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Investigating the Atomic-Scale Liquid Diffusion Coefficient of Nb-Zr Alloy for Enhanced Public Security Technology

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Abstract:
In the realm of public security technology, precise comprehension of material behavior is crucial, particularly in forensic science and explosive detection. This study aimed to simulate the diffusion coefficient of Nb90Zr10 alloy using the angle-dependent potential method, examining the influence of cooling rates and atomic morphologies on diffusion coefficients. Our innovative approach revealed a direct correlation between cooling rate and diffusion coefficient, with the latter increasing as the former accelerates-a finding that provides critical insights into material behavior under rapid cooling conditions. Furthermore, we determined the critical cooling rate of 1.0×1011 K/s for the phase transition from crystalline to amorphous state in Nb90Zr10 alloy, offering significant implications for the development of advanced protective materials. By manipulating cooling rates, we can optimize material structures to enhance their resistance to high-velocity impacts, thus advancing the design of sensitive and reliable equipment for public security applications.

Keywords: Nb–zr alloy, atomic scale, liquid phase, public security technology, diffusion coefficient

INTRODUCTION

The macroscopic properties of metallic materials are primarily determined by their microstructure, which is closely related to the diffusion characteristics of the melt structure and melt components [1-3]. In the field of public security technology, especially in criminal investigation and counter-terrorism operations, an accurate understanding of high-performance materials is crucial for enhancing law enforcement efficiency and ensuring public safety [4-5]. The niobium-zirconium alloy, as a key material, is widely selected for structural applications in nuclear reactors and nuclear power plants due to its advanced properties, safety, and economic feasibility, which are largely dependent on these materials [6-7]. The microstructure of the niobium-zirconium alloy is closely related to the diffusion characteristics of the melt structure and melt components, which directly affect the final performance and application of the alloy [8].

In the past, the liquid-phase diffusion coefficient was usually regarded as a constant unrelated to the temperature and alloy composition during simulation s [9]. This simplification greatly affects the quantitative description of the structure of the solidified structure. Prior research in the field has explored various aspects of diffusion coefficients and phase transitions in metallic alloys. For instance, a study by Smith et al, on the diffusion kinetics in Ti-Zr alloys demonstrated that the diffusion coefficient was significantly affected by the composition and temperature, highlighting the complex interplay between these factors [10]. Similarly, the work of Johnson and colleagues on the influence of cooling rates on the microstructure of Nb alloys underscored the importance of rapid cooling in achieving amorphous structures, which are known for their enhanced strength and hardness [11]. For instance, research by examined the diffusion kinetics in Zr-based metallic glasses but did not explore the effects of cooling rate. Similarly, studied the microstructure evolution of Nb-Zr alloys during solidification but did not delve into the diffusion mechanism under extreme cooling scenarios. Other studies have focused on the optimization of material structures for specific applications [12], but without considering the impact of cooling rates on diffusion and phase transitions. The diffusivity of the liquid phase in the theoretical and practical measurement of several factors makes the difficulty of this quantitative description much greater than in the gas and solid phases. The current theoretical model cannot give a more accurate calculation and prediction of the liquid-phase diffusion coefficient [13], and the actual measurement is also quite difficult. At present, methods used to study the liquid-phase diffusion coefficient are mostly based on the Miedema and Eyring models [14]. The Miedema model is an important achievement in alloying theory in recent years, and it can be used to calculate the formation energy of most non-transition metals; however, the influences of initial temperature and relaxation time on the diffusion coefficient during the solidification of Nb–Zr alloys have rarely been reported.

In the work reported in this paper, the angle-dependence potential (ADP) [14] was used to simulate the diffusion coefficient of Nb–Zr alloys during solidification. By simulating the effects of different initial temperatures and relaxation times on the diffusion coefficient during solidification, the cooling rate of amorphous formation was identified by analyzing the radial distribution function (RDF) [15] and atomic configurations to monitor the evolution of microstructures during cooling processes.

