JOURNAL OF NANOMATERIALS AND APPLICATIONS

Journal of Nanomaterials and Applications

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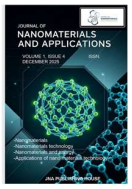

Glass Transition Mechanisms in Metallic Glasses: A Theoretical, Experimental, and Simulation Review

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Article info

Type of articles:

Original research paper

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Received: 08 October 2025

Revised: 22 December 2025

Accepted: 24 January 2026

Published: 28 January 2026

Abstract: Metallic glasses, as a distinct class of amorphous metals, exhibit a unique combination of mechanical robustness, thermal stability, and electronic functionality compared to their crystalline counterparts. Despite extensive studies, the microscopic origin of the glass transition and its dependence on structural heterogeneity remain subjects of ongoing debate. Experimental methods including Differential Scanning Calorimetry (DSC), Flash DSC, Dynamic Mechanical Analysis (DMA), nanoindentation and 5D Scanning Transmission Electron Microscopy (5D-STEM) are reviewed and analyzed. In addition, molecular dynamics (MD) and potential energy simulation models are investigated to establish a relationship with experimental data. Zr-based, Pd-based alloys and high-entropy metallic glasses are compared, in which β relaxation and glass-to-glass transitions are analyzed in detail. From this study, the combination of experiment and simulation has been emphasized as a key for accurate prediction of material properties, and outlines future research directions toward the development of optimized metallic glass systems.

Keywords: metallic glasses; glass transition; short-range order; medium-range order; β-relaxation; differential scanning calorimetry

1. Introduction

Metallic glasses represent a distinct class of non-crystalline metals characterized by the absence of long-

range atomic order. Unlike conventional crystalline alloys, their amorphous structure gives rise to unconventional mechanical and thermodynamic behavior, motivating extensive investigation into their glass transition mechanisms. The unique combination of superior mechanical properties, corrosion resistance, and excellent electrical and thermal properties has been noted as factors that make MGs an important research subject in the field of advanced materials [1, 2]. Over the past two decades, significant progress has been made in elucidating the glass transition mechanism at the microstructural level, along with the role of short-range order (SRO) and medium-range order (MRO) [3, 4]. The accurate determination of the glass temperature (T_g) along with the auxiliary phenomena such as β-relaxation has been considered as an important factor in guiding the design and optimization of metallic glasses (MGs). By accurately identifying T_g, the glassy state can be distinguished from the supercooled liquid regime and the onset of crystallization. β-relaxation, associated with local atomic or cluster motions in the amorphous structure, plays a crucial role in controlling ductility, deformability, and thermal stability in metallic glasses. As a result, the mechanical and thermal properties of the material can be effectively optimized by adjusting the fabrication conditions and alloy composition [5, 6]. Advanced experimental methods such as Differential Scanning Calorimetry (DSC), Flash DSC, Dynamic Mechanical Analysis (DMA), nanoindentation, and 5D Scanning Transmission Electron Microscopy (5D-STEM) have been developed and widely applied to accurately determine the T_g, investigate the microstructural mechanisms, and identify glass-to-glass transitions in Figure 1.

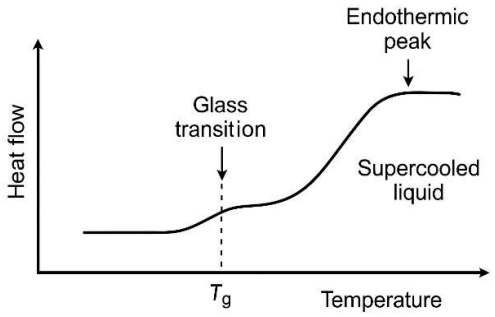

Figure 1. Schematic representation of calorimetric glass transition (T_g) determination using DSC, highlighting the change in heat capacity (ΔCp) during heating.

Through these techniques, subtle changes in the atomic structure and dynamics of materials have been recorded, thereby contributing to elucidating the nature of phase transition phenomena and structural stability mechanisms in amorphous metals [7–9]. In addition, thermodynamic and mechanical properties have been predicted through molecular simulations (MD) and machine-learning potentials, showing close correlation with experimental data and the applications [10–12]. In this review, recent theoretical, experimental, and simulation studies are summarized, focusing on the analysis of popular MG systems such as Zr-based, Pd-based, and high-entropy metallic glasses (HEMGs). At the same time, current controversies and potential research directions are also clarified. Special emphasis is placed on correlating calorimetric, mechanical, and microstructural observations with atomistic simulations, aiming to bridge experimental observations and theoretical interpretations.

