



# Molecular dynamics study of atomic-level structure in monatomic metallic glass



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## ABSTRACT

Molecular dynamics simulations have been performed to study the vitrification process and the local atomic structures in Ni monatomic metallic glasses (MG). The interatomic interactions are described by embedded atom method (EAM) potentials. Short-range order (SRO) and medium range order (MRO) in nickel monatomic MG is studied using several structural techniques such as the Radial distribution function (RDF); the Common neighbor analysis method (CNA) and the Voronoi tessellation. As a result, we found that the atomic packing in metallic glasses can be described globally as a superposition of the spherical-periodic order (SPO) and the local translational symmetry (LTS). From CNA method, we found that the majority of icosahedral clusters in Ni monatomic MG are connected together by vertex-sharing (VS), edge-sharing (ES), face-sharing (FS) and intercross-sharing (IS) rather than isolated clusters. These typical cluster connections constitute to the partial RDF of icosahedral atoms except the edge sharing which is hidden between the second and the third subpeaks of RDF. Furthermore, the visualization technologies are applied to follow the formation of clusters during rapid quenching. It is found that the clusters  $\langle 0,1,10,2 \rangle$  and  $\langle 0,2,8,4 \rangle$  are more dominant than the full icosahedral polyhedron  $\langle 0,0,12,0 \rangle$  in our monatomic system. Furthermore, the splitting of the second peak in RDF curve in Ni glass is not only caused by the icosahedral clusters, but also by the Voronoi polyhedrons  $\langle 0,1,10,2 \rangle$  and  $\langle 0,2,8,4 \rangle$ .

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## 1. Introduction

Metallic glasses have attracted considerable attention due to their unique properties, which are used in high technology applications [1, 2]. These improved properties, compared to their crystalline counterparts, depend on the atomic-level structures that are different from those found in the crystalline state. Recent studies confirm that the atomic packing within the medium-range order (MRO) controls the stability and mechanical properties of metallic glasses [3,4]. Generally, upon fast quenching of single, binary, ternary, and multicomponent metal systems the crystallization does not occur and the amorphous state forms without long-range structural correlation [5]. Therefore, a glass can be formed by cooling from a liquid where the atoms settle into a random arrangement [6], with the lack of boundaries unlike conventional polycrystalline metal thus the material becomes more viscous [7]. This amorphous phase is characterized by a glass transition temperature below which the high viscosity does not allow the structural rearrangements. Almost any metallic liquid can be vitrified into a glassy state if it is cooled rapidly to a lower temperature [8,9,10]. Mainly, the

quenching rate of conventional alloys is in the order of  $10^6$  K/s whereas in pure metals this critical rate is about  $10^{12}$  K/s [11,12,13] which is difficult to achieve experimentally.

The production of multicomponent metallic glasses (binary, ternary...) has been previously carried out by diverse experimental methods such as the mold casting [14,15,16], the melt spinning [17], the liquid splat-quenching [18], the pulsed laser quenching [19], the cast in argon and air atmosphere [20] and spark plasma sintering (SPS) [21]. Unfortunately, the vitrification of the single-component metallic glass is difficult because of the low glass-forming ability of the monatomic metallic [22]. Most recently, Li Zhong et al. [23] developed an experimental approach co-called ultrafast liquid-quenching which led to the vitrification of monatomic metallic liquids by achieving a high cooling rate of  $10^{14}$  K/s. By testing this method on transition metals of Ta, V, W and Mo, they successfully found that these metals can vitrify to form metallic glasses. Many computational approaches have been used to study the monatomic metallic glasses and explore their various properties. Recent studies highlight the significance of investigating the rapid solidification process and structural behavior in pure metallic glasses. For instance, the rapid quench and remelting of aluminum [2], the study of metallic glasses Cu using different cooling rates [24], the structural analysis of Al solidified under different pressures [25], the study of solidification of silver [26].

