}$ of VO₂ thin films grown on the same buffer layers, Pt (111) / SiO₂, but on different kinds of substrates.

2. Experimental

We chose four substrates materials, amorphous SiO₂ (fused silica), Si (001), Al₂O₃ (0001), and CaF₂ (001), whose α_{sub} values are widely ranging. 20 to 30 nm- thick SiO₂ layers and 100 nm- thick Pt layers were deposited by an RF sputtering method. 50 nm- thick VO₂ layers were then deposited with a pulsed laser deposition method. The deposition temperature for both Pt and VO₂ layers was set to 823 K. XRD $2\theta-\omega$ scans and temperature-controlled micro-Raman spectroscopy measurements were performed. To extract T_{tr} values, M1 phase occupation ratio at each temperature was evaluated from Raman spectra, with a method previously described.³

3. Results and discussion

The XRD peak around 40° in $2\theta - \omega$ profiles of each sample [Fig. 1(a)] is considered to be an overlap of diffraction signals from Pt 111 and VO₂ 020_{M1} planes. The difference of peak positions was clearly seen among the samples. Figure 1(b) shows the M1 ratio plotted against the temperature for all samples, again, demonstrating the difference of T_{tr} among them.

We define the linear shrinkage ratio ($\Delta L/L$) of the material during cooling from 823 to 293 K, as $\Delta L/L = \{L(293K) - L(823K)\} / L(823K)$ where L(T)is the in-plane lattice parameter (or simply the sample size in case of an amorphous material) at T K. Lattice spacings of Pt 111 and VO₂ 020_{M1} diffraction planes, estimated from deconvoluted XRD peak positions, and $T_{\rm tr}$ values are plotted in Fig. 2 as functions of $\Delta L/L$ of the substrates. One can see tendencies that the substrates with higher shrinkage ratio (higher α_{sub}) give larger out-ofplane spacings of both Pt and VO₂, and lower T_{tr} of VO₂ films, as expected. It is suggested that α of the substrate is a parameter that causes a significant influence onto phase transition properties of VO₂ thin films.

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Fig. 1 : (a) XRD $2\theta - \omega$ spectra of four samples. (b) Temperature dependence of M1 phase ratio of four samples.



Fig. 2 : (a) Out-of-plane lattice spacings of Pt 111 and VO₂ 020_{M1} diffractions, and (b) T_{tr} of VO₂ films, as functions of $\Delta L/L$ of the substrates.

 2θ (deg)