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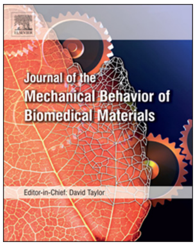

Short Communication

Origin of ultralow Young's modulus in a metastable β-type Ti–33Nb–4Sn alloy

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ABSTRACT

Although there is difficulty in growing a Ti–33Nb–4Sn single crystal due to its ultralow β-phase stability, the single-crystal elastic constants of metastable β-type Ti–33Nb–4Sn (wt%) alloy were extracted successfully from its polycrystal by in-situ synchrotron X-ray diffraction technique, to clarify the origin of the ultralow Young's modulus in its polycrystal. It is indicated that compared to binary TiCr, TiV and TiNb alloys, the Ti–33Nb–4Sn alloy possesses slightly lower β-phase stability with respect to $\{110\}<1\bar{1}0>$ shear (i.e., C') but much lower β-phase stability regarding to $\{001\}\langle 100\rangle$ shear (i.e., C_{44}). An analysis by the Hill approximation suggests that the ultralow isotropic polycrystalline Young's modulus (E_H) of Ti–33Nb–4Sn alloy originates from the extremely low shear modulus C_{44} as well as the relatively low C'. This indicates that in addition to C', C_{44} has a significant contribution to the Young's modulus of polycrystal, which challenges a conventional understanding that the Young's modulus of β-type Ti alloys is predominantly determined by C'.

1. Introduction

Titanium and its alloys have been widely used for hard tissue replacement materials due to their excellent biocompatibility, high corrosion resistance and good mechanical properties, especially relatively low Young's modulus (Geetha et al., 2008; Hao et al., 2007a, 2007b; Saito et al., 2003). Among the mechanical properties necessary for implant materials, Young's modulus is generally considered to be of dominant importance, because implant failure can occur due to the mismatch in Young's modulus between the implant materials and nature human bone (Geetha et al., 2008; Ho et al.,

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1999). As is well known, the most widely used Ti implant material, (α+β) type Ti–6Al–4V, exhibits a Young's modulus of ~110 GPa, which is much higher than that of human bone (~30 GPa) (Geetha et al., 2008). Thus, in the past few decades, much research effort has been devoted to the development of metastable β-type Ti alloys with lower Young's modulus, such as Ti–Mo (Oliveira et al., 2007), Ti–Nb–Ta–Zr (Morris et al., 2010), Ti–Nb–Zr–Sn (Hao et al., 2007a, 2007b), etc. Currently, β-type Ti alloys designed for hard tissue replacement have Young’s moduli in the range of 50–80 GPa, which still cannot match perfectly with human bone. Quite recently, a metastable β-type Ti–33Nb–4Sn (wt%) alloy, consisting entirely of non-cytotoxic elements, was fabricated by the present authors for biomedical applications (Guo et al., 2015). Upon cold deformation plus short-time annealing, this alloy can show an ultralow tensile Young's modulus of 36 GPa. This level of Young's modulus is the lowest ever recorded for the currently available biomedical Ti alloys, and is only ~6 GPa higher than that of human bone (Guo et al., 2015). However, the origin of the ultralow Young’s modulus in the Ti–33Nb–4Sn alloy has not yet been clarified in detail, although an in-depth understanding of this issue may provide a clear design concept for further decreasing the Young’s modulus in metastable β-type Ti alloys.

Previous investigations showed that the Young's moduli of polycrystalline body-centered cubic (bcc) metals are closely related to their single-crystal elastic constants (SECs), i.e., C_{11}, C_{12}, and C_{44} (Hill, 1952). As far as β-type Ti alloys with bcc structure, shear modulus C', which is equivalent to $(C_{11}-C_{12})/2$ and represents the stability of β phase with respect to $\{110\}<1\bar{1}0>$ shear, was once considered as the most important factor controlling the Young's modulus of polycrystal (Zener, 1947), because the Young's modulus decreases with decreasing the β-phase stability (Abdel-Hady et al., 2006; Guo et al., 2014). Thus, previous studies were mainly focused on clarifying the key role of shear modulus C' on the Young's moduli of polycrystalline β-phase Ti alloys (Hu et al., 2008; Obbard et al., 2011; Tegner et al., 2012). Actually, from the viewpoint of crystallography, in addition to C', C_{44} should also be considered as a key parameter for evaluating β-phase stability, since C_{44} represents resistance to $\{001\}\langle 100\rangle$ shear (Otsuka and Ren, 2005), being similar to C' corresponding to $\{110\}<110>$ shear. Therefore, the possible contribution of C_{44} to Young’s modulus of metastable β-type Ti alloys should be taken into account.

