JOURNAL OF APPLIED PHYSICS **107**, 074506 (2010)

Bending in VO_2-coated microcantilevers suitable for thermally activated actuators

Armando Rúa,[1,2] Félix E. Fernández,[1,a)] and Nelson Sepúlveda[3]
[1]*Department of Physics, University of Puerto Rico, Mayagüez, Puerto Rico 00681-9000, USA*
[2]*Doctoral Program in Physics, Graduate Center, City University of New York, New York 10016, USA*
[3]*Department of Electrical and Computer Engineering, University of Puerto Rico, Mayagüez, Puerto Rico 00681-9000, USA*

(Received 7 November 2009; accepted 18 February 2010; published online 9 April 2010)

The curvature of VO_2-coated silicon microcantilevers was measured as the temperature was cycled through the coating's insulator-to-metal transition (IMT), which drives the curvature change mainly through the strain generated during this reversible structural transformation. The films were grown by pulsed laser deposition (PLD) on heated substrates. Cantilever tip displacement was measured for a 130 μm long cantilever as the temperature was changed by recording the deflection of a laser beam, and the curvature change and estimated film stress were calculated from this data. A change in curvature of over 2000 m^{-1} was observed through the narrow temperature range of the IMT, with a maximum rate of ~485 m^{-1} per degree. Estimated recoverable stress was ~1 GPa through the transition region. These results suggest applications in actuator devices with reduced dimensions, including submicron lengths, multifunctional capabilities, and possibly with higher operational frequencies than other thermally actuated devices. © *2010 American Institute of Physics*. [doi:10.1063/1.3369282]

I. INTRODUCTION

Thermally activated transducers for miniaturized devices use mechanisms like differential thermal expansion (DTE) of two materials ($\Delta\alpha$) or changes through the martensitic type transformation occurring in shape memory alloys (SMAs). The first approach is adequate for sensitive thermal sensors.[1] If one of the two materials has a very high expansion coefficient, as certain polymers do, $\Delta\alpha$ can be as large as $\sim 10^{-4}$ K^{-1}. Deflections corresponding to a curvature change per degree $\Delta\kappa/\Delta T \approx 56$ m^{-1} K^{-1} have been demonstrated in polymer-coated cantilevers.[2] The second mechanism can exert much higher work per unit volume (10^6 to 10^7 J/m^3),[3] and is more suitable for microactuators. As reported here, an order of magnitude higher $\Delta\kappa/\Delta T$ values and high work/volume figures can be obtained in microcantilevers coated with VO_2 through this material's insulator-to-metal transition (IMT). The greatest potential for this response is in actuators with micron or submicron dimensions, which could also have additional functionality.

The IMT in VO_2 has been much studied since first reported by Morin.[4] The transition occurs at a temperature $T_C \approx 68$ °C (on heating) and exhibits temperature hysteresis, with a width of ~1 K or less in bulk crystals and at least several degrees in thin films. It can be classified as a martensitic transformation, as in SMAs, because it involves an ordered displacement of ions in the crystal structure. However, in the latter the transformation occurs between two phases with metallic bonding. In contrast, bonding in VO_2 is ionic, and the compound is a hard material, with Meyer hardness ~13 GPa,[5] comparable to that of quartz. Its conductivity in the "metallic" (high-temperature) phase ($\sigma \sim 10^3$ Ω^{-1} cm^{-1}), originating mainly from vanadium 3*d*-band electrons, is low compared with simple metals, and becomes four to five orders of magnitude lower still in its "insulating" (low-temperature) phase.

