World Academy of Science, Engineering and Technology
International Journal of Materials and Metallurgical Engineering
Vol:12, No:08, 2018

The Effects of Orientation on Energy and Plasticity of Metallic Crystalline-Amorphous Interface

Authors : Ehsan Alishahi, Chuang Deng

Abstract : Commercial applications of bulk metallic glasses (BMGs) were restricted due to the sudden brittle failure mode which was the main drawback in these new class of materials. Therefore, crystalline-amorphous (C-A) composites were introduced as a toughening strategy in BMGs. In spite of numerous researches in the area of metallic C-A composites, the fundamental structure-property relation in these composites that are not exactly known yet. In this study, it is aimed to investigate the fundamental properties of crystalline-amorphous interface in a model system of Cu/CuZr by using molecular dynamics simulations. Several parameters including interface energy and mechanical properties were investigated by means of atomic models and employing Embedded Atom Method (EAM) potential function. It is found that the crystalline-amorphous interfacial energy weakly depends on the orientation of the crystalline layer, which is in stark contrast to that in a regular crystalline grain boundary. Additionally, the results showed that the interface controls the yielding of the crystalline-amorphous composites during uniaxial tension either by serving as sources for dislocation nucleation in the crystalline layer or triggering local shear transformation zones in amorphous layer. The critical resolved shear stress required to nucleate the first dislocation is also found to strongly depend on the crystalline orientation. Furthermore, it is found that the interaction between dislocations and shear localization at the crystalline-amorphous interface oriented in different directions can lead to a change in the deformation mode. For instance, while the dislocation and shear banding are aligned to each other in {0 0 1} interface plane, the misorientation angle between these failure mechanisms causing more homogeneous deformation in {1 1 0} and {1 1 1} crystalline-amorphous interfaces. These results should help clarify the failure mechanism of crystalline-amorphous composites under various loading conditions.

Keywords : crystalline-amorphous, composites, orientation, plasticity
Conference Title : ICCM 2018 : International Conference on Composite Materials
Conference Location : Amsterdam, Netherlands
Conference Dates : August 06-07, 2018