PAPER ID:116

EFFECT OF VOLUME SHIFTS ON GLASS FORMATION IN BINARY ALLOYS

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ABSTRACT

Formation of glasses in metallic systems have received considerable attention since the discovery of the first metallic glass in the Au-Si system. This phenomenon has been variously explained through viscous dynamics of the liquid, mixing and mismatch entropy, enthalpy, free-energy, local structure, and lattice strain. These approaches each address a part of the puzzle of glass formation. Recently, few groups have developed synergistic models of glass formation, although the focus has been on bulk glasses in ternary or higher component systems rather than binary alloys. Nonetheless, the lower chemical complexity of binary metallic systems provides analytically simpler conditions for studying the interaction between various factors stated above. In this paper, we address this problem through theoretical studies on a few select systems, with the constituent elements chosen due to their differences in size and valence electrons. Co, Ni and Cu have near-identical atomic radius and are only separated by one electron each. We assess the glass-forming ability (GFA) where one element belongs to {Co,Ni,Cu} and the other belongs to Group IV of the periodic table with identical number of valence electrons but different atomic size.Wealsostudy theGFAin{Co,Ni,Cu}-{Y,Zr,Nb}systems with the latter three elements being separated by an electron each in while showing a trend in size. Through these investigations, we elucidate the synergistic effect of chemical (enthalpy) and structural (volume shifts) contributions on glass formation. It is shown that the presence of an extra valence electron can often result in larger volume shifts, as a result of which elements with similar molar volumes show different size during bonding in the glassy state, resulting in different glass-forming abilities.

Keyword: Glass forming ability, volume shift, binary metallic glasses, Miedema model