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First-principles Calculations of Ideal Tensile and Shear Strengths for Gum-Metal Approximants NAOYUKI NAGASAKO, Toyota Central R&D Labs., Inc., MICHAL JAHNATEK, University of Vienna, RYOJI ASAHI, Toyota Central R&D Labs., Inc., JÜRGEN HAFNER, University of Vienna — A newly developed bcc-type Ti-23Nb-0.7Ta-2Zr-O (mol%) alloy named Gum-Metal showed unusual properties including ultralow elastic modulus, ultrahigh strength, super-elastic-like behavior, and super-plastic-like behavior, in particular, accompanied by dislocation-free plastic deformation. [1]. As proposed in first-principles calculations, one of the requirements for the Gum-Metal is dramatic softening of the elastic shear modulus C'=(C11-C12)/2 $\sim$ 0, which happens at a valence electron concentration around 4.24. We also study ideal tensile and shear strengths for Gum-Metal approximants to understand microscopic origin of such unique mechanical properties. The most stable Gum-metal approximant among all the possible 1820 atomic configurations of Ti12Nb4 has been determined, and showed good agreement with the experimental elastic constants of Gum-Metal.

[1] T. Saito et al., Science 300, 464 (2003).

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