Near-infrared transmittance is low in the metallic phase, but increases sharply as the insulating phase is reached. The crystal structure of VO_2 is tetragonal in its metallic phase (rutile type, designated R). On cooling through the IMT, this changes to a monoclinic phase (designated M_1) by slight reordering of the vanadium ions, which causes a doubling of the unit cell.[6] Characteristics through the transition can be greatly affected by doping with other metallic elements,[6–8] or when the material is nanostructured.[9] Interest in VO_2 has been increased several years ago by the demonstration that its IMT can be induced by ultrashort laser pulses.[10–12] Very recently, it has been used also for novel frequency-agile metamaterials.[13]

II. EXPERIMENTAL PROCEDURES

For this work, VO_2 thin films were grown by pulsed laser deposition (PLD) on commercially available silicon microcantilever chips (MikroMasch) and on companion test substrates. The cantilever used for the detailed measurements had length, width, and thickness of, respectively, 130, 35, and 1.04 μm, and a spring constant of ~0.6 N/m. Thickness was determined from the first resonant frequency of the bare cantilevers in the chip, prior to film deposition.[14] This was required because the tolerance specified by the microcantilever manufacturer for the thickness value is too high and would have introduced unacceptable uncertainty in the calculations. A krypton fluoride excimer ($\lambda = 248$ nm) laser with fluence 4 J/cm^2, pulse duration ~20 ns, and repetition rate of 10 Hz was used for ablation of a vanadium metal

---

[a)] Electronic mail: felix.fernandez@upr.edu.

0021-8979/2010/107(7)/074506/4/$30.00

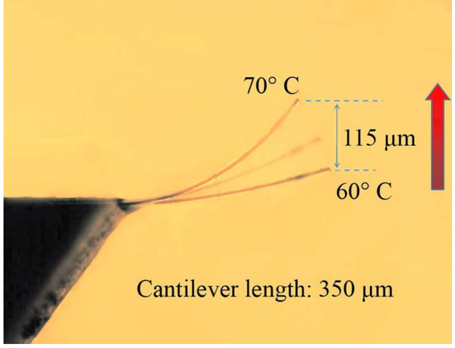

FIG. 1. (Color online) Multiple exposure picture of VO_2-coated silicon cantilever during heating. Temperature was measured with a thermocouple attached to the chip. The vertical displacement of 115 μm was estimated from the known cantilever length of 350 μm. A shorter cantilever was used for the detailed curvature measurements.

target. The PLD process was performed in vacuum chamber in an oxygen/argon atmosphere. Total gas pressure was 30 mTorr during depositions and substrate temperature was kept constant at $T=550$ °C. Film thickness was 240 nm, as measured with a stylus profilometer on reference steps created on the cantilever chip. X-ray diffraction scans on the test substrates show that the films are polycrystalline and strongly oriented with the monoclinic $(011)_M$ planes parallel to the substrate surface. When heated through the IMT, film structure changes reversibly to the tetragonal R phase, and the $(110)_R$ planes are then parallel to the surface.

In a preliminary observation the VO_2/Si cantilevers exhibited very large reversible changes in curvature as the IMT region was reached. The superimposed pictures in Fig. 1—for a 350 μm long cantilever—were taken through a low-power microscope as the temperature, measured with a thermocouple attached directly to the chip, was raised. Cantilever bending toward the side with the deposited film evidences increasing film tension. As the temperature was then reduced the reverse response was observed, with some noticeable hysteresis.

Cantilever tip displacement as a function temperature was measured for a shorter cantilever—130 μm long—using the setup described in Fig. 2. This particular arrangement was convenient for the large deflections observed. Light from a He–Ne laser (L) passing a spatial filter (SF) and from a white light source (W) are combined by a beamsplitter (BS1) and focused by an infinity-corrected microscope objective (F) onto the cantilever chip (C), so that the laser light is more tightly focused on the cantilever tip. Light reflected back through the lens is separated from the incoming beams by the second beamsplitter (BS2) and directed to the bare charge coupled device (CCD) element of the camera, where a magnified image of the cantilever ensemble (in white light) is produced. This image and scattered laser light illuminating the area near the cantilever can be observed in a video screen and adjustments of the chip made with the high-precision positioner. Laser light incident on the cantilever tip is reflected toward a mirror (M), and beam displacement is recorded by a position sensitive detector (PSD). The folded distance from the cantilever chip plane to the PSD plane was measured with a traveling micrometer. From this data the cantilever displacement Δz as a function of temperature was determined. For convenience, and since only the curvature changes were relevant for the present purpose, the initial radius of curvature was taken to be infinite (straight cantilever) although in fact there was observable curvature at room temperature.