2. Fundamental Concepts of Glass Transition in Metallic Glasses

The glass transition in metals refers to a gradual transformation from an amorphous solid to a supercooled liquid–like state as temperature increases. The glass temperature (T_g) is considered an important

parameter, because it clearly reflects the free energy and kinetic characteristics of the material system [13].

2.1. Short-range order and Medium-Range Order

Short-range order (SRO) refers to the ordered arrangement at the scale of a few atoms around each atom, while medium-range order (MRO) is used to describe the structural connections at the scale of a few nanometers larger than SRO but still not reaching the level of crystalline order [14]. The mechanical, thermal and deformational properties of MGs are believed to be directly influenced by SRO and MRO. According to studies, an increase in MRO connectivity is often associated with higher T_g and improved mechanical properties, depending on alloy composition and thermal history [3, 4]. Recent quantitative studies show that an increase in MRO connectivity can raise T_g by 20–60 K in Zr-based metallic glasses, as confirmed by recent combined experimental–simulation studies [15], while the activation energy of β-relaxation (E_β) typically ranges from 0.8–1.2 eV depending on alloy composition and heating rate.

2.2. The T_g value

The T_g value measured by the calorimetric method (calorimetric T_g) is determined through DSC technique, based on the change of specific heat when the material system is transformed into a thermoplastic state [7]. The dynamic T_g value (dynamic T_g) is determined through kinetic measurements such as Dynamic Mechanical Analysis (DMA), based on the change of elastic modulus with frequency and temperature [8]. It should be noted that calorimetric T_g and dynamic T_g may differ significantly due to their distinct kinetic origins and measurement timescales.

2.3. Influence of microstructure

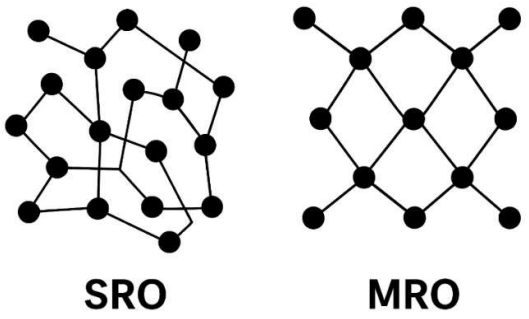

Figure 2: Schematic illustration of SRO and MRO in metals

The alloy ratio, atomic size and bond energy distribution are considered to be factors that directly affect T_g and the β relaxation process. Compared with Pd-based MGs, Zr-based MGs generally have higher T_g due to their more stable MRO structure [16] in Figure 2.

3. Experimental Approaches

Glass transition phenomena in metals have been extensively investigated using modern experimental techniques, to ensure that the determination of the glass temperature (T_g) is carried out accurately and reliably. In these studies, material samples are often prepared and processed according to strict procedures to avoid the influence of impurities or residual stresses, which can distort the measurement results. Methods such as Differential Scanning Calorimetry (DSC), Dynamic Mechanical Analysis (DMA), and mechanical vibration techniques at different frequencies are used to detect changes in the free energy, elastic modulus, and specific heat capacity of the material with increasing temperature. Through this, characteristics such as T_g, β-relaxation, as well as the microscopic phase transition mechanism are

identified and analyzed in detail. Other complementary measurements such as nanoindentation, 5D Scanning Transmission Electron Microscopy (5D-STEM) or in-situ X-ray scattering are also applied to directly observe the microstructural evolution in the phase transition region. By combining these methods, the transformation process from the solid state to the thermoplastic state in MGs is described more comprehensively, helping to clarify the relationship between structure, atomic dynamics and mechanical properties of the material system.

3.1. Differential Scanning Calorimetry

Although DSC is widely used to determine T_g, its accuracy strongly depends on heating rate and thermal history, limiting direct comparison with high-rate techniques such as Flash DSC. In this method, the difference in heat flow between the sample and the reference sample is recorded, from which T_g is determined accurately and reliably. In addition, Flash DSC technique was developed to extend the capabilities of the traditional method. With a much higher heating rate than conventional DSC, Flash DSC allows T_g to be measured under more severe dynamic conditions, while also facilitating clearer observation of glass-to-glass transitions that are difficult to detect with conventional DSC measurements [9]. However, reported T_g values obtained by Flash DSC may deviate by up to 30–50 K, particularly at heating rates above 10^4 K/s, as reported in recent fast scanning calorimetry studies, mainly due to the strong dependence on heating rate and thermal history, which complicates direct comparison with simulation predictions [17]. These high-rate calorimetric techniques have significantly improved the understanding of kinetic effects and non-equilibrium phenomena during the glass transition.