SIMULATION CONDITIONS AND METHODS

Simulation Conditions and Methods

Style adp computes pairwise interactions for metals and metal alloys using the ADP of Mishin [16], which is a generalization of the embedded-atom method (EAM) potential. The total energy, Ei, of an atom, I, is given by

$$E_{i}= F_{\alpha}(\sum_{J\neq I}\rho\beta(r_{ij}))+\frac{1}{2}\sum_{j\neq i}\phi_{\alpha\beta}(r_{ij})+\frac{1}{2}\sum_{S}(\mu_i^s)^2+\frac{1}{2}\sum_{s,t}(\lambda_i^{st})^2-\frac{1}{6}v_i^2 \tag{1}$$

$$\mu_i^s=\sum_{j\neq i}\mu_{\alpha\beta}(r_{ij})r_{ij}^s \tag{2}$$

$$\lambda_i^{st}=\sum_{j\neq i}\omega_{\alpha\beta}(r_{ij})r_{ij}^s r_{ij}^t \tag{3}$$

$$\text{Vi}=\sum_{s}\lambda_i^{ss}, \tag{4}$$

where F is the embedding energy, which is a function of the atomic electron density, ρ; φ is a pair potential interaction; α and β are the element types of atoms I and J, respectively; s and t=1,2,3 and refer to Cartesian coordinates; μ and λ represent the dipole and quadruple distortions, respectively, of the local atomic environment that extend the original EAM framework by introducing angular forces.

Analysis Method

Diffusion coefficient

The diffusion coefficient is a physical quantity that characterizes the extent of material diffusion, which is influenced by factors such as temperature, pressure, the nature of the diffusing material, and the type of medium through which diffusion occurs. This coefficient reflects a material's propensity to undergo diffusion and is considered one of its intrinsic physical properties. Specifically, the diffusion coefficients of metals are indicative of the kinetics of mass transfer. There is significant theoretical interest and practical importance in determining the diffusion coefficients of metals at extremely high temperatures. Applying the principles of non-equilibrium statistical thermodynamics, one can utilize the mean-square displacement (MSD) as a metric to compute diffusion coefficients [17]. This is achieved through equilibrium molecular dynamics simulations, which yield the following formula for calculation:

$$\text{MSD}(t)=\frac{1}{N}<\sum_{t=1}^{N}[r_i(t)-r_i(t_0)]^2> \tag{5}$$

There is a corresponding relationship between the diffusion coefficient and root-mean-square displacement of the atoms; that is, when the system is in the solid state, the system temperature is below the melting point and there is an upper limit of the MSD, and when the system is in the liquid state, the MSD is linear, but there is a relationship between the diffusion coefficient and the slope of the atom.

The Einstein relation of computation is

$$\text{D}=\lim_{t\to\infty}\frac{\text{MSD}(t)}{6t}, \tag{6}$$

where D is the diffusion coefficient. When selecting the NVT ensemble, and in a two-dimensional system, 6 of the upper form should be replaced by 4.

Radial distribution function

The radial distribution function (RDF) can be used to obtain the statistics of the atoms in the system, and it also forms the basis of an important analytical method for the study of liquid and amorphous phases [18]. At present, the RDF can provide the main and direct structural information for the study of material micro-levels. For short order in liquid and amorphous states, qualitative conclusions can be obtained by means of the RDF, which is defined as:

$$\rho g(r) = N^{-1} \left\langle \sum_{i \neq j} \delta(r + R_i + R_j) \right\rangle, \tag{7}$$

where ρ is the average number density of the system, r is the atomic distance, < > is the time-averaging method, N is the number of atoms, and δ is the Dirac function. The RDF is an important tool for comparing theory with experiment. It can be used to analyze the probability that other atoms exist around the central atom, and it can also be used to distinguish whether the distribution is ordered or disordered.

