Development of SMA Thin Film with Buffer Layer for Liquid Transportation Medical Device

Kazuyoshi Tsuchiya[1], Takehiro Sato [1] and Sam Davies[2]
[1] *Department of Precision Engineering, Tokai University, 4-1-1 Kitakaname, Hiratsuka, Kanagawa, 259-1292, Japan*
[2] *School of Engineering University of Warwick, CV4 7Al, UK*

esrmr@keyaki.cc.u-tokai.ac.jp

Abstract

In the design of TiNi SMA actuators, it is known that the selection of buffer layer influences crystal structure growth during the thin film deposition process so that TiNi SMA thin films can be epitaxially grown when the lattice parameter mismatch between a thin film and an buffer layer is small. In this study, a technique to control the strain in TiNi SMA thin films by optimum choice of buffer layer for matching lattice constants and to grow TiNi(110) which shows excellent shape recovery effect was investigated. Buffer layers of Nb, Mo, Ta, and W were selected for this investigation. Firstly, the number of atomic contact points between atoms on the thin film and those on the buffer layer were calculated corresponding to a given crystallographic orientation between the two. Secondly, TiNi films were deposited on various buffer layers by the ECR sputter deposition method on the SiO_2 substrate. Strains induced in the films by lattice constant mismatch with each buffer layer were also calculated from the shifted angles of diffraction based on ICDD (International Centre for Diffraction Data) database after XRD analysis. In conclusion, the number of atomic contact points between thin film and buffer layer seemingly influences the lattice constant to sufficiently induce strain into the film to grow TiNi(110) on the buffer layer and the X-ray intensity for TiNi(110) can be changed by the strain. Therefore, it is suggested that selectively changing such contact points by choice of appropriate buffer layers will enable strain in TiNi SMA thin films to be controlled.

1 Introduction

TiNi shape memory alloy (SMA) as a microactuator for a micropump in blood extraction has been investigated[1]. In a TiNi SMA actuator designing, the shape

memory effects as actuator properties such as output power, repeatable characterization, transformation temperature, depend on the chemical composition of TiNi SMA, are important. Moreover, it is changed by the strain generated in the heat treatment for crystalline growth[2]. And also, it is known that the selection of buffer layer influences the crystal plane to grow TiNi(110) which shows excellent shape recovery effect[3] in the thin film process. In this study, a technique to control the strain in the TiNi SMA thin film by the lattice constant of the optimized buffer layer for the deposition of the TiNi SMA thin film is investigated. First of all, TiNi films are deposited on various buffer layers, selected from the view point of the biocompatibility and the coefficient of thermal expansion, on the SiO_2 substrate. And the XRD intensity for TiNi with strain in the thin film deposited on an optimized buffer layer to control TiNi(110) crystal structure is evaluated by XRD and these strains in the films by changed lattice constants are also calculated from the sifted incident angles based on ICDD.

2 Selection of buffer layer and strain between selected buffer layer and deposited TiNi

The conditions for the buffer layer which must be satisfied are (1) biocompatibility for medical use, and (2) thermal expansion coefficient between Si and TiNi for prevention of peeling thin film from the substrate. Table 1 shows those thermal expansion coefficients and lattice constants. Here, SiO_2/Si(100) as a substrate was selected and the SiO_2 was 300 nm thickness. As the result, Nb, Mo, Ta, W and Pt were qualified as a candidate buffer layer of TiNi. Table 2 shows the ECR sputtering conditions for each buffer layer deposition and the substrate temperature is 600 degrees C to crystallize for buffer layer. Here, in this research, the thickness for buffer layer was fixed as 150 nm. According to FE-SEM results, it seems that Pt particles at surfaces on SiO_2 were diffused, therefore it must be difficult to control the lattice constant for TiNi by the buffer layer. Therefore, Nb, Mo, Ta and W are the candidates for TiNi buffer layer. Next, TiNi thin films were deposited on each buffer layers by using TiNi target changed in vacuumed chamber after buffer layers was deposited under the same sputtering conditions as for buffer layer shown in Table 2. TiNi thin films on each buffer layers were evaluated by XRD and the changed lattice constants calculated from the sifted incident angles based on ICDD (International

Centre for Diffraction Data). As the result, it is confirmed that the relationship between XRD intensities (Nb, Mo, Ta and W = 802, 597, 705 and 766 cps) and lattice constant changes (Nb, Mo, Ta and W = 0.380, 0.433, 0.413 and 0.370 deg) shows strong negative correlations (r=-0.927).

Table1: Properties for TiNi and various buffer layer materials.

	TiNi	Nb	Mo	Ta	W	Pt
a	2.885	3.303	3.1472	3.306	3.1648	3.9231
b	4.12	3.303	3.1472	3.306	3.1648	3.9231
c	4.622	3.303	3.1472	3.306	3.1648	3.9231
α	90°	90°	90°	90°	90°	90°
β	96.8°	90°	90°	90°	90°	90°
γ	90°	90°	90°	90°	90°	90°
Crystal structure	Monoclinic	Cubic (BCC)	Cubic (BCC)	Cubic (BCC)	Cubic (BCC)	Cubic (FCC)
CTE(10^{-6}/K)	10	7.1	4.8	6.5	4.3	8.9

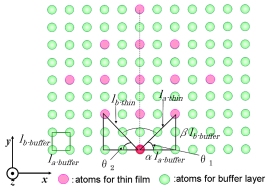
Table 2: Sputtering conditions for buffer layers deposition.

