Flow stress of Ni-rich NiTi thin films

FANLING MENG, YONGHUA LI, YUMING WANG, WEITAO ZHENG
Alan G. MacDiarmid Laboratory Department of Materials Science, Jilin University, Changchun 130023, People's Republic of China

Among several types of functional materials proposed for fabricating microactuators, TiNi shape memory alloys have great recovering force after deformation [1–3]. The environment temperature, the crystallographic texture, the grain size, and the thickness of film should affect the flow stress development [4]. It is interesting to predict the flow stress of thin film before its fracture. In this work the Hall-Patch coefficient was obtained.

The NiTi thin films were deposited onto copper substrates by magnetron sputtering in an argon atmosphere using a sputtering target of an equiatomic TiNi alloy. The copper substrate was 35 μm thick. The sputtering conditions were as follows: base pressure, $<1.0\times 10^{-3}$ Pa; argon pressure, 4×10^{-2} Pa; sputtering power, 640 w; deposition rate, 95 nm/min, substrate-to-target distance, 65 mm. The substrate temperature was about 400 °C. Under these conditions NiTi films were about 20 μm thick. The film composition determined by energy dispersive X-ray spectroscopies was Ti-51.45 at%Ni, which was a slightly Ni-rich TiNi film. To produce the crystallization of NiTi, the as-deposited films were first solution treated at 1073 K for 1 hr, and then aged at 773 K for 30 min. A vacuum furnace operating at higher than 10^{-4} Pa was used to anneal the films. Tensile tests were carried out at ambient temperature. The specimen size was 4.5 mm × 30 mm (gauge portion). The strain rate was 1.1×10^{-4} s^{-1}. The grain size of the NiTi thin film was obtained using scanning electron microscopy (SEM).

Griffin [5] and Bravman [6] recently showed that the strength of polycrystalline thin films depends on both their grain size and their thickness. The total flow stress is simply determined by the sum of two mechanisms [7]:

$$\sigma_{\text{flow,total}} = \sigma_{\text{flow}} + kd^{-1/2} \tag{1}$$

where d is median grain size and k is the Hall-Petch coefficient. Thompson [8] developed a model which considers a thin film predominantly composed of grains whose boundaries intersect both surfaces of the film. Each grain in such a film is a right polygonal cylinder. A further simplification is to treat each grain as a right circular cylinder of diameter d and height h. Consider the slip occurring by formation of dislocations at the top surface of the film. Once a dislocation has swept through the slip plane in the grain, the work done is given by

$$W_{\text{out}} = (\tau b)(ld) \tag{2}$$

$$\tau = \sigma\cos\lambda\cos\phi \tag{3}$$

where $l = h\sin\phi$, ϕ is the angle between the slip plane and the bottom of the grain, b is the Burgers vector of the dislocation, h is the film thickness, τ is the shear stress, and λ is the angle between the Burgers vector direction and the normal to the plane of the film [9, 10].

In accomplishing the work W_{out}, a dislocation loop going along the two sides of the grain and reaching the bottom of the grain has been created. This energy cost is given by

$$W_{\text{in}} = 2lW_{\text{side}} + dW_{\text{bottom}} \tag{4}$$

$$W_{\text{bottom}} \cong \frac{b^2}{4\pi(1-\upsilon)}\frac{2\mu_f\mu_s}{\mu_f+\mu_s}\ln\left(\frac{\beta h}{b}\right) \tag{5}$$

$$W_{\text{side}} = \frac{b^2\mu_f}{4\pi(1-\upsilon)}\ln\left(\frac{d}{b}\right) \tag{6}$$

where W_{side} and W_{bottom} are the energies per unit length of the respective dislocation segments [9, 10], ν is Poisson's ratio, β is a constant approximately equal to 1, μ_f and μ_s are the shear moduli of the film and substrate, respectively.

Assume that W_{side} and W_{bottom} are approximately equal

$$W_d \equiv W_{\text{side}} \cong W_{\text{bottom}}. \tag{7}$$

The net work done by the glide of the dislocation is then

$$\begin{aligned} W_{\text{net}} &= W_{\text{out}} - W_{\text{in}} \\ &= \frac{\sigma\cos\lambda\cos\phi}{\sin\phi}bhd - \left(\frac{2h}{\sin\phi}+d\right)W_d. \end{aligned} \tag{8}$$

For slip to occur $W_{\text{net}} \geq 0$, so that the flow stress is found by setting $W_{\text{net}} = 0$ therefore:

$$\sigma_{\text{flow}} = \left(\frac{W_d\sin\phi}{b\cos\lambda\cos\phi}\right)\left(\frac{2}{d\sin\phi}+\frac{1}{h}\right) \tag{9}$$

$$\sigma_{\text{flow}} = \frac{b\mu_f\sin\phi}{4\pi(1-\upsilon)\cos\phi\cos\lambda}\left(\frac{2}{d\sin\phi}+\frac{1}{h}\right). \tag{10}$$

For bcc structures, Chen [11] showed that real slip plane only occurred on the {110} plane. For a {110} oriented film, the slip direction is ⟨111⟩,