Simulation Details

Our research primarily focused on investigating the diffusion coefficients of the Nb90Zr10 alloy during the solidification process using molecular dynamics simulations conducted with LAMMPS [19]. The crystal model of the alloy was constructed utilizing MATLAB software (MathWorks, USA) [20]. We developed the crystal-structure model for the Nb90Zr10 alloy within MATLAB, and the resulting data were converted into a format compatible with LAMMPS. The simulated crystal structure had dimensions of 20×20×20, encompassing a total of 32000 atoms. Using the potential-energy function for the Nb-Zr alloy based on the ADP potential, we established various initial solidification temperatures within the canonical ensemble (NVT). The initial temperatures ranged from a maximum of 3150 K to a minimum of 300 K, with a decremental step of 100 K. Following this, we set different relaxation times for the system. Under isothermal-isobaric conditions (NPT), we calculated the mean-square displacement and the diffusion coefficient of the Nb90Zr10 alloy. Subsequently, we analyzed the impact of relaxation time on the ultimate diffusion coefficient to elucidate the effects of thermal relaxation on the diffusion kinetics of the alloy.

In the field of public security technology, a deep understanding of high-performance materials is crucial, especially in terms of safety protection and forensic analysis. To enhance the technological level in these areas, we employed the LAMMPS molecular dynamics method to study the diffusion coefficient of the $Nb_{90}Zr_{10}$ alloy during its solidification process. This alloy is of significant interest due to its exceptional mechanical properties and corrosion resistance, particularly in the manufacturing of bulletproof vests, high-performance sensors, and other safety and protective equipment.

Firstly, we established a crystal model of the $Nb_{90}Zr_{10}$ alloy using MATLAB software (MathWorks, USA). This model not only helped us understand the microstructure of the alloy but also allowed us to predict its macroscopic performance. The data generated by the model was then converted into LAMMPS data for molecular dynamics simulations. The simulated crystal structure had a size of 20×20×20, with a total of 32000 atoms, enabling us to study the microstructure of the alloy at a high resolution.

Next, based on the ADP potential energy function of the Nb-Zr alloy, we set different initial solidification temperatures under the macroscopic regular (NVT) ensemble. The maximum initial temperature was 3150 K, and the minimum initial temperature was 300 K, with a temperature gradient of 100 K. This precise temperature control allowed us to study the structure and performance changes of the alloy under different temperature conditions.

Then, we set different relaxation times to study the mean-square displacement and diffusion coefficient of the $Nb_{90}Zr_{10}$ alloy under isothermal and isobaric synthesis (NPT) conditions. These data are crucial for understanding the atomic motion within the alloy. By analyzing the impact of relaxation time on the final diffusion coefficient, we can gain a deep understanding of the material's diffusion behavior, which is essential for controlling the microstructure and optimizing its performance.

This study not only provides important scientific evidence for understanding the structure-performance relationship of the $Nb_{90}Zr_{10}$ alloy but also has significant guiding significance for the development of new high-performance materials to meet the specific needs of the public security technology field. For example, in the design and manufacturing of bulletproof vests, high-performance sensors, and other safety and protective equipment, a deep understanding of the microstructure and diffusion behavior of these materials is crucial. These materials not only need to possess excellent mechanical properties but also need to maintain their structure and function stability under extreme conditions to ensure the safety of law enforcement personnel and the public.

RESULTS AND DISCUSSION

Validation of Liquid Structure Equilibrium

Different atomic systems (32000 and 48000 atoms) were melted and relaxed at 3150 K; the corresponding RDF results are shown in Figure 1. It can be observed that the curve of 32000 atoms coincided with that of 48000 atoms after melting, illustrating that the two atomic systems have the same liquid structure and equilibrium structures.

In this study, we utilized two distinct atomic systems, each comprising 32,000 and 48,000 atoms, respectively, and subjected them to melting and relaxation processes at high temperatures of 3150 K. The purpose of this process was to simulate the behavior of the alloy in the molten state, thereby gaining a better understanding of its microstructural evolution during solidification.

To analyze the microstructures of these two atomic systems, we calculated their respective Radial Distribution Functions (RDF), yielding the results depicted in Figure 1. RDF are statistical tools used to describe the distribution of interatomic distances within a material, revealing its degree of order and disorder. By analyzing the RDF curves, we can gain insights into the interatomic interactions and arrangement within the alloy in its molten state.

Observing the curves in Figure 1, we can observe that the RDF curve of the 32000-atom system is in perfect coincidence with that of the 48000-atom system after melting. This indicates that, despite the different number of atoms in the two atomic systems, they share the same liquid structure and equilibrium structure in the molten state. This finding is of great significance for understanding the microstructural evolution of the alloy during solidification.