3.2. Dynamic Mechanical Analysis

DMA is used to measure the change in elastic modulus with frequency and temperature, thereby accurately determining the dynamic T_g. In this method, the material sample is subjected to harmonic mechanical vibrations at different frequencies, and the material response expressed in terms of storage modulus and loss modulus is recorded. With increasing temperature, the sharp decrease in the rheological modulus together with the appearance of a peak in the loss modulus is used to determine the dynamic T_g. By means of DMA, secondary relaxation processes such as β-relaxation are also more clearly recognized, thanks to the method's high sensitivity to micro-strains and atomic vibrations in the amorphous network. Parameters obtained from DMA help to elucidate the relationship between atomic dynamics, structural relaxation mechanisms and the deformability of metallic glass materials. When DMA is combined with other complementary measurements such as DSC or nanoindentation, a more comprehensive picture of the glass transition mechanism is formed. Through this combined approach, nonlinear deformation phenomena, internal energy distributions and microstructural restructuring processes in the transition region are analyzed in more detail [18, 19].

3.3. Nanoindentation

Nanoindentation is used to measure the mechanical properties of materials at the micro and nanoscale, by recording the relationship between the applied load and the indentation depth when the indenter is pressed into the sample surface. From the resulting load-unload curve, parameters such as hardness and elastic modulus are accurately determined. As a result, the local mechanical properties of metallic glasses (MGs) can be evaluated, directly reflecting the structure distribution and density of bonds in the material. When measurements are performed at various temperatures, the variation of hardness and elastic modulus with temperature provides indirect but important information about the T_g and structural relaxation processes. In the region near T_g, materials typically exhibit a marked decrease in hardness and

modulus, indicating increased atomic motion and structural rearrangements at the microscale. In addition, dynamic nanoindentation, in which a small oscillation is superimposed on a static load, allows for the investigation of transient changes in mechanical properties with respect to time and frequency. Due to its high resolution and ability to capture local material responses, this technique helps to clarify the relationship between β-relaxation, local motion of atomic clusters, and the resistance to plastic deformation of MGs. When combined with methods such as DSC or DMA, nanoindentation plays an important role in establishing the relationship between thermodynamics, atomic dynamics, and mechanical properties of metallic glasses, thereby contributing to a deeper understanding of the nature of phase transitions and relaxations in amorphous systems [20, 21].

3.4. 5D-Scanning Transmission Electron Microscopy

5D-STEM is considered one of the most advanced methods today in investigating the electronic structure and local deformation of materials at the atomic level. In this method, the scanning electron beam is controlled with high precision over each point of the sample, while diffraction data are collected simultaneously in space and diffraction angle, creating a "5-dimensional" data set including two-dimensional position, two-dimensional diffraction angle, and one-dimensional signal intensity. Owing to its atomic-scale resolution, 5D-STEM allows direct identification of short-range ordered (SRO) and medium-range ordered (MRO) regions in metallic glass materials, as well as their distribution in space. Through the analysis of the diffraction intensity and direction at each point, the local deformation zones, structural dislocations, and the degree of homogeneity of the amorphous network can be determined in detail. When combined with DSC and DMA measurements, 5D-STEM provides valuable complementary information, helping to clarify the relationship between the microstructure, thermodynamics, and mechanical properties of the material. The changes in SRO and MRO before and after the glass transition can be directly observed, thereby providing a deeper understanding of the mechanism of atomic rearrangement and structural relaxation in the vicinity of T_g [22, 23]. By simultaneously recording both structural and dynamic information at the atomic level, 5D-STEM serves not only as an observational tool, but also as an important means to verify and refine simulation models, contributing to the understanding of the microscopic nature of the glass transition in amorphous metallic materials.

3.5. Validation of results

Comparison of the methods shows that each technique provides complementary information: DSC measures calorimetric T_g, DMA measures dynamic T_g, nanoindentation provides mechanical properties, and 5D-STEM investigates the microstructure in the Table 1.

Table 1. Comparison of T_g values obtained by different experimental and simulation methods.

Method	Typical heating rate	T_g range (K)	Strengths	Limitations
DSC	10–40 K/min	Reference T_g	Standard, reproducible	Rate dependent
Flash DSC	10^3–10^4 K/s	+30–50 K	Captures fast kinetics	Difficult comparison
DMA	Frequency dependent	Higher T_g	Sensitive to β-relaxation	Not calorimetric
MD	$\sim 10^{12}$ K/s	Overestimated T_g	Atomic insight	Timescale mismatch
ML potentials	—	< 5% error	High accuracy	Data-dependent

A comparison of T_g values obtained by different experimental and simulation approaches is presented in Table 1, highlighting the influence of timescale and measurement principle on the reported glass transition

behavior.