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The atomic structure of disordered solids remains one of the most interesting problems in materials science, since the mechanism of glass transition is a complex process. The direct observation of the atomic structure in metallic glasses has not been achieved experimentally using the conventional techniques. However, many structural models have been already proposed to analyze the atomic arrangement of glassy solids such as Bernal's 'dense random packing' [27], Gaskell's 'short-range order' [28] and the recent 'solute-centered quasi-equivalent cluster' [29,30]. In this sense, numerous studies have tried to reveal the structural properties of metals during rapid solidification. As a result, the efficient atomic packing has been recently developed. It has been shown that the full icosahedral cluster is the major unit in metallic glasses and plays a critical role in the formation of these materials. Wu et al. [31] used MD simulation to study the short-range order in amorphous  $\text{Cu}_{80}\text{Si}_{20}$ . From Honeycutt Andersen index, Voronoi tessellation method, and the atomistic cluster alignment method, they found that the icosahedral cluster is predominant in the system. In Wang and Wong's study [32]; MD simulations revealed that the amount of icosahedral clusters increases with the addition of Al concentration to Zr—Cu alloys. However, recent study demonstrated that the full icosahedral clusters are unstable in some metallic glasses, such as Zr-rich Cu—Zr glasses and CaMgCu MGs [4,33,34]. Ju et al. [35] applied MD technique to investigate the local structures of  $\text{Mg}_{67}\text{Zn}_{28}\text{Ca}_5$  and  $\text{Mg}_{50}\text{Zn}_{30}\text{Mg}_{20}$ . They found a fundamental difference in the sense that the full icosahedral cluster is the more abundant in  $\text{Mg}_{67}\text{Zn}_{28}\text{Ca}_5$  while in  $\text{Ca}_{50}\text{Zn}_{30}\text{Mg}_{20}$  glass the distorted icosahedral unit is predominant.

The purpose of the present study is to explore the atomic structures in a Nickel metallic glass. As it is well known, this metal plays an important role in our daily lives, it possess very good oxidation resistance, good corrosion resistance, greater toughness, and a range of special magnetic and electronic properties. Therefore, it is used for the production of batteries, and some other uses, such as mobile phones, medical equipment, and transport. The Nickel is also used as catalyst of several important reactions, including the hydrogenation. For all these reasons, we will study the atomic-level structure of Nickel using the molecular dynamics simulation, which may provide a new viewpoint to understand the transition from liquid to glass in monatomic metallic materials. For this specific study, we will use the radial distribution function (RDF) and highlighted the splitting of the second peak of RDF, which is a sign of vitrification in metallic glasses. Several techniques have been widely proposed to obtain details of atomic-level structures in amorphous materials. Among them we employed the common neighbor analysis [36] and the Voronoi tessellation [37] to show good ability in describing the local structure in our simulated system. The results exhibited that the icosahedral clusters in Ni monatomic MG are connected together by vertex-sharing (VS), edge-sharing (ES), face-sharing (FS) and intercross-sharing (IS) rather than isolated clusters. We have found that there is a difference between monatomic and multicomponent metallic glasses. The Voronoi polyhedrons  $\langle 0,1,10,2 \rangle$  and  $\langle 0,2,8,4 \rangle$  are more abundant than the full icosahedral polyhedron  $\langle 0,0,12,0 \rangle$  in monatomic systems. While it is generally observed that in multicomponent metallic glasses the full icosahedral units present a higher percentage. Furthermore, we showed that the splitting of the second peak of RDF may be interpreted by the formation of other polyhedra in conjunction with the full icosahedral.

This paper is organized as follows: In Section 2, we describe the MD approaches and the optimized EAM for Ni metal used to simulate the Ni metallic glass. In Section 3, we present a series of results obtained throughout the cooling process. Finally, we close this work by emphasizing our main conclusions.