Generally, the elastic constants of β-type Ti alloys, i.e., C_{11}, C_{12}, and C_{44}, can be obtained by measuring their corresponding single crystals using resonant ultrasound spectroscopy and/or electromagnetic acoustic resonance (Hermann et al., 2012). However, although many Ti single crystals have been grown successfully in binary β-type Ti alloys (Ahlberg et al., 1978; Hermann et al., 2012), it is still difficult or even impossible to grow single crystals for ternary or quaternary β-type Ti alloys, especially for Ti–33Nb–4Sn alloy. The difficulties in growing a Ti–33Nb–4Sn single crystal lie in the following two aspects: on one hand, the Ti–33Nb–4Sn alloy exhibits a mixture of β- and α"- phases in the solution treated state due to its ultralow β-phase stability caused by low content of β stabilizers; on the other hand, severe cold deformation plus short-time annealing is necessary for Ti–33Nb–4Sn alloy to achieve ultralow Young’s modulus (Guo et al., 2015).

Previous studies have revealed that the valence electrons per atom (*e/a* ratio) have a dominant influence on the elastic constants (Lee et al., 2012; Tane et al., 2008). The *e/a* ratio is the valence based on the total d plus s electrons in the free atom configuration and corresponds to the position of Fermi level (Ikehata et al., 2004). Generally speaking, the *e/a* ratio is determined by the type and content of β stabilizers and increases with the increasing amount of β stabilizers (Hao et al., 2007a, 2007b). In binary β-type Ti alloys, shear modulus C' and bulk modulus *B* decrease with decreasing *e/a* ratio while the shear modulus C_{44} keeps almost unchanged, thus it is obvious that the Young's modulus can be reduced by decreasing *e/a* ratio (Tane et al., 2010). Therefore, it is helpful to investigate the relationship between the SECs and *e/a* ratio so as to elucidate the cause of low Young's modulus and finally reduce the Young's modulus of β-type Ti alloys. In the study, an attempt was made to extract the SECs of metastable β-type Ti–33Nb–4Sn alloy from its polycrystal by in-situ synchrotron X-ray diffraction technique and Eshelby–Kroner–Kneer elastoplastic self-consistent (EPSC) model (Talling et al., 2008). Compared with the dependence of SECs on *e/a* ratio in binary β-type alloys, the origin of ultralow Young's modulus in a metastable β-type Ti–33Nb–4Sn alloy was discussed.

2. Experimental procedure

An ingot with a nominal composition of Ti–33Nb–4Sn (wt%) was arc melted in an argon atmosphere using high purity Ti (99.99%), Nb (99.95%) and Sn (99.95%). The ingot was homogenized, forged and then solution treated at 1073 K for 1 h, followed by quenching into water (~298 K). The test samples that were spark cut from the solution treated billet will be denoted as ST specimens henceforth. The ST billet was cold rolled at a thickness reduction of 87%, and then annealed at 673 K for 20 min followed by quenching into water. These resultant specimens will be referred to as CRA specimens henceforth. A more detailed description of fabricating Ti–33Nb–4Sn alloy can be seen in our previous reference (Guo et al., 2015).

X-ray diffraction (XRD) measurements were performed by a Rigaku D/max 2550 diffractometer with Cu Kα radiation. The texture of β phase was also characterized by XRD and the data were dealt with using preferred orientation package from Los Alamos National Laboratory. Microstructure observation was conducted on a FEI Tecnai F20 transmission electron microscope (TEM). Uniaxial tensile test was performed along the rolling direction, using an Instron-8801 testing system at a strain rate of $1\times10^{-3}\,s^{-1}$. The in-situ synchrotron X-ray experiments were conducted on the 11-ID-C beam-line of Advanced Photon Source at Argonne National Laboratory, and the data were obtained from a ±5° region for grains with crystal planes perpendicular to the loading direction.