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THE EFFECT OF MO ADDITION ON STRUCTURE AND GLASS FORMING ABILITY OF NI-ZR ALLOYS

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Understanding the structure and glass forming ability (GFA) of metals is crucial to establishing metallic glass theory and producing advance materials with excellent properties. The classical molecular dynamics simulation was conducted to investigate the effect of Mo atom addition upon atomic structure and glass-forming ability (GFA) of Ni64Zr36-xMox (x=0, 6, 12, 18, 21, 24, 27) metallic glasses (MGs), in terms of the system energy, radial distribution functions, and the largest standard cluster analysis. It is found that the Mo atoms do not simply replace Zr atoms, but change the chemical order, resulting in more stable and compact structures that are much complex indicated by the split of the first major peak on pair distribution function curves. Further analysis reveals that the addition of Mo atoms does not favour the formation of icosahedrons but enhances that of topologically close-packed (TCP) structures that are not only fully responsible for the shape evolution of the first major peak on the PDF curves, but also positive correlation with the glass forming ability (GFA) predicted by formation enthalpy. Thus TCP structures are the essential characteristic of MGs and the higher the forming ability of TCP structures, the better the GFA of Ni64Zr36-xMox alloys. These findings shed a new light on the understanding of microstructure and the structure-GFA relationship of MGs.

Biography

Zean Tian has completed his PhD at 2009 from Hunan University and Postdoctoral studies from the University of New South Wales. He has published more than 80 papers in reputed journals.

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