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Cooling-Rate Dependent Structural Evolution and Glass Formation in $Cu_{50}Ti_{42}Ni_8$ Alloy: A Molecular Dynamics Study

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Abstract- ***Molecular dynamics (MD) simulation based on the Embedded Atom Method (EAM) potential was used to study the structural evolution and glass forming ability of the ternary Cu50Ti42Ni8 alloy. The alloy system was melted and quickly cooled down to give an amorphous structure. The radial distribution functions were used to study the structural evolution during solidification, showing the changes in the atomic packing and short-range order. Incorporation of Ni contributes to the generation of stable Cu–Ti–Ni atomic clusters, thereby enhancing the structural stability and mechanical performance of the alloy. Glass transition temperature and crystallization resistance, thermal properties, indicate the enhanced glass-forming ability which is attributed to the increased thermal stability and suppressed crystallization***

Keywords: Short Range Order, Molecular Dynamics, Radial Distribution Function, Metallic Glass

I. INTRODUCTION

Bulk metallic glasses (BMGs) have an amorphous atomic structure that offers superior mechanical, thermal and corrosion resistant properties to conventional crystalline alloys. Understanding the factors governing the glass-forming ability (GFA), especially at the atomic scale where the structural ordering and the atomic dynamics are strongly correlated with the glass formation, still remains as a major challenge. Whereas high GFA is usually found in multicomponent alloys [1-4], the simpler binary and ternary systems provide useful model systems to study the fundamental mechanisms that are responsible for the amorphization.

In metallic glass forming systems, Cu-based alloys have been extensively studied because of their good mechanical properties and relatively high GFA. Previous studies showed that atomic packing, chemical short-range order and interatomic interactions are key factors controlling the liquid dynamics and resistance to crystallization. In Cu–Ti alloys [5], the strong chemical interaction between Cu and Ti atoms influences the structural evolution on cooling, while the addition of Ni can further modify the local atomic arrangements and enhance the thermal stability [6].

In the present work we study the structural evolution and glass forming ability of ternary Cu50Ti42Ni8 alloy by using molecular dynamics simulations. Particular attention is paid to the knowledge of the development of short-range order, atomic packing characteristics and the influence of Ni on thermal stability and glass forming ability of the alloy on rapid solidification.

II. METHOD

The molecular dynamics (MD) simulations of the $Cu_{50}Ti_{42}Ni_8$ alloy were carried out by the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) [7] with the constant number of particles, pressure and temperature (NPT) ensemble. The interactions between atoms were described by the Embedded Atom Method (EAM) potential. The simulation cell contained 5000 atoms on a face-centered cubic (FCC) lattice, with Cu, Ti and Ni atoms randomly distributed according to the desired alloy composition. In order to avoid surface effects, periodic boundary conditions were applied in all three spatial directions. The system was initially equilibrated at 300 K and then heated to 3000 K where it was maintained for 400 ps in order to assure the complete melting and to erase any memory of the initial crystalline configuration. The molten alloy was then cooled rapidly to 2100 K and quenched to 300 K

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with a cooling rate of 1×10^{11} K s^{-1}, to get the amorphous structure. The structural and thermodynamic properties were averaged over 80 ps in each temperature step. All simulations were performed using a time step of 2 fs.

III. RESULTS & DISCUSSION

The first peak of the Radial Distribution Function (Figure 1) appears very sharp, which indicates a high probability to find neighboring atoms at this distance which is a around 2.5–2.7 Å. This also suggests that the amorphous structure has a high degree of atomic short-range ordering and dense packing of atoms. a characteristic for strong interatomic interactions between Cu, Ti and Ni atoms. The first peak is followed by a deep minimum indicating a well-defined first coordination shell separated from the surrounding atomic environment.

