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Molecular dynamics Simulation of the Turnbull Criterion for Predicting the Glass Forming Ability (GFA) in the Binary Fe100-XZrX Metallic Alloy

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Abstract: In order to better understand the glass forming ability, we have evaluated the reduced glass transition temperature (Trg) as one of the potential factors in molecular dynamics simulations of the binary Fe100-XZrX (X=10,12) system. Our investigation indicates that the calculated Trg values for Fe88Zr12 and Fe90Zr10 are 0.537 and 0.535, respectively, which are close to the minimum requisite T_rg≅0.4 the Turnbull criteria for glass formation in alloys.

Index Terms- Molecular dynamics, reduced glass transition temperature, metallic glass.

I. INTRODUCTION

Bulk metallic glasses (BMGs) have attracted considerable attention from both scientific and industrial sectors since their introduction [1]. Bulk metallic glasses (BMGs), owing to their superior features, such as corrosion resistance, fatigue resistance, elastic strain limit, and improved strength in comparison to crystalline materials, may serve as possible options for structural applications due to their amorphous structure. The requirement for a higher cooling rate (106 K/s) to prevent crystallization has constrained the viable casting thickness of BMG alloys. Consequently, new families of these alloys with greater dimensions and enhanced glass forming ability (GFA) necessitate further examination before their application. Inoue [2] has come up with three real-world criteria for creating bulk metallic glasses (BMGs) with better glass-forming ability (GFA), based on observations made in experiments. To meet these criteria, researchers have combined components like Fe, Zr, Pd, Mg, Cu, Ca, and La to create bulk metallic glasses (BMGs) [3-8], which feature reduced cooling rates, improved dimensions (diameter/thickness), and superior glass-forming ability (GFA). Researchers have conducted simulation studies on several binary alloys to establish a foundation for designing a multi-component alloy system with enhanced glass-forming ability (GFA) [8]. Research on Fe-based bulk metallic glasses (BMGs) has predominantly focused on their magnetic properties [9] or crystallization behavior [10], whereas investigations into their structural development remain few. Therefore, it is crucial to investigate the compositions that form glass in iron-based systems for potential structural applications. The aim of this study is to investigate glass-forming compositions based on the lowered glass transition temperature requirements established by Turnbull.

We have employed molecular dynamics (MD) simulations to examine the structural and dynamic properties, with the aim of understanding glass formation in several simple amorphous alloys [11,12]. In light of these considerations, we chose the Fe100-XZrX (X=10,12) system and performed molecular dynamics simulations on the alloy in both its liquid and amorphous forms. The investigation of Trg involved analyzing the volume temperature curve, the Wendt-Abraham parameter, and the radial distribution functions (RDFs) above the glass transition point.

II. METHOD

The Iron-zirconium alloy's molecular dynamics simulation (MD) was performed using a constant number of particles-pressure-temperature (NPT). The Fe100-XZrX (X=10,12) alloy systems were simulated using EAM potentials from Large-scale atomic/molecular massively parallel simulator software (LAMMPS) [13]. The simulated system contained 4000 atoms in a cubic unit cell of the B2 structure with periodic boundary conditions. First, the model system was heated to 300 K to relax it, then the temperature was increased to 3000 K and maintained there for 400 picoseconds (ps) to allow atoms to forget their initial structure. The system was immediately cooled to 2100 K, then gradually chilled from liquid to 300 K at a rate of 1 × 1011 K/s. At each temperature, the amounts of interest were calculated by taking averages over 80 ps. The simulation used an MD time step of 2 fs (1 fs = 1 × 10 −15 second).

III. RESULTS AND DISCUSSION

Radial distribution function

The radial distribution function (RDF) can be used to calculate a system's structural properties, particularly in

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liquids and amorphous materials. The RDF is determined as follows:

$$4\pi\rho \int_0^{\infty} g(r).r^2 dr = N - 1$$

In the simulation cell, N denotes the number of atoms in the shell with thickness ***dr*** and distance ***r***.

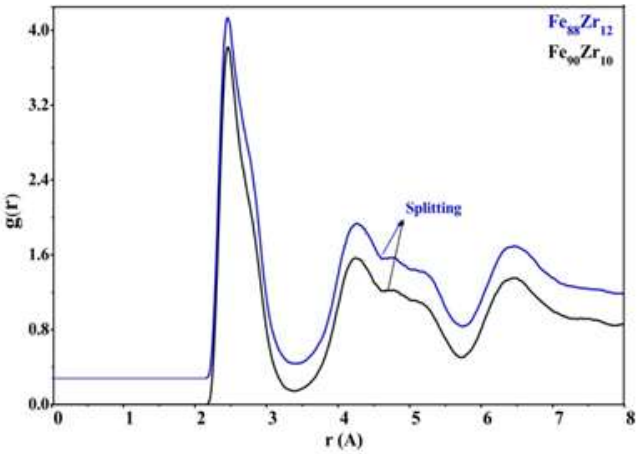


Figure 1 RDF of the model structure Fe100-XZrX (X = 10, 12)

Figure 1 displays the RDF of the model structure Fe100-XZrX (X = 10, 12) quenched just above the glass transition temperature at approximately 800 K. We initiated our simulation with the FCC structure, and the RDF reveals that dissimilar atoms have filled the first-nearest-neighbour positions, while only similar atoms occupy the second-nearest-neighbour positions.