## 2. Simulation method

All simulations have been performed using the LAMMPS code (Large-scale Atomic/Molecular Massively Parallel Simulator) [38, 39]. We choose the EAM (embedded atom method) interaction

potential parameterized by Baskes et al. [40] to model the interactions between the atoms of nickel. The simulations are performed with a cubic *fcc* sample consisting of 5324 atoms in 3D cubic box of size  $11\text{\AA} \times 11\text{\AA} \times 11\text{\AA}$  with periodic boundary conditions (PBC) applied in the three directions of the MD cell. Newton's movement equations are numerically integrated using the Verlet [13] algorithm with a time step of 1 fs used in all simulations. Firstly, MD simulations were carried out by increasing temperatures from 200 K to 2500 K with a heating rate of  $10^{12}$  K/s under the isothermal isobaric (NPT) ensemble [29], where moles (N), pressure (P), and temperature (T) are conserved. Ni liquid is reached at a temperature as high as 2500 K. This temperature is far above the melting point of the nickel in order to allow atoms to diffuse far from their initial positions. Then, the system is relaxed for a supplementary 100 ps at 2500 K under Canonical NVT ensembles (constant number, volume, and temperature) to reach the equilibrium liquid state. This high temperature relaxation avoids any memory effect where atoms may keep locally their crystalline environment. Afterwards, based on (NPT-MD), we cool down the system from 2500 K to 200 K at different cooling rates to test the effect of the cooling rate on the transition process (see Fig. 1).

It is well known that the interatomic potentials play a very important role on the accuracy of an atomistic simulation. For this reason, we adopted the EAM potential, which is currently the method of choice for performing semi-empirical calculations of the properties of metallic systems. This potential type has been successfully employed to a wide range of aspects such as the grain boundary structure [41], alloys [42, 43,44] and surface structural order-disorder transitions [45]. The principal advantage of this potential is much less in computational time and it can handle a large number of atoms compared to the ones using the density functional theory (DFT).

The EAM is a semi-empirical technique for computing the energy of an arrangement of atoms. In this approach, the energy of each atom is computed from the energy required to embed an atom into the local-electron density as provided by the other atoms of the metal. In particular, the total energy of system is given by [29]:

$$E_{\text{tot}} = \sum_i F_i(\rho_{h,i}) + \frac{1}{2} \sum_{i \neq j} \phi_{ij}(r_{ij}); \quad (1)$$

where  $F_i$  denote the energy to embed atom  $i$  into the electron density  $\rho_{h,i}$ ,  $\phi_{ij}$  is the pair interaction between atoms  $i$  and  $j$ , and  $\rho_{h,i}$  represents the host electron density at atom  $i$  due to the other atoms of the system.

In the present work, the electron density for nickel is calculated from [46]

$$\rho(r) = \psi \left( \frac{r-r_c}{h} \right) [A_0 z^y e^{-\gamma z} (1 + B_0 e^{-\gamma z} + C_0)]; \quad (2)$$

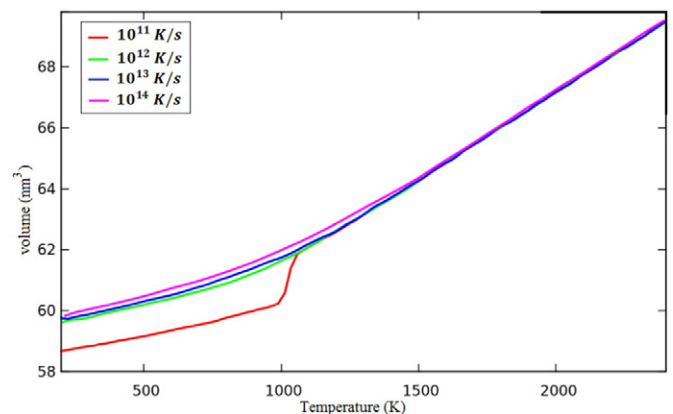


Fig. 1. Volume change as temperature decreases during the cooling process for three different cooling rates.

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