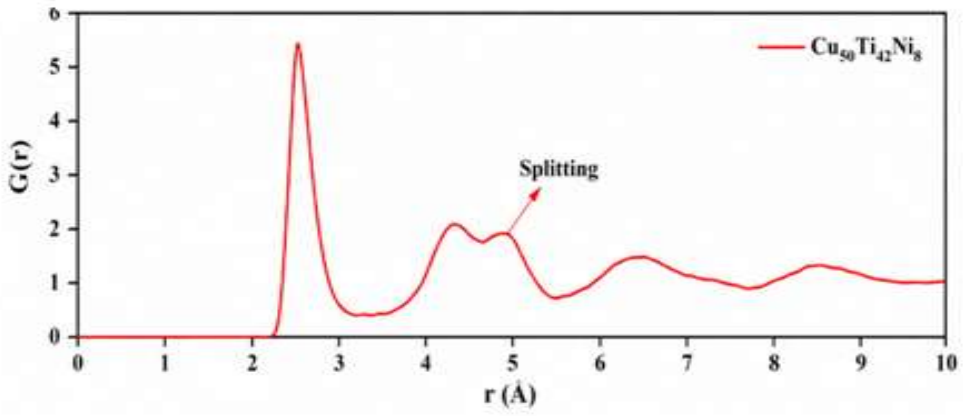

Figure 1 Radial distribution function of Cu50Ti42Ni8 at supercooled state

A notable characteristic of the RDF is the splitting of the second peak, occurring approximately between 4.3 and 5.2 Å. This splitting is widely recognized as a structural signature of metallic glasses and amorphous alloys. It originates from the presence of multiple local atomic environments and indicates the development of medium-range order beyond the first coordination shell. The split-second peak suggests the formation of densely packed clusters, including distorted icosahedral and Kasper-type polyhedra, which are known to enhance structural stability and suppress crystallization.

Voronoi tessellation analysis was employed to investigate the evolution of local atomic structures in the $Cu_{50}Ti_{42}Ni_8$ alloy over the temperature range of 900–1200 K.The results indicate that the local atomic environment is dominated by a few characteristic Voronoi polyhedra, indicating a pronounced short-range order in the undercooled liquid and amorphous states. The population of the Cu-centered (figure 2(a)) and Ti-centered (figure 2(b)) atoms in the

⟨0,1,10,2⟩ polyhedron is found to be highest at all the studied temperatures of the order of 12-16% which indicates the formation of the densely packed and energetically favorable local atomic configurations. Significant portions of polyhedra like ⟨0,3,6,5⟩, ⟨0,2,8,4⟩, ⟨0,3,6,4⟩ and ⟨0,1,10,4⟩ imply the existence of distorted icosahedral and Kasper-type polyhedra [8-10], which are generally regarded as crucial structural motifs in metallic glasses due to their efficient packing of atoms and resistance to crystallization .

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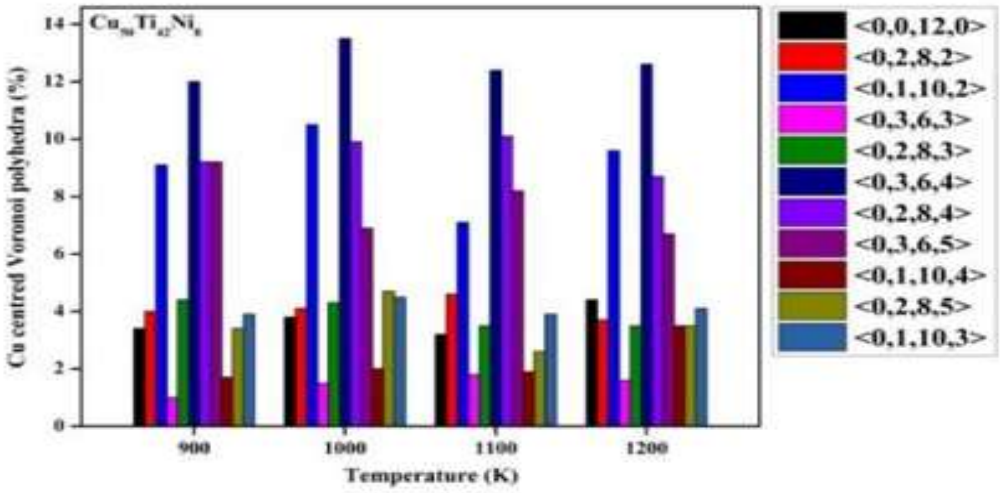
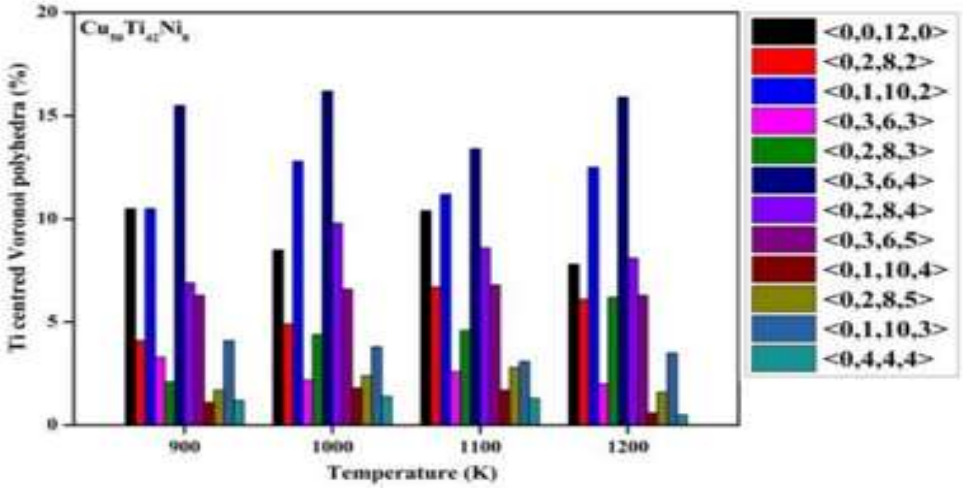
(a)