Target	Nb	Mo	Ta	W	Pt
Sputtering Time (min)	41	36	59	72	24
Film thickness (nm)	150				
Ar gas flow rate (sccm)	0.6				
Micro wave power (W)	100				
Vaccum pressure (Pa)	5×10^{-3}				
Accelerating voltage (eV)	2000				
Substrate	SiO_2/Si(100)				
Substrate temperature (deg C)	600				

3 Mismatch rate calculation

Mismatch rate for lattice constants was defined as a difference of lattice constants between substrate and thin film. When mismatch rate is small, it has an advantage that the thin film can be epitaxially grown. Here, the lattice constant for thin film is defined as l_{thin} and the lattice constant for buffer layer is defined as l_{buffer}. In general, the mismatch rate is described as the difference between lattice constants for each unit cells, under the ideal condition, shown in Equ.(1). In this study, the mismatch rates for some unit cells were calculated including consideration of thin film rotation. Here, the crystal structure can be also grown on buffer layer at a rotated angle against the lattice axis for a buffer layer, shown in Fig.2. For example, one lattice length (for example $l_{a\text{-}buffer}$ on the lattice axis in the direction of <100>) with several fold ("α" or "β") bond length (minimum length of lattice) on lattice axis was defined as basic length for buffer layer in Fig.2, and the lattice axis is rotated at the angle of θ_1 to bond the atoms for thin film. Therefore, the actual lattice length is shown in Equ.(3). The other lattice length l_{thin} with several fold ("m" or "n") bond length on lattice axis was defined as basic length for TiNi thin film, and the mismatch rates for some unit cells were calculated by the Equ.(2), where α, β, m and n are 2, 2, 1 and 1, respectively. By using equations shown above, the contact points for atoms between substrate and buffer layer were counted under the all possible lattice plane combinations between buffer layer and TiNi thin film shown in Table 3, where the mismatch rate is less than 1 %, as maximum numbers for "α", "β", "m" and "n" of bond length on lattice axis were defined as 25. Table 4 shows the results. As the result, the numbers for contact

points of TiNi on Mo were the largest, on the other hand, the numbers for contact points of TiNi on Nb were the smallest. Table 4 shows the XRD intensities for TiNi deposited on various buffer layers and the calculated contact points satisfied lattice mismatch rate under 1 %. The relationship between XRD intensities and the contact points for atoms between buffer layer and TiNi thin film with one lattice length with several fold bond length on lattice axis shows negative correlations. Therefore, it is suggested that the changing contact points by buffer layer can control the strain in TiNi SMA thin film.



$$\varepsilon = \frac{l_{thin} - l_{buffer}}{l_{buffer}} \times 100[\%] \quad \cdots \text{Equ.(1)}$$

$$\varepsilon = \frac{m \times l_{a-thin} - n \times \sqrt{(\alpha \times l_{a-buffer})^2 + (\beta \times l_{b-buffer})^2}}{n \times \sqrt{(\alpha \times l_{a-buffer})^2 + (\beta \times l_{b-buffer})^2}} \times 100[\%]$$

$$l_{buffer} = \sqrt{(\alpha \times l_{a-buffer})^2 + (\beta \times l_{b-buffer})^2} \quad \cdots \text{Equ.(2)} \quad \cdots \text{Equ.(3)}$$

Figure 2: Image of thin film(001) on buffer layer(001)[bcc].

Table3: Correlation coefficient between contact point and TiNi intensity.

	TiNi on Nb	TiNi on Mo	TiNi on Ta	TiNi on W
Contact points satisfied lattice mismatch rate under 1%	1043	1338	1059	1247
TiNi all intensity[cps]	802	597	705	766
Correlation coefficient between contact point and TiNi intensity	-0.664714154			

Table4: Combination of TiNi thin film and buffer layers plane direction.

Buffer layer plane direction	TiNi thin film plane direction
[100]	[100],[010],[001],[110],[101],[011],[-101],[111],[1-11]
[110]	[100],[010],[001],[110],[101],[011],[-101],[111],[1-11]
[111]	[100],[010],[001],[110],[101],[011],[-101],[111],[1-11]

4 Conclusion

In this study, a technique to control the strain in the TiNi SMA thin film by the lattice constant of the optimized buffer layer to improve shape memory effect for TiNi is proposed. It is suggested that the changing contact points by buffer layer can control the strain in TiNi SMA thin film.

References:

[1] Kazuyoshi Tsuchiya *et.al.*, Biomedical Microdevices 7:4, pp.347-353(2005).

[2] K. Tsuchiya, and T. Sato, Proceedings of IEEE Conference on Optoelectronic and Microelectronic Materials and Devices 2010, pp.193-194(2010).

[3] H. Inoue, N. Miwa and N. Inakazu, Acta mater., 44, pp.4825-4834(1996).