This combination allows for a comprehensive description of the glass transition [24, 25]. When comparing the different experimental methods, we found that each technique provides a type of complementary information, contributing to the overall picture of the glass transition in metals. Specifically, DSC is used to determine the calorimetric T_g through the change in specific heat capacity; meanwhile, DMA allows to determine the dynamic T_g based on the variation of elastic modulus with frequency and temperature. In addition to these two techniques, nanoindentation is applied to obtain data on hardness and elastic modulus, which directly reflect the local mechanical properties of the material. Meanwhile, 5D-STEM allows to observe the microstructure and local arrangement of orders (SRO, MRO) at the atomic level, providing direct evidence of the structural evolution in the transition region. When the results from DSC, DMA, nanoindentation, and 5D-STEM are compared and analyzed simultaneously, a comprehensive and unified view of the glass transition is formed. This combination of thermodynamic, mechanical, and microstructural data not only helps to more accurately describe the phase transition mechanism, but also aids in the calibration of simulation models, contributing to the elucidation of the dynamic and structural nature of metallic glasses [26, 27] in Figure 3.

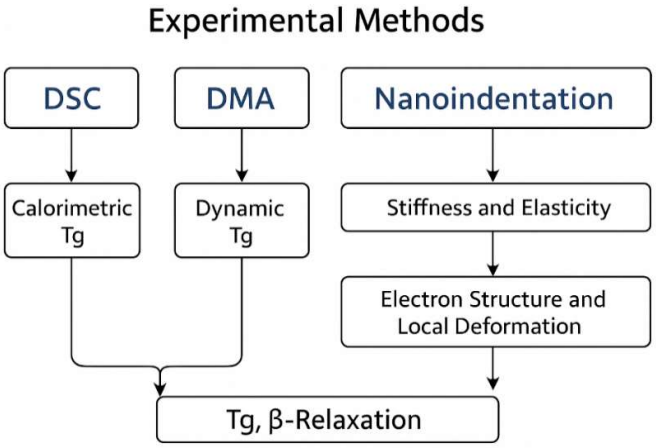

Figure 3: Schematic illustration of the main experimental methods in metallurgical research

4. Simulation and Theoretical Modeling

Simulation methods and theoretical models are considered important tools in elucidating the mechanism of the glass transition and establishing a connection between computational results and experimental data. Through these models, microscopic processes which are difficult to observe directly by experimental methods are reproduced and analyzed in more detail. In recent studies, molecular dynamics (MD) simulations and machine-learning potential models have been widely used to describe the movement of atoms, the formation of amorphous structures, as well as the structural relaxation process when materials are heated or cooled [28]. These simulations allow for direct assessment of the changes in binding energy, atomic density, and local order (SRO, MRO) during the phase transition. Through simulation methods, many potential dynamic mechanisms of the glass transition that are difficult to determine experimentally have been clarified, such as the rearrangement of atomic clusters, the propagation of local deformation zones, or the formation of intermediate structures. When compared with experimental data obtained from DSC, Dynamic Mechanical Analysis (DMA) or 5D Scanning Transmission Electron Microscopy (5D-STEM), the simulation results help to enhance the reliability and integrity of the analysis. Therefore, the use of simulation and theoretical modeling has become an integral part of the study of metallic glasses, as it allows

complex phase transition phenomena to be described more clearly, and provides a scientific basis for the design and optimization of material properties at the atomic level.

4.1. Molecular Dynamics

MD simulations are widely used to study the motion of atoms in amorphous metals at different temperatures. By tracking atomic trajectories over time, the microscopic characteristics of the material system are reproduced, allowing accurate prediction of the glass temperature (T_g), analysis of β-relaxation, as well as assessment of the influence of short-range order (SRO) and medium-range order (MRO) on material properties [29-31]. In MD simulations, the interaction between atoms is described through interatomic potentials, which faithfully reflect the relationship between energy and structure. When the temperature is changed, displacements, vibrations and rearrangements of atomic clusters are recorded, thereby describing the phase transition from solid to thermoplastic state in detail at the atomic level. In particular, MD simulations predict glass-to-glass transitions in Zr-based metallic glasses driven by changes in medium-range order and local packing motifs. However, experimental validation remains controversial: while some Flash DSC studies suggest multiple transition events, others report no clear separation, highlighting the sensitivity to heating rate and sample preparation [32]. These results demonstrate the pivotal role of SRO and MRO evolution in controlling T_g, relaxation, and stability of the amorphous structure. Due to its ability to describe atomic dynamics with high precision, MD methods not only help to explain experimental results but also open up the possibility of predicting material behavior under untested conditions, thereby making an important contribution to understanding the transition mechanism and guiding the design of high-performance metallic glasses. However, limitations related to accessible timescales and cooling rates in MD simulations must be carefully considered when comparing with experimental T_g values.