Lowering the temperature to 800K at a rate of 30 K/ps reveals the long-range disorder feature in RDF and the distinct splitting of the second peaks of g(r) shows that an amorphous phase has formed. The first peak of unlike pairings is sharper than that of like atom pairs, indicating a preferential interaction between unlike atom pairs. But the RDFs of Fe100-XZrX (X = 10, 12) show a similar pattern with compositions. We don't fully understand this, but it could be due to the fact that thermal entropy in alloys doesn't change as much as configurationally entropy, a key factor in the formation of glasses.

Volume Temperature Curve

The volume-temperature curve in Figure 2 demonstrates a noticeable elevation during the heating process. The alteration in slope is attributable to a first-order phase transition, commonly referred to as melting. The system was modeled as an ideal crystal. The calculated melting temperature of Fe100-XZrX exceeded the experimental melting temperatures owing to homogeneity in the absence of any free surface.

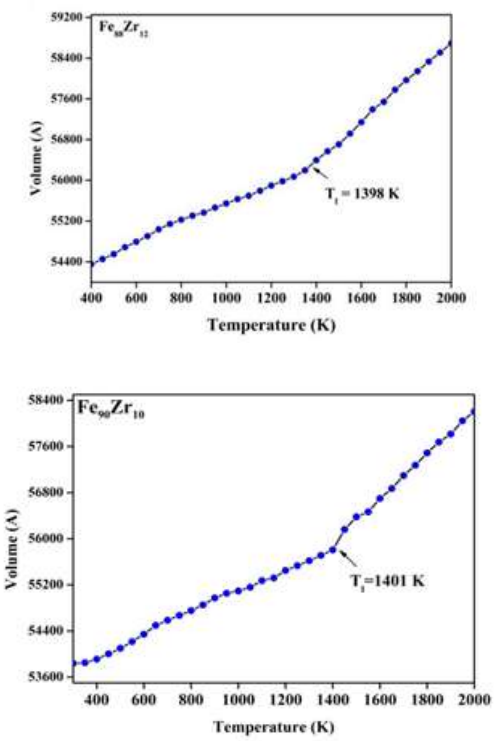


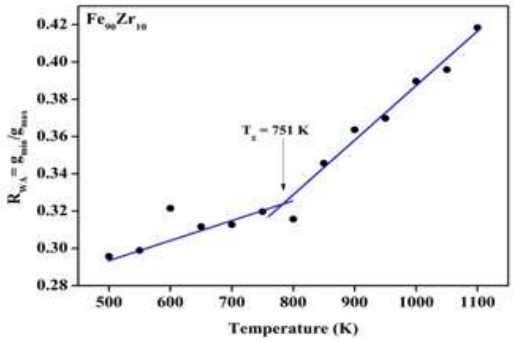
Figure 2 Volume-Temperature melting curve for Fe100-XZrX (X = 10, 12)

Wendt-Abraham Parameter (RWA)

Wendt- Abraham Parameter (RWA) parameter serves as a structural indicator for determining the glass transition temperature (Tg) and analyzing the local arrangement of particles during the transition from a liquid to a glass state.

$$R_{WA} = \frac{G_{min}}{G_{max}}$$

Where Gmin is the value of G(r) at the first minimum and Gmax is the value of g(r) at the first maximum in RDF curve. Figure 3 is the plot between RWA versus temperature for Fe100-XZrX (X = 10, 12), Tg value has been deduced from the intersection point shown in the plot.



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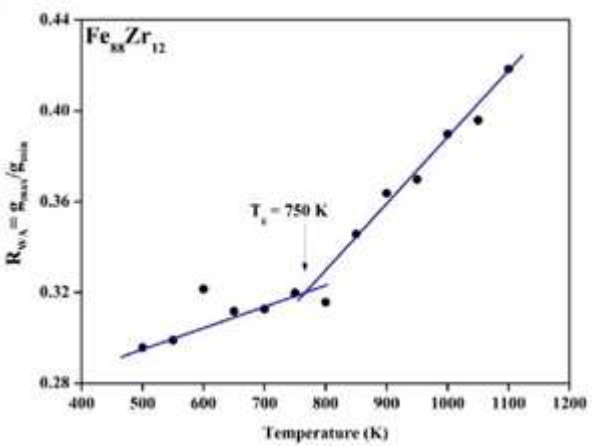

Figure 3 is the plot between R_{WA} versus temperature for $Fe_{100-X}Zr_X$ (X = 10, 12)

V. CONCLUSION

In summary, our investigation of Turnbull's criterion ($T_{rg} \cong$ 0.4.) for glass formation in $Fe_{100-X}Zr_X$ (X = 10, 12, T_{rg} 0.535 and 0.537 respectively) via molecular dynamics simulations indicates that materials with a high melting temperature ratio have enhanced glass-forming abilities since they transition to glass without crystallization.

Table 1 The simulated T_l, T_g and T_{rg} values for $Fe_{100-X}Zr_X$ (X=10,12)

Compositions	T_l (K)	T_g (K)	T_{rg}
$Fe_{88}Zr_{12}$	1398	751	0.537
$Fe_{90}Zr_{10}$	1401	750	0.535

This ratio in table 1 in conjunction with Wendt-Abraham's structural analysis and the characteristics of the volume-temperature curve creates a comprehensive structure for understanding glass-forming ability (GFA) in reported Fe-Zr binary alloy.

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