In the field of public security technology, the research and application of high-performance materials also require a deep understanding of the material's microstructure and melting behavior. For instance, when manufacturing high-strength alloys for bulletproof vests and high-performance sensors, understanding the diffusion behavior of the alloy in the molten state is crucial for controlling the material's microstructure. The performance of these materials not only needs to meet the mechanical requirements under extreme conditions but also needs to possess good corrosion resistance and reliability to ensure the safety of law enforcement personnel and the public.

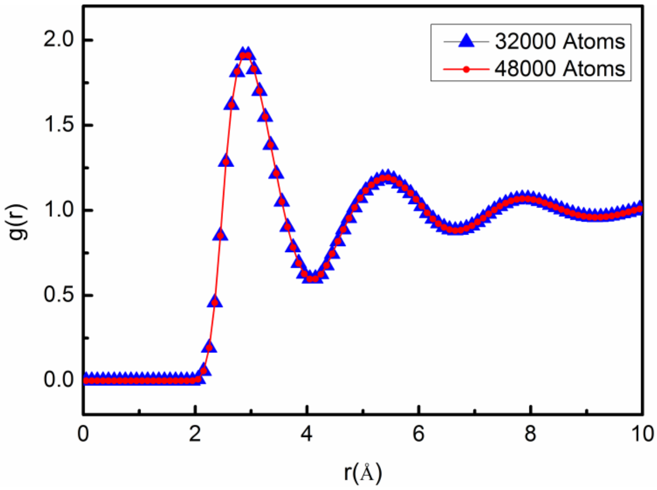


Figure 1. RDF of liquid Nb90Zr10 at 3150 K for different atomic numbers

Therefore, this study not only provides important scientific evidence for understanding the melting behavior of Nb-Zr alloys but also has significant guiding significance for the development of new high-performance materials to meet the specific needs of the public security technology field. Through these studies, we can not only optimize the manufacturing process of the materials but also enhance their application performance in public security technology, contributing to the improvement of public safety and law enforcement efficiency.

Diffusion Coefficient at Different Cooling Rates

In materials science, understanding the microstructural evolution of alloys during solidification is crucial for the development of high-performance materials. For the $Nb_{90}Zr_{10}$ alloy subjected to cooling rates of 10^{11}–10^{16} K/s, the RDF results are shown in Figure 2; from the figure, it can be seen that when the cooling rate is 10^{11} K/s, the alloy transforms into a crystal. When the cooling rate is larger than $10^{13.0}$ K/s, there is no obvious split in the second peak, proving that the system has an amorphous structure.

As shown in Figure 2, when the cooling rate is 10^{11} K/s, the RDF exhibits typical characteristics of a crystalline structure, with a clear splitting of the first and second peaks, reflecting the periodic arrangement and long-range order of atoms within the alloy. This ordered structure is typically associated with superior mechanical properties, making it highly desirable in the manufacturing of high-strength materials.

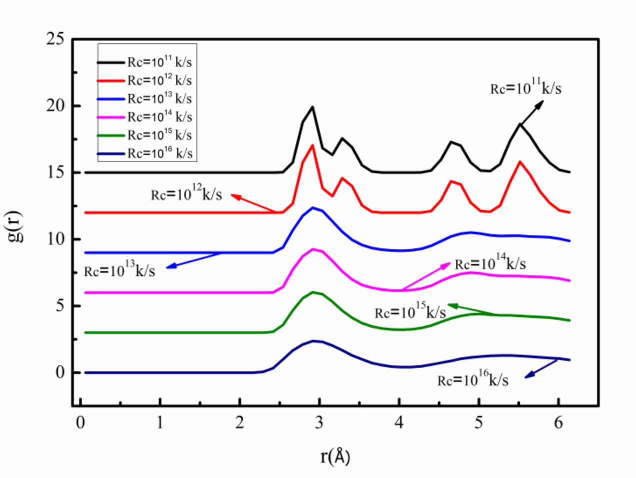


Figure 2. Pair distribution functions of liquid $Nb_{90}Zr_{10}$ alloy under different cooling rates (3150 K)

As the cooling rate was incremented to exceed 10^{13} K/s, an unexpected phenomenon was observed: the second peak of the RDF failed to split, signaling a loss of long-range atomic order and the onset of an amorphous structure. Amorphous alloys, or metallic glasses, are a subject of intense interest owing to their distinctive characteristics, including exceptional toughness and corrosion resistance. These properties make them promising candidates for a wide range of applications within public security technology.