4.2. Machine-Learning Potentials

Machine Learning Potentials (ML potentials) have been developed to overcome the limitations of traditional potentials in material simulation, especially for metallic glasses (MGs) with complex structures and many components. In this method, machine learning models are trained based on energy and force data obtained from ab initio calculations (usually DFT – Density Functional Theory), thereby relearning the relationship between atomic structure and energy with almost the same accuracy as quantum simulation, but at a significantly faster computational speed. With this ability, machine learning potentials allow simulation of multi-component MGs over a much larger spatial and temporal range than traditional methods. Recent developments after 2019 demonstrate that machine-learning potentials trained on quantum-accurate datasets can reproduce T_g and elastic properties of metallic glasses with errors typically below 5% when benchmarked against experimental T_g values [28, 31]. This represents a major advancement over classical potentials, particularly for compositionally complex and high-entropy systems. This is especially useful for high-entropy metallic glasses (HEMGs) materials with high complexity in composition and structure. With ML potentials, characteristics such as T_g, average binding energy, local degree of order (SRO, MRO), as well as mechanical and thermodynamic properties can be reliably predicted [33, 34]. In addition to the advantages of speed and accuracy, ML potentials also allow for flexible description of nonlinear effects, such as local changes in bond energy during structural relaxation or plastic deformation under external loading phenomena that are difficult to describe with classical potentials. Therefore, the machine learning potential method has become a promising approach in the simulation of amorphous materials, helping to narrow the gap between theoretical and experimental calculations, and

expanding the ability to predict and design new generation metallic glasses with superior and more stable properties.

4.3. Connecting with Experiments

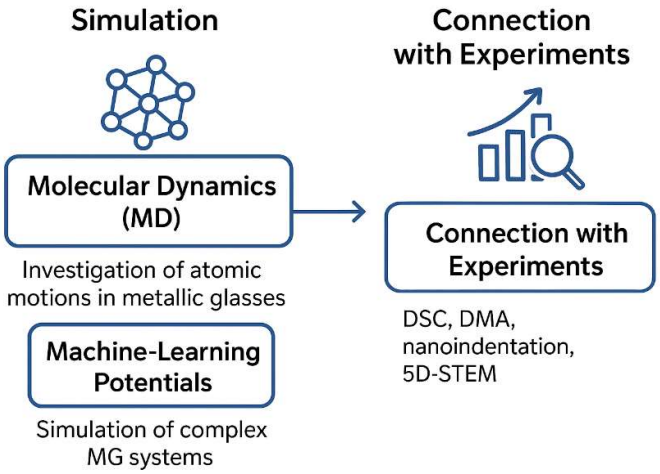

Figure 4: Schematic illustration of simulation methods and their connection to experiments

Combining MD and ML simulations with DSC, DMA, nanoindentation and 5D-STEM data helps to validate the results and deeply understand the microstructural mechanisms affecting T_g. This connection forms the basis for designing MGs with optimal properties [1, 25]. These experimental datasets also serve as essential benchmarks for validating simulation models, as discussed in Section 3.5. This close connection not only strengthens the accuracy of computational models but also opens up new approaches to deeply understand the formation and structural evolution mechanisms of materials. As a result, researchers can more effectively guide the design and optimization of metallic glasses (MGs) with desired properties [1, 28] in Figure 4.

5. Comparative Case Studies

This review examines typical metallic glasses (MGs) systems such as Zr-based, Pd-based, and high-entropy metallic glasses (HEMGs). Each system has its own structural, thermodynamic, and mechanical characteristics, reflecting the relationship between the medium-range order (MRO), the glass transition mechanism, and ancillary phenomena such as β-relaxation or glass-to-glass transitions in the Table 2 .

Table 2. Reported glass transition temperature (T_g) and β-relaxation characteristics in representative metallic glass systems.

