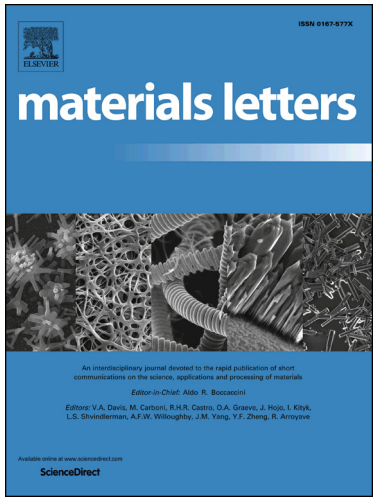

Understanding and designing good glass formers in Zr-Al-Co-(Nb) system combining clusters and mixing entropy

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Understanding and designing good glass formers in Zr-Al-Co-(Nb) system combining clusters and mixing entropy

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Abstract

Bulk alloy compositions in Zr-Al-Co-(Nb) system were understood and designed using our clusters- and mixing entropy-related method. Glass formers in Zr-Al-Co system were regarded as a mixture of Zr-Al and Zr-Co binary clusters with specific ratio. Icosahedral atomic clusters Co-Co_3Zr_9, Co-Co_6Zr_6, Al-Al_4Zr_8 and an Archimedean octahedral anti-prism cluster Al-Al_2Zr_8 were obtained and used. The coefficients of clusters were designed by mixing entropy. Only four compositions were designed. Among those, alloy with highest GFA was achieved at the composition of $Zr_{53.6}Al_{18.6}Co_{27.8}$ which enjoyed the same glass forming ability (GFA) as the well-known $Zr_{56}Al_{16}Co_{28}$ under the same condition. A series of compositions minor alloyed by Nb were further designed and analyzed. The results show that the optimum addition content of Nb could further enhance the GFA. Through the perspective of clusters and mixing entropy, it was assayed qualitatively the origin of enhancing GFA by minor-alloying element, which might help build a foundation for quantitative analysis of minor alloying.

Key words: Cluster, Amorphous materials, Biomaterials, Zr-based bulk metallic glass

Since Zr-based glassy alloys with large supercooled liquid region found in Zr-Al-TM (TM=Fe, Co) system, researchers paid lots of attention to Zr-based bulk metallic glasses (BMGs)[1]. One of the reasons is their potential application as biomaterials due to their unique chemical property and super corrosion resistance. However, up to date, most of Zr-based glass formers contain elements Ni, Be and Cu, which hinders their potential application as biomaterials. Among Zr-based glassy systems, minimal Zr-based glass formers without those elements have been developed[2]. **Zr-Co based BMGs have less cytotoxicity and better application foreground**.[3]However, the glass forming ability (GFA) is sensitive to compositions, so, it's full of challenge to develop new glass formers with high GFA especially in complex system.

Recently, with an aim to design glass formers with high GFA in a complex system, a new method was