β-Ti bio-alloys with low Young's moduli interpreted by cluster-plus-glue-atom model

β-Ti biomedical alloys with low Young's moduli require multiple alloying using both BCC stabilizers and low-E elements. I attempted to introduce the cluster-plus-glue-atom model in the composition interpretation of Ti-Zr-Mo-Nb-Sn alloys. I found out quite interesting composition rules in terms of valence electron concentration and atomic size.

Ti-based alloys are useful biomaterials for their low Young's modulus (low-E), high strength, excellent biocompatibility and corrosion resistance [1]. They usually have BCC □β-Ti structure containing multiple non-toxic elements such as Mo, Nb, Ta, Zr, etc. The alloying elements play two major roles apart from being non-toxic: stabilizing the BCC structure and decreasing the Young's modulus of β-Ti alloys.

In light of our cluster-plus-glue-atom model [2,3], we here attempt to obtain the composition formula of the low-*E* β-Ti solid solution alloys with high structural stabilities.

According to enthalpies of mixing ΔH's, the cluster-plus-glue-atom model specific to Ti-Zr-Mo-Nb-Ta-Sn BCC β-Ti alloys is proposed as $[(Mo,Sn)_1(Ti,Zr)_{14}]Nb_x$. Alloys conforming to composition formula were prepared at Dalian and the data on BCC stability and mechanical properties were collected there.

The correlations between the *E* value and elemental properties such as valence electron concentration and average atomic size were analyzed and summarized in Fig. 1.

Two conclusions can be drawn from this figure. First, all the low-*E* alloys, both ours and from the literature, are located in the same narrow region, with valence electron concentration per atom being 4.1~4.3 and average atomic size being 0.145~0.148 nm. Second, the alloys showing the lowest *E* values are further grouped towards the lower edges of the composition region. It is interesting to note that the latter zone is quite close to that of pure Ti, with valence of 4 and atomic radius of 0.146nm. This figures then points out a practical way to design Ti-based biometals with low Young's moduli, by controlling the overall valency of the alloy to about 4.1 and the average atomic radius to about 0.146-0.147nm.

Besides the research, I have visited a few professors, including Dr. W Zhang, Dr. YM Wang, Dr. Nojiri, and Dr. Nakai.. In particular, the discussion with Dr. Nakai was quite useful to guide our future alloy design work. I also gave an open seminar (Fig. 2), entitled "Composition formulas of multi-component complex alloys issued from the cluster-plus-glue-atom model", which was attended by an audience of about forty.

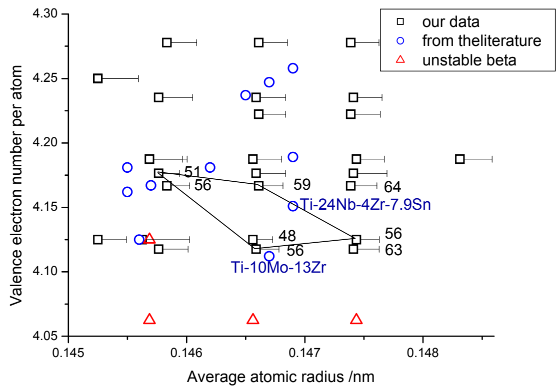

Fig. 1 Compositions of low-*E* alloys in a 2D map coordinated by valence electron concentration and atomic size. The data are both from our experiment (□) and from the literature (○). The non-BCC alloys are marked with △. The Young's moduli *E* below 65GPa are shown near the alloy compositions.

Fig. 2 NEDO Lab. Special Lecture on Nov. 29, organized by Dr. Yamaura and Dr. Zhang,

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Key Words

Ti alloys, solid solution model, Young modulus

Contact to

Chuang DONG (Dalian University of Technology, China)

E-mail: dong@dlut.edu.cn

http://mmlab.dlut.edu.cn