MG system	Composition (example)	T_g (K)	β-relaxation (E_β or T_β)	Method	Reference
Zr-based	$Zr_{55}Cu_{30}Al_{10}Ni_5$	650–690	$E_\beta \approx 0.9$–1.2 eV	DSC + DMA	[15, 16]
Pd-based	$Pd_{40}Ni_{40}P_{20}$	580–610	Strong β-relaxation	DMA	[27]
Fe-based	$Fe_{75}B_{20}Si_5$	520–550	Weak β-relaxation	DSC	[14]
HEMGs	(TiZrHfCuNi)	700–750	Broad β-relaxation	MD + ML	[28, 35]

To facilitate a direct comparison across different metallic glass systems, Table 2 summarizes representative values of glass temperature (T_g) and β-relaxation characteristics reported in previous experimental and simulation studies. This comparison helps to better visualize how the nature of atomic bonding and microstructure influence the stability and performance of the material in practice.

5.1. Zr-based Metallic Glasses

The Zr-based MGs system, known for its high glass temperature (T_g) and outstanding mechanical strength, is one of the most studied groups of materials in the field of metallic glasses. Experimental and simulation results show that the existence of stable MRO plays a key role in controlling β-relaxation and glass-to-glass transitions. The icosahedral atomic clusters in this system often maintain a stable structure even when the material is heated or stressed, which increases the resistance to plastic deformation and improves thermal stability [15, 36]. Therefore, Zr-based MGs are considered an ideal platform to study the relationship between microstructure, phase transition and mechanical properties in more complex metallic glasses.

5.2. Pd-Based Metallic Glasses

Pd-based metallic glasses typically have lower T_g than Zr-based systems, but exhibit higher ductility and deformability, making them well suited for applications that require materials with good load-bearing and processability. Results obtained from dynamic mechanical analysis (DMA) and molecular dynamics (MD) simulations show that the β-relaxation process in this system is strongly influenced by the arrangement of short-range order (SRO) and the presence of weak regions in the structural network. These structural regions act as trigger points for local deformation, and regulate the atomic displacements in the period near T_g [1, 37]. Due to this mechanism, Pd-based MGs exhibit remarkable plastic deformation while maintaining structural stability, making them one of the typical objects to study the relationship between atomic dynamics and mechanical properties in metallic glasses.

5.3. High-Entropy Metallic Glasses

HEMGs are formed by mixing many elements with nearly equivalent content, thereby creating a complex MRO structure rich in dynamic features [36]. Due to the large number of participating elements, the atomic structure of HEMGs often exhibits a wide distribution of binding energies and many local heterogeneities, making it more difficult to determine the glass transition mechanism than that of conventional MGs systems. In recent studies, machine-learning potentials have been applied to simulate the atomic behavior of HEMGs with higher accuracy and wider simulation range than classical potentials. As a result, Tg values are reliably predicted, and the β-relaxation mechanism and glass-to-glass transitions can be analyzed in more detail [27, 32].

5.4. Analysis of β-relaxation and glass-to-glass transitions

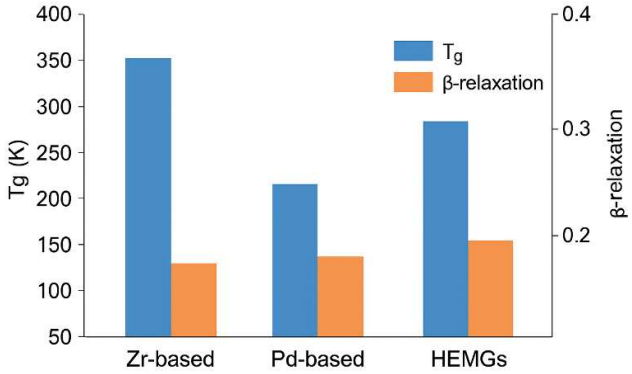

Figure 5 Comparison chart of T_g and β-relaxation between MGs systems.

The β-relaxation phenomenon and glass-to-glass transitions have been noted to be strongly influenced by the MRO, alloy composition ratio, and the distribution of interatomic bond energies. As the MRO becomes more stable, local heterogeneities are restricted, leading to a decrease in the β-relaxation intensity and an increase in the T_g transition temperature. On the contrary, in systems with poorly developed MRO or

unevenly distributed bond energy, β-relaxation occurs more strongly, reducing the thermal and mechanical stability of the material. By comparing different metallic glass systems, it can be seen that this mechanism plays a key role in determining the ductility and strength of the material. Understanding the correlation between MRO, bond energy and β-relaxation is considered an important basis for guiding the design of metallic glasses with optimal mechanical properties and higher resistance to deformation [33, 34] in Figure 5. These observations support the view that β-relaxation serves as a structural precursor linking atomic-scale heterogeneity to macroscopic deformation behavior.