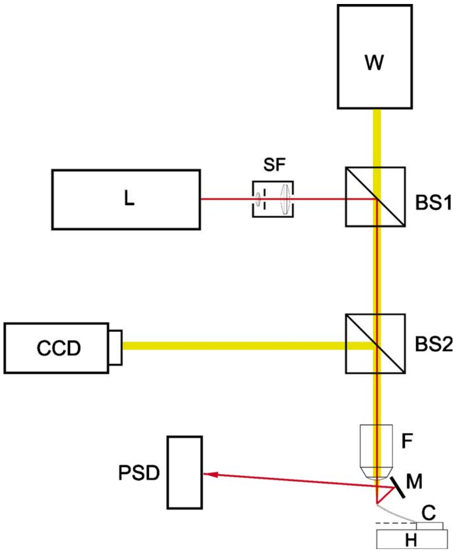

FIG. 2. (Color online) Setup used to measure microcantilever tip displacement as a function of chip temperature. White light and He–Ne laser beams are combined by a beamsplitter and focused on the cantilever tip. The reflected laser beam is recorded by a PSD. Scattered light is separated from the incoming light by the second beamsplitter and forms an image of the cantilever on the bare CCD camera.

III. RESULTS AND DISCUSSION

From each tip displacement Δz measured, the corresponding curvature (1/R) was calculated by solving the transcendental equation relating these quantities and the cantilever length L. The results for a full heating-cooling cycle are presented in the graph in Fig. 3, where the left-hand vertical axis is the curvature in m^{-1}. Repeated heating-cooling cycles produced the same reversible behavior. Film stress (σ_f) causing the bending was estimated from

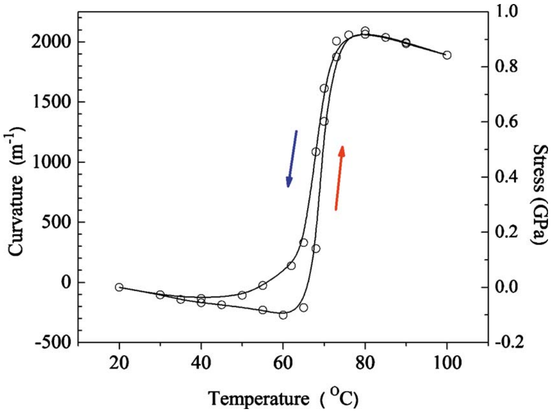

FIG. 3. (Color online) Microcantilever curvature (in m^{-1}, left axis) as a function of temperature through the IMT of VO_2, determined from the measured tip displacement. The right axis gives the estimated film stress (in GPa).

$$\sigma_f = \left(\frac{t_s^3 E_s}{6t_f^2(1-\nu_s)\mathrm{R}}\right)\frac{1}{1+B}, \tag{1}$$

where t_f is the film thickness and t_s, E_s, and ν_s are the substrate's thickness, Young's modulus, and Poisson's ratio, respectively, while $B=t_f/t_s$ is the thickness ratio between film and substrate. Equation (1) is a better approximation than Stoney's well known formula, particularly in a case in which film thickness is not negligible in comparison with the substrate's.[15] A value of 180.5 GPa was used for $E_s/(1-\nu_s)$, the biaxial modulus for the substrate, because the Si cantilever employed has surfaces parallel to {100} planes and this value is constant for directions within these planes for cubic crystals.[16,17] Results for calculated stress change are given by the right-hand vertical axis in Fig. 3. The change through the transition represents a recoverable stress of ~ 1 GPa, an extremely high value. The stress change rate through the IMT was ~ 0.1 GPa/K.