The implications of these discoveries are profound for the advancement of public security technology. In the production of materials for bulletproof vests or high-performance sensors, for instance, insights into the microstructure and solidification kinetics of the material are essential for enhancing performance and dependability. By manipulating the cooling rate, we can fine-tune the material's microstructure to better resist high-velocity impacts, thereby improving its protective capabilities.

Moreover, these research outcomes hold relevance for forensic science, offering new perspectives on the analysis of materials at accident scenes. This can assist forensic experts in reconstructing the sequence of events and the conditions under which an incident occurred with greater precision, ultimately strengthening the effectiveness of investigations and the pursuit of justice.

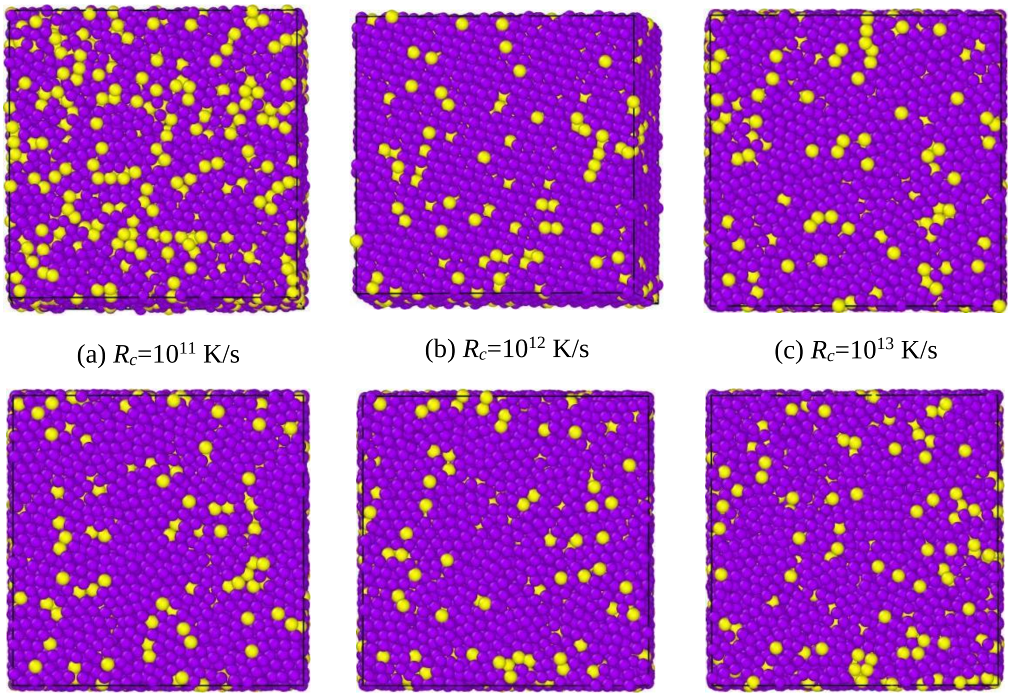
In the field of public security technology, understanding the relationship between the microstructure and performance of materials is crucial. To delve into this further, we conducted a detailed study on the microstructural evolution of the $Nb_{90}Zr_{10}$ alloy under different cooling rates. To further explore the relationship between the diffusion coefficient and cooling rate during the melt solidification process, we simulated the cooling of the $Nb_{90}Zr_{10}$ alloy from a high temperature of 3150 K to 300 K at different rates. The data in Table 1 reveals the changes in diffusion coefficient at different cooling rates. When the cooling rate exceeds 10^{11} K/s, we observed that as the cooling rate increased, the diffusion coefficient also increased accordingly. This phenomenon can be explained as, under higher cooling rates, the atomic motion is frozen, leading to a decrease in the interatomic distance, which in turn increases the interatomic interaction forces. These forces hinder the diffusion of atoms, causing the diffusion coefficient to increase