(b)



(c)

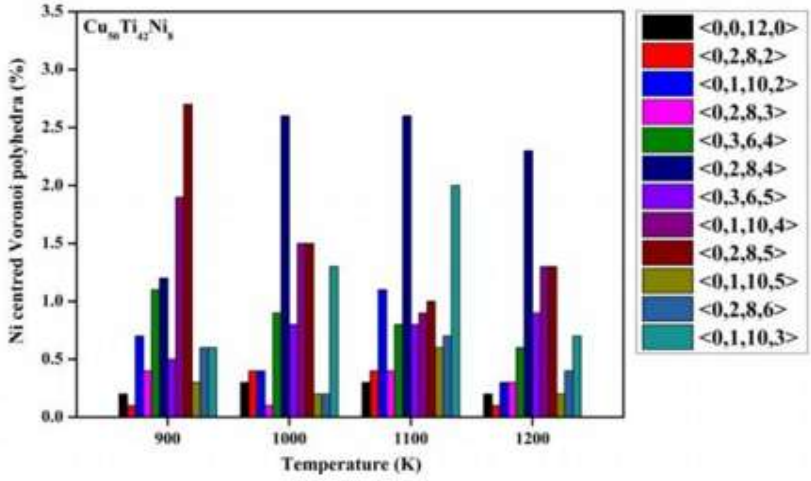


Figure 2: (a) Copper centred (b) Ti Centered and (c) Ni Voronoi Polyhedron from 900 K- 1200K

These cluster occurrences suggest the development of medium-range structural correlations which stabilize the amorphous phase. When the temperature is lowered from 1200 K to 900 K, the fractions of these dominant polyhedra usually increase, indicating the gradual establishment of chemical and topological short-range order on cooling. Ti-centered polyhedra are found to be especially rich in ordered motifs, indicating that Ti atoms may be playing a key role in stabilizing the glassy network. On the other hand, Ni-centered polyhedra (figure 2(c)) are less populated due to the low Ni concentration (8 at.%) but clusters such as ⟨0,1,10,2⟩, ⟨0,1,10,4⟩ and ⟨0,3,6,5⟩ are stable in the whole temperature range studied, which suggests that Ni atoms are sitting in specific local environments and promote favorable chemical ordering between adjacent Cu and Ti atoms. The abundant distorted icosahedral and Kasper-type clusters, coupled with the absence of prevailing crystalline motifs, lead to a substantial structural frustration that obstructs long-range atomic ordering and thereby crystal nucleation. Therefore, the formation and stabilization of these densely packed local structures improve the glass-forming ability of the Cu 50 Ti 42 Ni 8 alloy through increasing the structural stability, decreasing the atomic mobility, and facilitating the retention of an amorphous structure under the process of rapid solidification.

IV. CONCLUSION

The structural evolution and glass forming ability of Cu50Ti42Ni8 alloy were studied by the radial distribution function (RDF) and Voronoi polyhedral analysis. The RDF results show a strong first peak indicating strong nearest-neighbor atomic correlations and a clear splitting of the second peak which is a characteristic of amorphous metallic glasses. The absence of long-range periodicity and the gradual attenuation of the atomic correlations at larger distances confirm the formation of a stable amorphous structure. The observed second-peak splitting suggests that there are a significant medium-range order and densely packed local atomic arrangements, which prevent crystallization upon rapid cooling.

Voronoi analysis also shows that the local structure consists of polyhedra such as ⟨0,1,10,2⟩, ⟨0,3,6,4⟩, ⟨0,2,8,4⟩ and ⟨0,3,6,5⟩ for distorted icosahedral and Kasper-type atomic clusters. The presence and growth of these clusters with decreasing temperature is an indication for the gradual formation of short range and medium range order in the undercooled liquid. Ti- and Cu-centered polyhedra had the highest populations, suggesting the importance of these polyhedral units for the stabilization of the amorphous network, while Ni atoms contributed to the chemical ordering and formation of stable Cu-Ti-Ni local environments.

In summary, the RDF and Voronoi polyhedral analysis taken together indicate that the Cu50Ti 42Ni8 alloy is characterized by a densely packed and structurally heterogeneous atomic network with prevailing distorted icosahedral and Kasper type clusters. local atomic arrangements impede crystal nucleation, enhance thermal stability and favor glass formation. However, the addition of Ni significantly enhances the structural stability and glass-forming ability of the Cu–Ti alloy system, and $Cu_{50}Ti_{42}Ni_8$ is a promising composition for metallic glass formation.

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