$\sin\phi/\cos\phi\cos\lambda = 2.121.$

$$\sigma_{\text{flow}} = 2.121 \times \frac{b\mu_{\text{f}}}{4\pi(1-\upsilon)} \ln\left(\frac{d}{b}\right) \times \left(\frac{2}{0.866d} + \frac{1}{h}\right) \quad (11)$$

$$\sigma_{\text{flow,total}} = 2.121 \times \frac{b\mu_{\text{f}}}{4\pi(1-\upsilon)} \ln\left(\frac{d}{b}\right) \times \left(\frac{2}{0.866d} + \frac{1}{h}\right) + kd^{-1/2}. \quad (12)$$

The stress-strain curves of the free-standing NiTi thin film were obtained from the experimental stress-strain curves of copper substrate together with the thin film adherent to the substrate compared with the stress-strain curves of copper substrate without film. These are shown in Fig. 1. The total flow stress was about 160 MPa. Fig. 2 shows the microstructures of the thin film after heat treatment. The grain size was estimated to be 1.5 μm. For NiTi alloy [12], $\mu_{\text{f}} = 27 \times 10^3$ MPa, $b = 0.2596$ nm, $\upsilon = 0.28$. From Equation 12, the Hall-Patch coefficient was calculated, $k = 205$ MPa $\mu\text{m}^{1/2}$. Ishida [13] showed that the total flow stress of Ti-51.5 at%Ni thin film was about 600 MPa at 317 K, $h = 8\ \mu$m, $d = 0.5\ \mu$m. The Hall-Patch coefficient was calculated to be 383 MPa·$\mu\text{m}^{1/2}$ from Equation 12. It seems that the Hall-Patch coefficient decreases with increasing film thickness which agrees with Venkatraman's work [6].

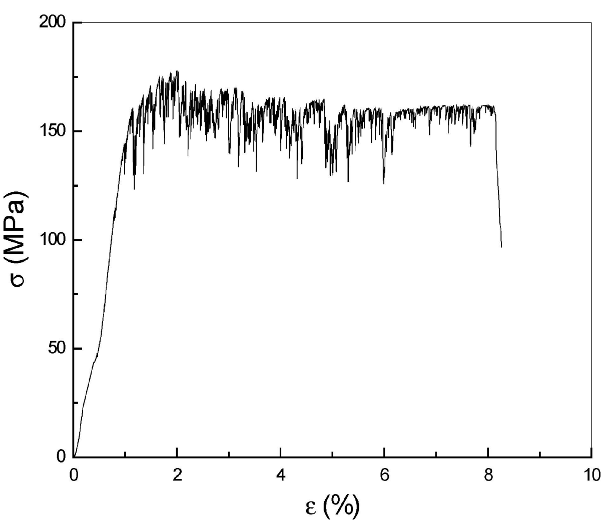

Figure 1 stress-strain curve of free-standing NiTi thin film.

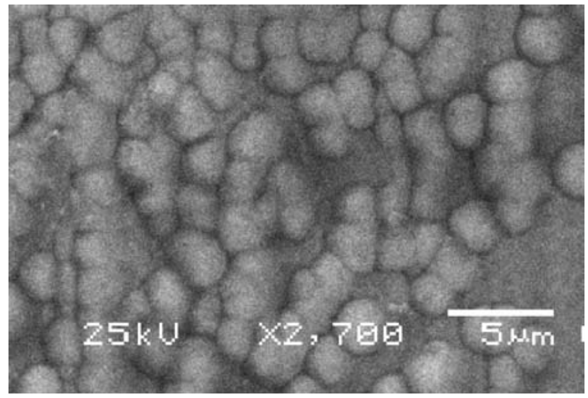

Figure 2 SEM micrographs of NiTi thin film.

Acknowledgments
The supports from National Doctorate Fund and Science and Technology Committee of Jilin Province are highly appreciated.

References
1. S. MIYAZAKI, Y. OHMI and K. OTSUKA, *J. Phys. (France)* **43** (1982) C4-255.
2. S. MIYAZAKI, in "Engineering Aspects of Shape Memory Alloys," edited by T. W. Duerig, K. N. Melton, D. Stockel and C. M. Wayman (Butterworth-Heinemann, Guildford, UK, 1990), p. 394.
3. S. MIYAZAKI and K. Otsuka, *ISIJ Int.* **29** (1989) 353.
4. J. E. SANCHEZ and E. ARZT, *Scripta Metall. Mater.* **27** (1992) 285.
5. A. J. GRIFFIN, F. R. BROTZEN and C. DUNN, *Scripta Metall.* **20(9)** (1986) 1271.
6. R. VENKATRAMAN and J.C. BRAVMAN , *J. Mater. Res.* **7** (1992) 2040.
7. P. RICHARD and J. J. VLASSAK, *Annu. Res. Mater. Sci.* **26** (1996) 431.
8. C. V. THOMPSON, *J. Mater. Res.* **8** (1993) 237.
9. W. D. NIX, *Metall. Trans.* **20A** (1989) 2217.
10. L. B. FREUND, *J. Appl. Mech.* **54** (1987) 553.
11. R. MADDIN and N. K. CHEN, *Progr. Met. Phys.* **5** (1954) 53.
12. F. SHAN, Y. HUO, F. TENG and Y. WANG, *Rare Metal. Mater. Engng. (Chinese)* **27** (1998) 199.
13. A. ISHIDA, M. SATO, T. KIMURA and S. MIYAZAKI, *Philosoph. Mag.* A **80** (2000) 967.

Received 2 May 2003
and accepted 3 June 2004