11th International Conference on Advanced Materials
Rio de Janeiro Brazil
September 20 - 25
ICAM2009

Critically-Percolated Cluster-Packed Structure in Zr-Al-Ni Bulk Metallic Glass Created with Molecular Dynamics Simulations Based on Plastic Crystal Model

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Abstract – The local atomic arrangements of a $Zr_{0.60}Al_{0.15}Ni_{0.25}$ bulk metallic glass (BMG) was studied with molecular dynamics (MD) simulations based on plastic crystal model (PCM). After a $Zr_{0.73}Ni_{0.27}$ glassy alloy that possesses critically-percolated Ni atoms had been created with atomistic MD simulation through quenching from a liquid, a $Zr_{0.618}Al_{0.146}Ni_{0.236}$ (~ $Zr_{0.60}Al_{0.15}Ni_{0.25}$) was created with MD-PCM. In MD-PCM, the Zr and Ni atoms in the $Zr_{0.73}Ni_{0.27}$ glassy alloy was replaced with randomly-oriented icosahedral and tetrahedral clusters, respectively, followed by structural relaxation after adjusting the density for the ternary alloy. The analyses revealed that the critically-percolated cluster-packed structure enhances the glass-forming ability.

Molecular dynamics (MD) simulations were performed for a $Zr_{0.618}Al_{0.146}Ni_{0.236}$ alloy to derive the general features of the local atomic arrangements of a $Zr_{0.60}Al_{0.15}Ni_{0.25}$ bulk metallic glass (BMG). The $Zr_{0.618}Al_{0.146}Ni_{0.236}$ alloy was selected due to its feature in terms of atomic fractions of the constituent elements. The $Zr_{0.618}Al_{0.146}Ni_{0.236}$ alloy can be describable as $Zr_{\phi^{-1}}Al_{\phi^{-3}}Ni_{\phi^{-4}}$ with a value of Golden Mean (ϕ ~ 1.618), which predicts the presence of a critically-percolated cluster-packed structure of icosahedral and tetrahedral clusters [1]. The present study aims to confirm this prediction by computational methods. As well as conventional atomistic MD simulations, MD simulations based on plastic crystal model (PCM) [2] were performed by utilizing the features of the model. Specifically, MD-PCM includes random rotations of hypothetical clusters around each center of gravity and subsequent structural relaxation [2]. The procedures for creating the $Zr_{0.618}Al_{0.146}Ni_{0.236}$ alloy have two steps. First, the $Zr_{0.73}Ni_{0.27}$ glassy alloy comprising 125 atoms with a density (ρ) of 7.254 Mg/m^3 was created by a conventional MD simulation through a quenching process from 2500 to 500 K under Universal Force Field (UFF) potential, the Number of atoms, Temperature, and Pressure (constant-NTP) ensemble and periodic boundary conditions, as shown in Fig. 1a, with keeping percolated Ni atom structure as demonstrated in Fig. 1b. Then, the $Zr_{0.618}Al_{0.146}Ni_{0.236}$ alloy comprising 1353 atoms with ρ of 6.53 Mg/m^3 was created from the $Zr_{0.73}Ni_{0.27}$ glassy alloy through MD-PCM under Generalized Embedded Atom Method (GEAM) potential, as shown in Fig. 1d, after the Zr and Ni atoms in the $Zr_{0.73}Ni_{0.27}$ glassy alloy had been replaced with the icosahedral and tetrahedral clusters, respectively, as illustrated in Fig. 1c from Fig. 1a. Assumptions include the presence of icosahedral and tetrahedral clusters, which comprise 13 atoms (8Zr, 3Ni and 2Al) and 5 atoms (3Zr, Ni and Al), respectively, and the ratio of their number density of the clusters being ϕ^2 : 1 [1]. The analysis with total pair-distribution functions shown in Fig. 1e revealed that a liquid-like structure containing distorted clusters forms in the $Zr_{0.618}Al_{0.146}Ni_{0.236}$ alloy after relaxation through MD-PCM (Fig. 1 d). The critically-percolated distorted tetrahedral clusters are the origin of the $Zr_{0.618}Al_{0.146}Ni_{0.236}$ alloy to be formed in BMG.

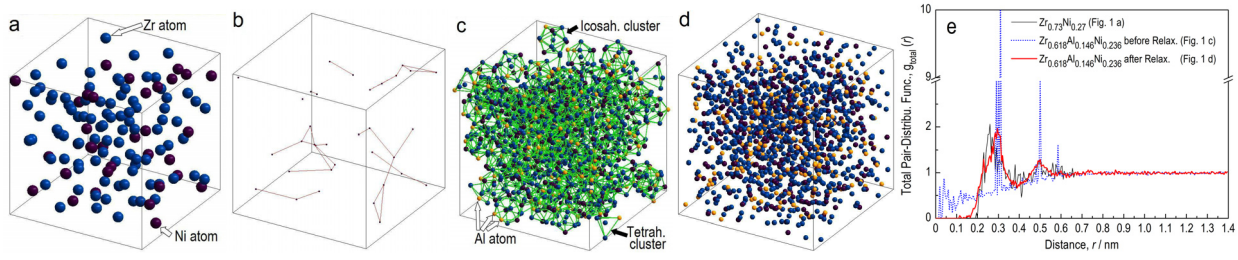

Figure 1: (a–d) Ball and stick views for arrangements of components (atoms and clusters) and (e) total pair distribution functions. **a)** The $Zr_{0.73}Ni_{0.27}$ glassy alloy, **b)** Percolated Ni atoms in the $Zr_{0.73}Ni_{0.27}$ glassy alloy in Fig. 1 a), **c)** The initial arrangements of components before structural relaxation for the $Zr_{0.618}Al_{0.146}Ni_{0.236}$ alloy, and **d)** $Zr_{0.618}Al_{0.146}Ni_{0.236}$ alloy glassy alloy created with MD-PCM. **e)** Pair-distribution functions of the $Zr_{0.73}Ni_{0.27}$ and the $Zr_{0.618}Al_{0.146}Ni_{0.236}$ alloys. The black profile corresponds to the atomic arrangemetns of the $Zr_{0.73}Ni_{0.27}$ alloy in Fig. 1 a), while blue and red profiles correspond to those of the $Zr_{0.618}Al_{0.146}Ni_{0.236}$ alloys before and after relaxations, respectively.

References

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