For cantilever detectors sensitivity becomes rapidly smaller as dimensions are reduced. Sensitivity is often quoted in terms of tip displacement per degree, but since Δz increases as L^2, it is better to compare performance in terms of curvature change per degree, at least when the acting mechanism is the same. Results for the VO_2/Si cantilevers demonstrate an extremely high rate of change in curvature of up to $\sim 485\ \mathrm{m}^{-1}\ \mathrm{K}^{-1}$ near T_C, which is almost an order of magnitude higher than for the best cases reported for polymer-coated or SMA-coated cantilevers, even though the quoted spring constant for the microcantilever used was an order of magnitude higher than for the similar but longer cantilevers used for the work reported in Ref. 2. This suggests that cantilevers or similar structures coated with VO_2 can be used as thermally driven transducers with very small dimensions. Unfortunately, applications as sensor devices would be comparatively limited because (1) devices would need to be "primed" by bringing them near the transition temperature, (2) hysteresis would complicate calibration, and (3) the latent heat of transformation must be provided through the transition. In relation to the last point, it should be mentioned that temperature sensitivity, which would be ~ 1.6 nm/mK in the present case, can be a misleading way of comparing sensors based on different actuation principles. Ultimately, detectivity in a thermal detector depends on the energy which must be absorbed to cause a measurable change in the monitored parameter. For DTE-based cantilever sensors the energy absorbed per degree change and per unit mass, neglecting all losses, is just the weighted specific heat capacity of the materials and is hence ~ 1 kJ/kg or less. In contrast, for the case of interest here the strain change mechanism is essentially the structural change through the IMT. The latent heat for the $M_1 \rightarrow R$ transition in VO_2 is over 51 kJ/kg,[18,19] which is higher than for typical SMAs, including Ni-Ti, and the transition occurs over a few degrees, so it is clear that this mechanism is energetically much more demanding. While this limits applicability in sensor devices, it implies that large driving forces are associated with the transition in VO_2. Actuators based on this material can exert higher forces and perform more work per unit volume than similar ones based on DTE and possibly also than those based on SMAs.

The curvature κ of a bilayered cantilever with rectangular cross section can be calculated from the expression[20]

$$\kappa \equiv \frac{1}{\mathrm{R}} = \frac{6(1+B)^2\varepsilon}{t[3(1+B)^2+(1+AB)(B^2+1/AB)]} = \frac{\Gamma\varepsilon}{t}, \tag{2}$$

where $t=t_f+t_s$ is the total thickness of the bilayer, ε is the strain (unitless), $B=t_f/t_s$ as defined before, and $A=E_f'/E_s'$, where E' stands for the biaxial modulus of the material, while the function $\Gamma=\Gamma(A,B)$ is implicitly defined. For fixed geometry, a change in curvature $\Delta\kappa$ is proportional to the change in strain $\Delta\varepsilon$, which can be caused by different mechanisms. For DTE, $\Delta\varepsilon=\Delta\alpha\Delta T$. Neglecting other considerations such as vibration tolerance or work performance, temperature sensitivity $(\Delta\kappa/\Delta T)$ can be increased by using a pair of materials with higher $\Delta\alpha$, maximizing Γ, or—within practical limits—reducing the total cantilever thickness. However, if the cantilever will be used as an actuator the amount of work it can perform becomes an important issue and a different design compromise is needed. The restoring force at the cantilever tip (for rectangular section cantilevers) is proportional to the third power of its thickness.[21] Selection of a pair of materials to maximize $\Delta\alpha$ implies a simultaneous selection of the A ratio. Since polymers have very low elastic moduli ($E\sim 1$ GPa) the restoring force and the work performed in bending, both of which are proportional to the composite cantilever elastic modulus, will be low. Use of stiffer materials will allow exertion of larger forces, but then $\Delta\alpha$, and hence $\Delta\varepsilon$, will not be as high.

