1P1-9

Elastic constant of alpha and beta tungsten films studied by picosecond ultrasonics

ピコ秒超音波法を用いたタングステン薄膜の弾性率計測

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1. Introduction

Tungsten thin films are widely used for many applications such as transition edge sensors,[1] diffusion barriers and adhesion layers in semiconductor fabrication,[2] masks for X-ray lithography,[3] soft X-ray mirrors,[4] and so on. Especially, due to high mechanical strength and heat resistance, tungsten is also used as mechanical tools and nuclear fusion reactors. For these applications, structure of tungsten is important. Tungsten naturally shows thermally stable body centered cubic structure (α-W) as shown in **Fig. 1(a)**. However, thin-film tungsten often shows meta-stable A15 structure (β-W) as shown in Fig. 1(b), which plays important roles in the properties and functions of tungsten films. For example, superconductive transition temperature of β-W is about 3 K[6] while that of α-W is lower than 70 mK.[1] β-W also exhibits large spin Hall angle which reaches 0.5[7] whereas that of α-W is less than 0.07.[8]

Although the relationship among the deposition conditions, structures, and some electric properties have been investigated, their mechanical properties remain unclear. Previous studies suggest that β-W films often include oxygen.[9-14] For nuclear fusion reactors and other mechanical tools, the surface properties of tungsten are the most important. Therefore, in this study, we measure the elastic constant of tungsten thin films deposited under various conditions, and measure their elastic constants by picosecond ultrasonics. Moreover, we calculate the elastic constants of alpha and beta tungsten by using the density functional theory.

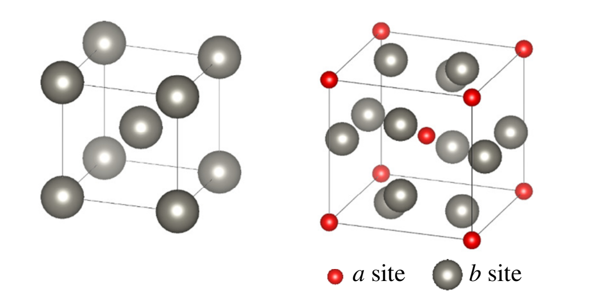

Fig. 1 The structure of (a) α-W and (b) β-W.

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2. Sample deposition and film structures

We deposited tungsten thin films by DC sputtering methods on Si (111) substrates. We changed the Ar pressure P_{Ar} between 0.2 and 2.7 Pa to control the structure. Sputtering power is 150 or 30 W.

We measure the film structures by the X-ray reflection (XRR) and X-ray diffraction (XRD) methods using a Co target. By comparing the calculated and measured reflectivity in a low incident angle region, we can determine the film thickness d, roughness and mass density ρ from the oscillation period, oscillation amplitude, and critical angle, respectively. The tungsten structure is estimated from the XRD spectra. **Figure 2** shows typical XRR and XRD spectra for an α-W film deposited under P_{Ar} = 0.2 Pa. The calculated reflectivity agrees well with the measurement result, resulting in the film thickness d = 46.0 nm and the same mass density as the reported

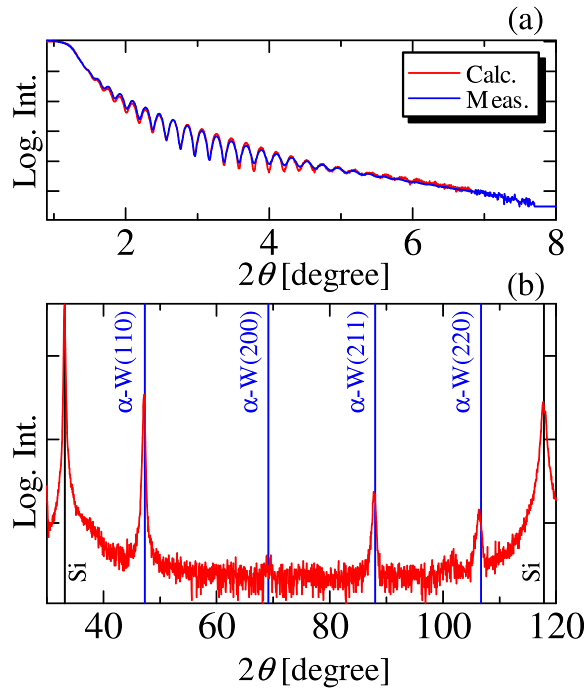

Fig. 2 (a) XRR and (b) XRD spectra for an α-W film.

bulk value. We observed all of the diffraction peaks from α-W in Fig. 2(b), which suggests that the film is isotropic pure α-W including no β-W. We also synthesized pure β-W thin films.

2. Elastic constants

We measured elastic constants of thin films by using the picosecond ultrasonics,[15,16] which excites and detects sub-THz ultrasound by fs pulse light. **Figure 3** shows typical observed acoustic resonances of the through-thickness modes for a thin film and pulse echoes for a thick film. From the film thickness and resonance frequencies or the travel time of the echoes, we determined longitudinal sound velocity v and corresponding elastic constants $C=\rho v^2$.

