



Full length article

Microscopic study of gum-metal alloys: A role of trace oxygen for dislocation-free deformation



Naoyuki Nagasako^{a,*}, Ryoji Asahi^a, Dieter Isheim^{b,c}, David N. Seidman^{b,c},
Shigeru Kuramoto^{a,1}, Tadahiko Furuta^a

^a Toyota Central Research and Development Laboratories, Inc., Nagakute, Aichi 480-1192, Japan

^b Department of Materials Science and Engineering, Northwestern University, 2220 Campus Drive, Evanston, IL 60208, United States

^c Northwestern University Center for Atom-Probe Tomography (NUCAPT), 2220 Campus Drive, Evanston, IL 60208, United States

ARTICLE INFO

Article history:

Received 15 May 2015

Received in revised form

2 October 2015

Accepted 6 December 2015

Available online xxx

Keywords:

First-principles calculation

Three-dimensional atom-probe tomography

Dislocation-free deformation mechanism

Ti alloys

ABSTRACT

A class of Ti–Nb–Ta–Zr–O alloys called gum metal are known to display high strength, low Young's modulus and high elastic deformability up to 2.5%, simultaneously, and considered to deform by a dislocation-free deformation mechanism. A trace of oxygen (~1%) in gum metal is indispensable to realize such significant properties; however, the detailed mechanism and the role of the oxygen has not been understood. To investigate an effect of trace oxygen included in gum metal, first-principles calculations for gum-metal approximants including zirconium and oxygen are performed. Calculated results clearly indicate that oxygen site with less neighboring Nb atom is energetically favorable, and that Zr–O bonding has an important role to stabilize the bcc structure of gum metal. The three-dimensional atom-probe tomography (3-D APT) measurements for gum metal were also performed to identify compositional inhomogeneity attributed to the trace elements. From the 3-D APT measurements, Zr ions bonding with oxygen ions are observed, which indicates existence of Zr–O nano-clusters in gum metal. Consequently, it is found that (a) coexistence of Zr atom and oxygen atom improves elastical stability of gum metal, (b) inhomogeneous distribution of the compositions induced by the trace elements causes anisotropical change of shear moduli, and (c) Zr–O nano-clusters existing in gum metal are expected to be obstacles to suppress movement of dislocations.

© 2015 Acta Materialia Inc. Published by Elsevier Ltd. All rights reserved.

1. Introduction

The dislocation theory [1–3] has long been considered to be a standard mechanism to explain plastic deformation of metals, namely, why yield strength is about one-fifth to one-tenth lower than ideal strength. However, in the last decade, several materials whose properties can not be understood by the conventional deformation theory have been found [4–6]. Among them, a class of Ti–Nb–Ta–Zr–O alloys called "gum metal", whose typical composition is Ti–23Nb–0.7Ta–2Zr–1.2O in atomic %, are known to display high strength, low Young's modulus, simultaneously, which have been considered to be conflicting properties in metallic materials. In addition, elastic anormal properties of gum metal

including high elastic deformability up to 2.5%, Inver property and Elinvar property, have attracted a great deal scientific and industrial interests [4].

In our previous first-principles calculations [7], we investigated composition dependence of elastic properties systematically for D0₃-type TiX₃, TiX₃, and B2-type TiX ordered binary alloys, where X = V, Nb, Ta, Mo and W, to clarify an origin of the low Young's modulus of gum metal. As a result, vanishing of the tetragonal elastic constant $C'=(C_{11}-C_{12})/2$ was found to be a key to develop the low Young's modulus and, simultaneously, the high elastic deformability in gum metal. In addition, it was also found that vanishing of C' can be achieved by controlling compositions of gum metal such that composition-averaged valence-electron concentration per atom (e/a) is close to 4.24. Actually, it was experimentally confirmed that Young's modulus and elastic deformability are drastically lowered and improved, respectively, when e/a is controlled to be around 4.24 [4].

As already known, in body-centered-cubic (bcc) metals, ideal

* Corresponding author.

E-mail address: nagasako@mosk.tytlabs.co.jp (N. Nagasako).

¹ Present address: Department of Mechanical Engineering, Ibaraki University, Hitachi, Ibaraki 316-8511, Japan.

strength τ_{max} can be roughly estimated from the shear modulus G according to the empirical formula [8],

$$\tau_{max} \approx 0.11G = 0.11 \times \frac{3C_{44}(C_{11} - C_{12})}{C_{11} - C_{12} + 4C_{44}}. \quad (1)$$

In short, vanishing of C' implies a possibility of significant reduction of the ideal strength.

Based on the possibility of small ideal strength and several experimental observations, we have proposed a dislocation-free plastic deformation mechanism [4,6,9] to explain the properties of gum metal. In the dislocation-free deformation mechanism, materials are considered to be able to deform near their ideal strength under the two conditions below: (1) ideal strength itself becomes significantly small due to elastic softening only along a certain direction, and (2) some kinds of obstacle prevents moving of dislocations under the condition that ideal strength is kept to be small. As a result, elastic deformation is assumed to occur until load stress reaches ideal strength and then plastic deformation suddenly occurs nearly ideal strength.

To verify if gum metal actually deforms by the dislocation-free deformation mechanism, it is important to know the both yield strength and ideal strength of gum metal. Our recent first-principles calculations [10,11] showed that G1-type $Ti_{12}Nb_4$ structure featured with Nb–Nb chain along [111] direction is better gum-metal approximant than the previously used $D0_3$ -type model (see Fig. 1). Then, ideal strength of G1-type $Ti_{12}Nb_4$ for $\langle 111 \rangle \{211\}$ shear deformation was predicted to be 1.65 GPa from calculated stress–strain curve [11].