Because film strain developed during the IMT in VO_2-coated cantilevers originates from structural transformation of the coating and over a small temperature change, it is mostly unrelated to $\Delta\alpha$ between film and substrate. The maximum strain developed during the transformation can be estimated as follows. Noting that the unit cell crystal of M_1 phase VO_2 corresponds to two unit cells of the R phase along the monoclinic c direction, and using the unstressed lattice parameters of these two phases,[22] it is readily calculated that twice the volume of the tetrahedral unit cell is slightly larger than that of the monoclinic unit cell (0.32% larger). However, because the film crystal planes parallel to the substrate surface are $(011)_M$ for $T<T_C$ but $(110)_R$ for $T>T_C$, the extension of these planes as the IMT is traversed must be considered. From the lattice parameters, the calculated area for the $(011)_M$ and $(110)_R$ planes bounded by, respectively, the monoclinic and doubled tetragonal unit cells along these nearly parallel planes is actually *decreased* by $\sim 1.7\%$ for a single crystal on heating through the transition. This shows that a substantial strain of up to approximately -0.0083 on heating through the IMT in VO_2 is possible in principle. Since the polycrystalline films, although well oriented, have no "in plane" texture, this result cannot be expected to apply directly. Also, in the bilayer the strain is partially restricted by the substrate, which is precisely what generates the stress causing it to bend. The actual strain developed can be estimated from Eq. (2) and the measured $\Delta\kappa$. While the elastic moduli for VO_2 are not well known, and although these (and hence A) should change through the IMT, it seems reasonable to assume $A\sim 1$ for VO_2/Si in Eq. (2).[5,23,24] With $B=0.23$, the strain change during the transition can be estimated to have been nearly -0.003. While higher strain changes can be produced in other physical situations, it should be noted that in the present case this resulted from a temperature change of ~ 10 K. Comparing with DTE-driven cantilevers, this is equivalent to $\Delta\alpha = 3\times 10^{-4}$ K^{-1}, which is higher than for the best bilayer pairs available.

The work per unit volume which can be performed by the cantilever can be calculated from the strain energy density, which is the product $(1/2)E\varepsilon^2 = (1/2)\varepsilon\sigma$, where σ is the stress generated. For bilayered cantilevers the relevant elastic modulus is the weighted average of the biaxial moduli of the two materials. For the present case, assuming again that $A\sim 1$ in order to calculate Γ, and using the measured maximum curvature change, the strain energy density was estimated to have been $\sim 8\times 10^5$ J/m^3. Comparable work/volume characteristics can only be obtained with DTE-driven cantilevers by driving them over hundreds of degrees. Better work/volume figures have been achieved with SMA-based cantilevers, but it should be noted that the VO_2/Si cantilevers used for the present work were not optimized for any particular application and higher figures of merit are possible. As can be expected, the work performed by the cantilever is just a small fraction of the heat required to produce the phase transition. Neglecting all heat losses and the energy required to heat the silicon substrate in the cantilever, the work performed was equivalent to $\sim 1.8\%$ of the heat absorbed to produce the phase transition in the VO_2 film. But while transition-driven thermal actuators are not thermodynamically efficient, they can still be useful in low-grade energy harvesting devices because they can operate between sources and sinks near ambient temperatures, and with a small differential (of just ~ 10 K or less for VO_2).

IV. CONCLUSIONS

Very large reversible curvature changes with large recoverable stress were demonstrated for VO_2-coated silicon microcantilevers over the small temperature range of the film's IMT. These results suggest that thermally activated actuators of this type and with micron or submicron lengths can offer controllable motions with nanometer resolution and capable of applying large forces. While these capabilities can be obtained from piezoelectric microdevices, thermally activated ones would be much simpler to fabricate and operate. An interesting aspect which remains to be probed is the switching speeds for mechanical actuation by direct thermal or optical excitation. These can be expected to be high in comparison with SMAs, considering the hardness and stiffness of the material. In this context, the possibility of reduced dimensions is also relevant, since the input energy required to cause a given temperature change scales inversely with the mass of the device's active region. Increased operational frequency—which is very low in thermally activated devices in comparison with piezoelectrics—would increase the applicability of thermal actuators. Because IMT characteristics in VO_2 can be strongly affected by doping and by controlling its microstructure, there is ample scope for engineering the mechanical response of this material and designing actuators for novel electromechanical or optomechanical microdevices.