The elastic constants of pure α-W and β-W are 5–10% lower than a reported bulk value for α-W.[17] Thin films often exhibit lower stiffness due to many defects or large strain.[18] Since the elastic constants of β-W have not been reported, we calculate those of α-W and β-W by using the density functional theory with the Vienna Ab initio simulation packages (VASP). The calculated lattice parameter and elastic constants of α-W agree well with reported values[17,19] within 0.3 and 7% deviation, respectively. The lattice parameter of β-W agrees with reported value within 0.5% deviation, too. Our measured and calculated elastic constants of β-W agree within 10% deviation, therefore, we succeeded in determining the elastic constants of β-W.

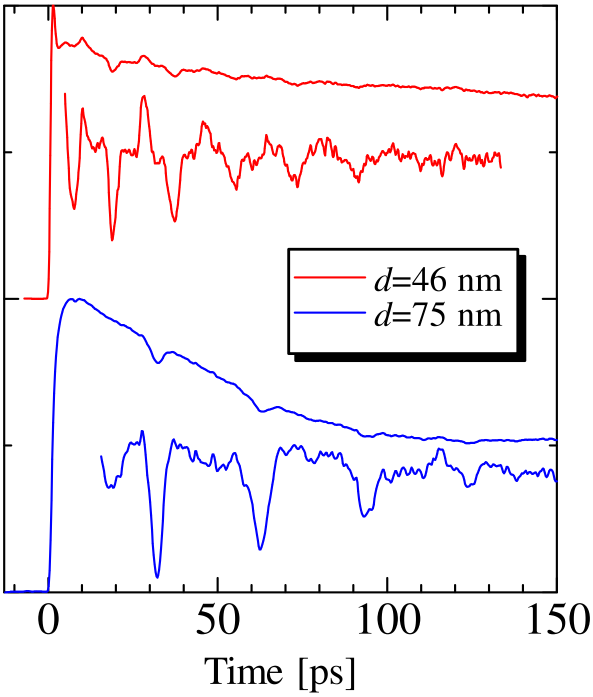

Fig. 3 Observed acoustic resonances and pulse echoes for thin (d=46 nm) and thick (d=75 nm) films, respectively.

References

1. A. E. Lita, D. Rosenberg, S. Nam, A. J. Miller, D. Balzar, L. M. Kaatz, and R. E. Schwall, IEEE T. Appl. Supercon. **15** (2005) 3528.
2. S. M. Rossnagel, I. C. Noyan, and and C. Cabral, J. Vac. Sci. Technol. B **20** (2002) 2047.
3. M. Itoh, M. Hori, and S. Nadahara, J. Vac. Sci. Technol. B **9** (1991) 149.
4. T. Salditt, D. Lott, T. H. Metzger, J. Peisl, G. Vignaud, P. Hoghoj, O. Scharpf, P. Hinze, and R. Lauer, Phys. Rev. B **54** (1996) 5860.
5. J. E. Hirsch, Phys. Rev. Lett. **83** (1999) 1834.
6. W. L. Bond, A. S. Cooper, K. Andres, G. W. Hull, T. H. Geballe, and B. T. Matthias, Phys. Rev. Lett. **15** (1965) 260.
7. K. U. Demasius, T. Phung, W. Zhang, B. P. Hughes, S. H. Yang, A. Kellock, W. Han, A. Pushp, and S. S. P. Parkin, Nat. Commun. **7** (2016) 10644.
8. C. F. Pai, L. Liu, Y. Li, H. W. Tseng, D. C. Ralph, and R. A. Buhrman, Appl. Phys. Lett. **101** (2012) 122404.
9. G. Hagg. N. Schonberg, Acta Cryst. **7** (1954) 351.
10. P. Petroff, T. T. Sheng, A. K. Sinha, G. A. Rozgonyi, and F. B. Alexander, J. Appl. Phys. **44** (1973) 2545.
11. I. A. Weerasekera, S. I. Shah, D. V. Baxter, and K. M. Unruh, Appl. Phys. Lett. **64** (1994) 3231.
12. Y. G. Shen and Y. W. Mai, J. Mater. Sci. **36** (2001) 93.
13. N. Radica, A. Tonejc, J. Ivkov, P. Dubcek, S. Bernstorff, and Z. Medunic, Surf. Coat. Technol. **180** (2004) 66.
14. K. Salamon, O. Milat, N. Radic, P. Dubcek, M. Jercinovic, and S. Bernstorff, J. Phys. D **46** (2013) 095304.
15. C. Thomsen, J. Strait, Z. Vardeny, H. J. Maris, and J. Tauc, Phys. Rev. Lett. **53** (1984) 989.
16. H. Ogi, M. Fujii, N. Nakamura, T. Yasui, and M. Hirao, Phys. Rev. Lett. **98** (2007) 195503.
17. F. H. Featherston and J. R. Neighbours, Phys. Rev. **130** (1963) 1324.
18. N. Nakamura, H. Ogi, T. Yasui, M. Fujii, and M. Hirao, Phys. Rev. Lett. **99** (2007) 035502.
19. F. C. Nix and D. MacNair, Phys. Rev. **61** (1942) 74.