On the other hand, yield strength of gum metal was measured by an in-situ nano-indentation experiment [12] with gum-metal nanopillars, which were confirmed to consist of single grain and had no dislocations by the transmission electron microscopy. As a result, nanopillar strength of gum metal was found to be 1.75 GPa,

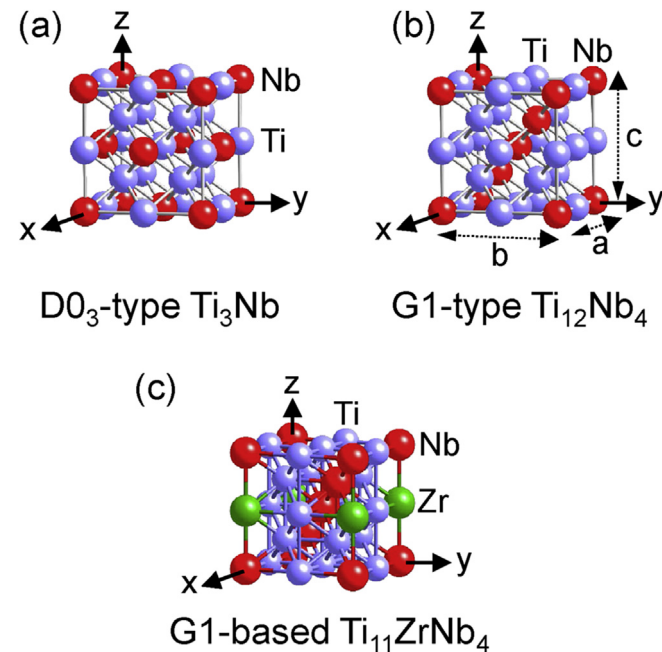


Fig. 1. Crystal structures assumed in the present calculations. (a) $D0_3$ -type Ti_3Nb , (b) G1-type $Ti_{12}Nb_4$, and (c) G1-based $Ti_{11}ZrNb_4$. The blue, red, green and black spheres indicate Ti, Nb, Zr and O atoms, respectively. Figures (a) and (b) adapted with permission from Ref. [11]. Copyrighted by the American Physical Society. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

which agrees well with the predicted ideal strength of the G1-type $Ti_{12}Nb_4$.

In addition to lowering of ideal strength, some kinds of obstacle which prevents moving of dislocations have to exist to deform near ideal strength. From several experimental results, trace elements included in gum metal such as Ta, Zr and O have been considered to have important roles as such an obstacle. For instance, the X-ray absorption fine structure (XAFS) measurements [4] indicated that trace oxygen does not exist near Nb atoms but exists near Zr atoms. The small-angle X-ray scattering (SAXS) analysis [13] showed that inhomogeneous distribution of the compositions less than 1 nm in size exists in gum metal although actual local structure has not yet been identified.

So far, Several experimental measurements [9,12,14–19] and theoretical calculations [7,10,11,20–23] have been reported. The effects of trace oxygen in gum metal have already been investigated experimentally by Tane et al. [24,25]. They clarified temperature dependence of the elastic constants of single crystalline gum metals and influence of the amount of trace oxygen on the elastic properties. They suggested that oxygen addition to gum metal suppresses a creation of the ω and the α'' phases. On the other hand, Takesue et al. clarified that single-crystalline gum metal containing trace oxygen undergo extensive transformation during loading along $\langle 110 \rangle$ direction [18]. In addition, Morris et al. performed a theoretical investigation for such an extensive transformation [19]. Tahara et al. investigated effect of trace oxygen in Ti–Nb binary alloys and suggested a mechanism to explain superelasticity in β -Ti–Nb–O alloys [26,27]. Kim et al. investigated the microstructure of gum metal to clarify the correlation between nanodomain structure and thermal expansion behavior [28]. Recently, Dai et al. investigated an effect of trace oxygen in Ti–X (X = Nb, Zr or Sn) and Ti2448 (Ti–24Nb–4Zr–8Sn in weight %) alloys by the first-principles calculations [29]. They estimated elastic constants of Ti2448 with oxygen and concluded that oxygen has a weak effect on the elastic moduli in Ti2448.

The experimental results clearly show the importance of these trace elements. However, the detailed distributions of the trace elements and the mechanism to prevent the motion of dislocation have not yet been understood. Therefore, in the present study, we investigated effect of trace elements on phase stability and elastic properties, especially focused on oxygen, by calculating the most stable oxygen site in the G1-type $Ti_{12}Nb_4$ and its related composition, $Ti_{11}ZrNb_4$ (see Fig. 1(c)), by the first-principles calculation method. The three-dimensional atom-probe tomography (3-D APT) measurements for gum metal were also performed to identify compositional inhomogeneity attributed to the trace elements. These theoretical and experimental results lead to comprehensive discussion to understand unique mechanical properties realized in gum metal.

2. Computational methods

2.1. Total energy calculations

First-principles calculations in this study were performed with the projector augmented wave method [30,31] based on the density functional theory as implemented in the Vienna ab-initio simulation package (VASP) [32,33]. The cutoff energy for the wave function was set to be 350 eV. Occupancies of electronic states at each wave vector were determined by the first-order Hermite-Gaussian smearing method [34] with the smearing width of 0.2 eV. The integration in the reciprocal space was performed with k -point mesh of (8, 8, 8). We assumed the generalized gradient approximation for the exchange-correlation energy and potential, and adopt the functional proposed by Perdew, Burke and Ernzerhof

Download English Version:

<https://daneshyari.com/en/article/7879099>

Download Persian Version:

<https://daneshyari.com/article/7879099>

[Daneshyari.com](https://daneshyari.com)