[1] J. R. Barnes, R. J. Stephenson, M. E. Welland, C. Gerber, and J. K. Gimzewski, Nature (London) **372**, 79 (1994); J. K. Gimzewski, Ch. Gerber, E. Meyer, and R. R. Schlittler, Chem. Phys. Lett. **217**, 589 (1994); J. R. Barnes, R. J. Stephenson, C. N. Woodburn, S. J. O'Shea, M. E. Welland, T. Rayment, J. K. Gimzewski, and Ch. Gerber, Rev. Sci. Instrum. **65**, 3793 (1994).

[2] M. C. LeMieux, M. E. McConney, Y.-H. Lin, S. Singamaneni, H. Jiang, T. J. Bunning, and V. V. Tsukruk, Nano Lett. **6**, 730 (2006).

[3] P. Krulevitch, A. P. Lee, P. B. Ramsey, J. C. Trevino, J. Hamilton, and M. A. Northp, IEEE J. Microelectromech. Syst., **5**, 270 (1996).

[4] F. J. Morin, Phys. Rev. Lett. **3**, 34 (1959).

[5] P. Jin, S. Nakao, S. Tanemura, T. Bell, L. S. Wielunski, and M. V. Swain, Thin Solid Films **343–344**, 134 (1999).

[6] M. Marezio, D. B. McWhan, J. P. Remeika, and P. D. Dernier, Phys. Rev. B **5**, 2541 (1972).

[7] W. Bruckner, U. Gerlach, W. Moldenhauer, H. P. Bruckner, B. Thuss, H. Opperman, E. Wolf, and I. Storbeck, J. Phys. (Paris) **37**, 63 (1976).

[8] M. Ghedira, H. Vicent, M. Marezio, and J. C. Launay, Solid State Commun. **2**, 423 (1977).

[9] R. Lopez, L. A. Boatner, T. E. Haynes, L. C. Feldman, and R. F. Haglund, Jr., J. Appl. Phys. **92**, 4031 (2002).

[10] A. Cavalleri, Cs. Tóth, C. W. Siders, J. A. Squier, F. Ráksi, P. Forget, and J. C. Kieffer, Phys. Rev. Lett. **87**, 237401 (2001).

[11] S. Lysenko, V. Vikhnin, F. Fernandez, A. Rua, and H. Liu, Phys. Rev. B **75**, 075109 (2007).

[12] S. Lysenko, A. Rúa, V. Vikhnin, F. Fernández, and H. Liu, Phys. Rev. B **76**, 035104 (2007).

[13] T. Driscoll, H.-T. Kim, B.-G. Chae, B.-J. Kim, Y.-W. Lee, N. M. Jokerst, S. Palit, D. R. Smith, M. Di Ventra, D. N. Basov, Science **325**, 1518 (2009).

[14] N. Sepúlveda, A. Rúa, R. Cabrera, and F. Fernández, Appl. Phys. Lett. **92**, 191913 (2008).

[15] C. A. Klein, J. Appl. Phys. **88**, 5487 (2000).

[16] W. A. Brantley, J. Appl. Phys. **44**, 534 (1973).

[17] J. J. Wortman and R. A. Evans, J. Appl. Phys. **36**, 153 (1965).

[18] C. N. Berglund and H. J. Guggenheim, Phys. Rev. **185**, 1022 (1969).

[19] F. Pintchovski, W. S. Glausinger, and A. Navrotsky, J. Phys. Chem. Solids **39**, 941 (1978).

[20] S. Timoshenko, J. Opt. Soc. Am. **11**, 233 (1925).

[21] D. Sarid, *Scanning Force Microscopy* (Oxford University Press, New York, 1991).

[22] Powder Diffraction Files nos. 82–0661 and 79–1655, International Centre for Diffraction Data, Pennsylvania.

[23] K. Y. Tsai, T. S. Chin, and H. P. Shieh, Jpn. J. Appl. Phys., Part 1 **43**, 6268 (2004).

[24] M. Guntersdorfer, Solid-State Electron. **13**, 355 (1970).