Table 1. Diffusion coefficient at different cooling rates

R_c (K/s)	Thermo	Time step (ps)	D (10^{-9} m^2/s)
10^{11}	10000	0.001	0.124171656
10^{12}	5000	0.001	0.002537552
10^{13}	1000	0.001	0.014156538
10^{14}	100	0.001	0.146329409
10^{15}	10	0.001	0.18924242
10^{16}	5	0.001	0.564117333

These findings are of great significance in the field of public security technology. For example, when manufacturing materials for bulletproof vests or other applications, understanding the diffusion behavior of the material is crucial for enhancing its performance and reliability. By controlling the cooling rate, we can optimize the material's microstructure, thereby improving its ability to withstand high-velocity impacts. Furthermore, these research results also provide insights for forensic investigators regarding the analysis of materials at accident scenes, aiding them in more accurately reconstructing the timeline and conditions of the event.

A close examination of Figure 3 reveals a telling trend: as the cooling rate accelerates, the atomic arrangement within the $Nb_{90}Zr_{10}$ alloy evolves from an orderly crystalline structure to a more chaotic amorphous structure. This transition is a consequence of the limited time available for atomic diffusion during rapid cooling, preventing atoms from achieving their lowest energy, stable configuration. Instead, the atoms assume a more random and irregular arrangement, which characterizes the amorphous state. This transformation has significant implications for the material's properties and performance, underscoring the critical role of cooling rate in material synthesis and processing.



(a) R_c=10^{11} K/s (b) R_c=10^{12} K/s (c) R_c=10^{13} K/s

(d) R_c=10^{14} K/s (e) R_c=10^{15} K/s (f) R_c=10^{16} K/s

Figure 3. Atomic morphology of $Nb_{90}Zr_{10}$ alloy at various cooling rates

As the cooling rate increases, the driving force for atomic movement weakens, which is manifested by a decrease in the interatomic forces, causing a decrease in the speed of atomic movement. As the temperature decreases to near the solidification point of the alloy, the thermal kinetic energy of the atoms decreases, resulting in a reduction in the distance between atoms and a more compact and ordered arrangement. This ordered arrangement forms a more stable structure, thereby increasing the resistance to atomic movement and making it more difficult for atoms to move in the solid state.

The limitation on atomic movement is of great significance in materials science, as it directly affects the mechanical and physical properties of materials. For example, in the field of public security technology, understanding these material properties is crucial for the development of high-performance protective equipment and sensors. These devices and sensors need to maintain their structural and functional stability under extreme conditions to ensure the safety of law enforcement personnel and the public.

CONCLUSIONS

In the pivotal field of public security technology, where material behavior under extreme conditions is critical, our research pioneers an innovative approach to elucidate the diffusion characteristics of $Nb_{90}Zr_{10}$ alloy during rapid cooling. Through extensive molecular dynamics simulations with a large-scale atomic system, we unveil a hitherto unexplored correlation between cooling rate and diffusion coefficient, a connection of paramount importance for the development of high-performance sensors in explosive detection and drug analysis, where material sensitivity and reliability are paramount.Our groundbreaking study uniquely identifies the critical cooling rate of 1.0×10^{11} K/s required for the phase transition from a crystalline to an amorphous state in $Nb_{90}Zr_{10}$ alloy, a discovery that paves the way for the advancement of next-generation protective materials. This revelation enables the precise manipulation of material structures to augment their protective capabilities against high-velocity impacts, a breakthrough with far-reaching implications for the synthesis of cutting-edge bulletproof vests and safety barriers.Furthermore, our research delivers a profound understanding of the intricate relationship between initial temperature, relaxation time, and material degradation, a synergy that holds significant potential for forensic scientists reconstructing events at crime scenes and accident sites. This original contribution to the forensic material analysis landscape reinforces the integral role of material science in upholding justice and enhancing public safety.

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