6. Discussion

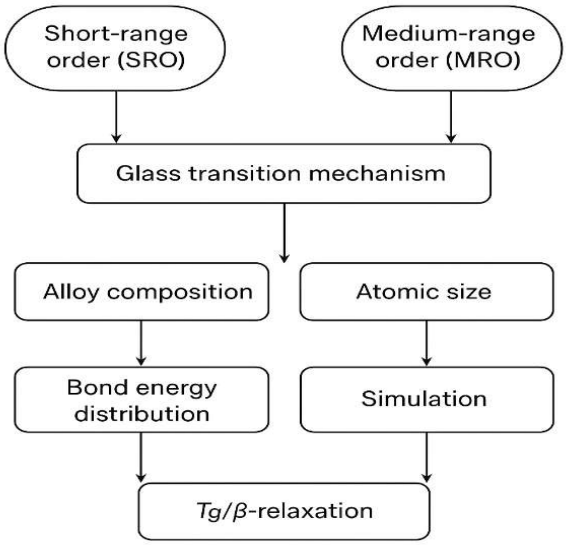

Figure 6: Schematic diagram of factors affecting T_g and β-relaxation

From the results obtained through theoretical, experimental and simulation studies, it can be seen that the glass transition mechanism in metals is strongly influenced by the microstructural characteristics at both short-range order (SRO) and medium-range order (MRO). The influence of factors such as alloy composition ratio, atomic size and the distribution of bond energy between atomic clusters are also determined to play a decisive role in controlling the phase transition. These correlations show that the formation and stabilization of the glass phase is not only the result of thermal kinetics but also influenced by the spatial structure inside the material. When SRO and MRO reach high stability, the free energy of the system is reduced, leading to an increase in T_g and improvement in mechanical properties. On the contrary, heterogeneity in MRO or uneven distribution of bond energy can promote β-relaxation and reduce the structural strength [15, 26]. Different experimental methods such as DSC, Flash DSC, Dynamic Mechanical Analysis (DMA), nanoindentation and 5D Scanning Transmission Electron Microscopy (5D-STEM) have been used to investigate the glass transition in metals. Each technique provides complementary observations, contributing to the elucidation of the thermal and mechanical properties of the materials. However, the T_g and β-relaxation values obtained from these methods sometimes do not agree completely. Such inconsistencies are often attributed to differences in heating rates, sample preparation conditions and resolution limitations of each measurement technique. Therefore, combining multiple methods and adjusting experimental parameters is considered necessary to obtain accurate and comparable results [14]. Molecular dynamics (MD) simulations and machine-learning potentials have been used to elucidate

the role of the MRO in glass-to-glass transitions. Through these simulations, the mechanism of atomic rearrangement in the transition region has been observed more clearly, helping to explain the variation of T_g and β-relaxation phenomena at the microscopic level. However, there is still debate regarding how to accurately model high-entropy metallic glasses (HEMGs) systems, due to the diversity of compositions and the complex interactions between the constituent elements. Quantitative prediction of β-relaxation in these systems remains a major challenge, requiring a closer combination of simulations, theoretical models and experimental data to achieve higher reliability [21]. An open research direction is the development of higher-speed T_g measurement techniques, allowing accurate recording of phase transitions in a short time. In addition, the application of artificial intelligence (AI) in the simulation and structural analysis of HEMGs systems is considered a potential tool to handle complex material systems. By combining experimental data and simulation results, comprehensive predictive models of the glass transition mechanism and material properties can be built, helping to shorten the gap between theory and practical applications. This approach promises to expand the design and optimization of metallic glasses for advanced industrial fields such as electronics, energy materials and precision mechanical technology [32] in Figure 6.

7. Future Perspectives

Research on metallic glasses (MGs) is still opening up many new approaches to gain a deeper understanding of the phase transition mechanism and optimize material properties. Some specific research directions are proposed as follows:

7.1. Development of fast T_g measurement techniques

High-precision measurement of the glass temperature (T_g) remains a major challenge, especially for MGs with complex structures. Therefore, methods such as Flash DSC and high-speed Dynamic Mechanical Analysis (DMA) need to be further improved to be able to record glass-to-glass transitions and β-relaxation processes in real time. These improvements include increased thermal sensitivity, precise control of heating rates, and synchronization of data obtained from multiple measurements. Through this, T_g and the secondary phase transitions can be more clearly identified, leading to a deeper understanding of the microscopic dynamics of MGs and laying the foundation for the design of materials with high thermal stability [35, 36].

7.2. Application of artificial intelligence in simulation

The application of artificial intelligence (AI) in material simulation has been considered a potential research direction, especially for high-entropy metallic glasses (HEMGs) systems with complex compositions. Through the use of machine-learning potentials and deep learning models, properties such as T_g, β-relaxation process and mechanical properties of materials can be predicted with higher accuracy [37]. By learning from large datasets and automatically identifying structure–property relationships, AI models allow for a significant reduction in computational time compared to traditional simulations. At the same time, the reliability of the results is also improved through calibration using experimental data. This approach opens up the possibility of constructing a materials map for HEMGs, supporting the design of new materials with properties tailored to specific requirements [33, 34].

7.3. Exploring complex HEMG systems

The study of HEMGs systems with multiple components and complex medium-range order (MRO) structures is considered an important development direction in current materials science. These systems are characterized by a diversity of atomic sizes and binding energies, creating a microstructure rich in interactions and difficult to predict by traditional models. Through the combination of simulations,

experimental measurements and advanced analytical techniques, the formation, stability and phase transition mechanisms of HEMGs can be elucidated. These insights not only expand the range of applications of MGs in advanced industrial fields such as heat-resistant, wear-resistant, and highly ductile materials but also lay the foundation for the development of new generation amorphous alloys with performance tailored to specific engineering requirements [36, 38]. Recent experimental AI integrated studies further confirm the feasibility of designing HEMGs with tailored T_g and relaxation behavior [37].

7.4. Comprehensive integration of experimental and simulation data

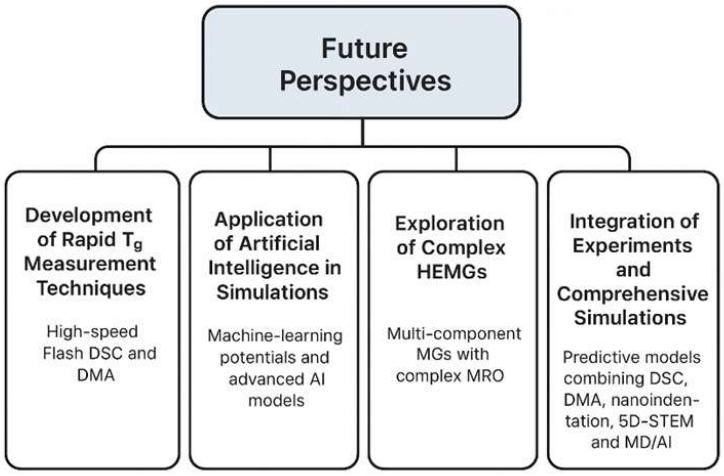

Figure 7. Summary of key findings and future directions in metal research

The simultaneous integration of experimental and simulation data is considered a key research direction to improve the prediction and design of metallic glasses (MGs). Data obtained from DSC, DMA, nanoindentation, and 5D Scanning Transmission Electron Microscopy (5D-STEM), when integrated with molecular dynamics (MD) simulations and artificial intelligence (AI) models, will form a comprehensive database that clearly reflects the relationship between microstructure and macroscopic properties of materials. Based on this integrated data platform, multi-scale predictive models can be built, allowing the determination of T_g, analysis of β-relaxation process and prediction of mechanical properties of MGs with higher accuracy. This approach opens up prospects for optimal MGs material design, flexibly meeting the requirements of mechanical performance, thermal stability and applications in advanced industries [26] in Figure 7.

8. Conclusion

Metallic glasses represent a unique class of materials whose properties are governed by non-crystalline atomic arrangements. The glass transition in metallic glasses (MGs) is determined to be strongly influenced by the short-range order (SRO) and medium-range order (MRO) microstructures, along with factors such as alloying ratios and interatomic bond energy distributions. By combining advanced experimental methods including DSC, Flash DSC, Dynamic Mechanical Analysis (DMA), nanoindentation, and 5D Scanning Transmission Electron Microscopy (5D-STEM) with molecular dynamics (MD) simulations and machine-learning potentials, the formation and transformation mechanisms of T_g, β-relaxation, and glass-to-glass transitions have been elucidated at the atomic level. Comparisons between Zr-based, Pd-based, and high-entropy metallic glasses (HEMGs) show that differences in SRO and MRO lead to significant variations in the mechanical properties, thermal stability, and phase transition kinetics of the materials.

This review also addresses the existing academic debates and suggests new research directions, including: improving fast Tg measurement techniques, applying artificial intelligence (AI) to material simulation, and extending research to HEMGs with complex compositions. This review highlights the critical role of multiscale integration in advancing both the fundamental understanding and practical application of metallic glasses.

Funding: The work received no funding.

Data Availability Statement: The data that support the findings of this study are available from the corresponding authors upon reasonable request.

Competing interests: The authors declare that they have no competing interests.

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