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REVIEW

# Relaxation Behavior in Metallic Glasses and Related Mechanisms by Simulation Method: A Brief Review

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**Abstract:** The relaxation dynamics of metallic glasses, as one of the most challenging issues, is complex. The relaxation, including $\alpha$ relaxation, slow $\beta$ relaxation, and fast $\beta$ relaxation, occurs at different temperatures. Taking advantage of the microscopic atomic information of simulation, the characteristics and mechanisms of these three typical relaxations were summarized to discuss their influence on mechanical properties of metallic glasses. Recent progresses on dynamical, structural, and physical mechanisms by simulation method were discussed. This review is beneficial to understand the nature of glass and to establish the dynamics-structure-property relationship of glassy materials.

**Key words:** metallic glasses; relaxation; dynamics; structure; mechanism

Glass materials are ancient materials, which have been used for thousands of years[1–3]. New information and potential applications of glass materials continue to emerge[1]. However, the nature of glass is still obscure, which restricts the application of glass materials. Metallic glasses (MGs) attract much attention as good model materials due to their simple structures in glass family[4–8].

MGs are usually prepared by rapid quenching of MG forming liquid. If the cooling rate is not fast or the temperature is not high enough, crystalline forms instead[9]. Therefore, MG is normally at non-equilibrium state. When MG is approaching the equilibrium state, relaxation behavior occurs[9–11]. Different from long range ordered structure in crystalline, disordered structures result in more complex relaxation behavior of MG[6,12]. The relaxation behavior is mainly investigated for conventional glass materials, such as molecular glasses and polymers. Many factors influence the relaxation behavior of MGs, forming various relaxation modes. From the perspective of frequency, the glass materials suffer $\alpha$ relaxation at low frequency (about $10^{-2}$ Hz), subsequently $\beta$ relaxation, and fast relaxation process at high frequency of $10^{6}$ Hz[3]. From the perspective of temperature, $\alpha$ relaxation occurs at very high temperatures; with decreasing the temperature, $\alpha$ relaxation and $\beta$ relaxation simultaneously occur; $\alpha$ relaxation can even be frozen at glass transition temperature ($T_g$) and $\beta$ relaxation becomes the main relaxation mode at low temperatures[9]. Initially, MG is found in the AuSi system[13]. Subsequently, the relaxation behavior of Pd- and La-based MGs has been researched[13–14]. Recently, the formation of bulk MGs promotes the further investigation of relaxation behavior in MGs[4,15–16]. It is normally considered that the $\alpha$ relaxation is related to the cooperative motion, and the $\beta$ relaxation is governed by local rearrangement[10–11]. Notably, the relationship between relaxation behavior and properties also attracts extensive attention, such as glass transition[17], crystallization[18], fragility[19], mechanical properties[20–21], and shear banding dynamics[22–23]. Many new relaxation modes have gradually been reported, including fast relaxation mode, slow relaxation mode, and fast $\beta$ relaxation mode[24–25], as shown in Fig. 1. Therefore, it is of great significance to study the relaxation mechanism for the deep investigation of the nature of MGs and the modification of properties. Taking the

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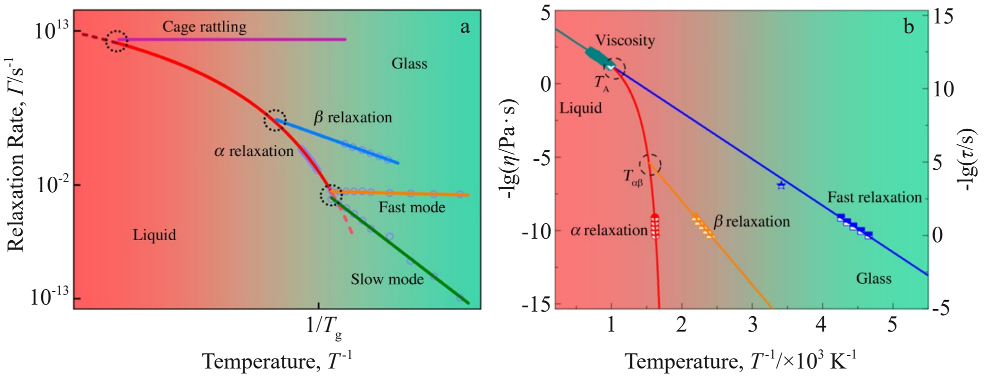

Fig.1 Schematic diagrams of relaxation modes in MGs: (a) dynamical behavior including fast modes and slow modes inherited from supercooled liquid of MGs[24]; (b) α relaxation, β relaxation, and fast relaxation[25]

advantage of simulation methods, the information of atomic structures and trajectories can be obtained, which is beneficial to investigate the relaxation mechanism[26]. Although numerous reviews discuss the relaxation modes in MGs[22,27–29], the relaxation mechanisms investigated by simulation methods are rarely reviewed.

In this review, the development of multiple relaxation modes and related mechanisms investigated by simulation method was summarized. The relationships among relaxation modes, dynamics, and structure properties were also discussed.

## 1 Relaxation Measurement by Simulation Method

In polymer or molecular glasses, dielectric spectroscopy is commonly used to study the relaxation behavior due to the wide frequency range[3]. However, dielectric spectroscopy cannot be applied on MGs because they are conductive. Therefore, dynamical mechanical analysis is used to measure the relaxation behavior for MGs[30]. The simulation and dynamical mechanical spectroscopy (DMS) are combined to obtain the stress response after the sinusoidal strain is applied on MG model[31]. To obtain accurate data, the stress response is collected at least 20 times at a given temperature with the same initial configuration but random momenta based on the Maxwell-Boltzmann distribution in the simulation[32]. Using the equation $\sigma(t)=\sigma_0+\sigma_A\sin(2\pi t/t_p+\delta)$, the stress data can be well fitted, and the phase shift ($\delta$) between the strain and stress can be obtained, as shown in Fig. 2[33]. Then, the equations $E'=\sigma_A/\varepsilon_A\cos(\delta)$ and $E''=\sigma_A/\varepsilon_A\sin(\delta)$ are used to compute the storage and loss moduli, respectively. Loss modulus can present the relaxation behavior. By simulation method, the dynamical and structural properties during the relaxation behavior can be obtained.

The activation relaxation technique can supply representative potential energy landscape samplings in amorphous systems. Although dynamical relaxations can be detected by annealing or activation relaxation techniques[34], DMS can achieve more obvious dynamics behavior. In DMS method, the first principles method is not appropriate due to its small system. Therefore, the molecular dynamics (MD) method is used to calculate the relaxation behavior of large systems. MD method mainly relies on Newtonian mechanics to simulate the atomic motions, and the potential functions in MD method are established based on the experiment data and Newtonian mechanics, which lack the electronic structure information. Thus, there are some gaps in results between experiment and simulation. In this case, some consistent qualitative results between experiment and simulation can be obtained.

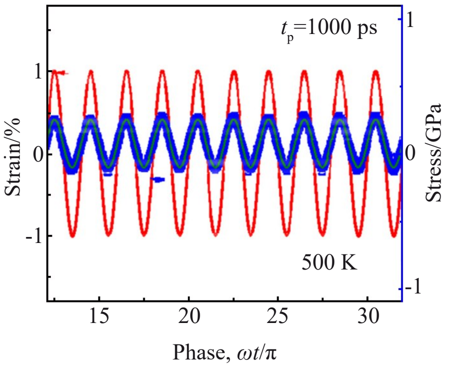

Fig.2 Simulated DMS data of MGs[33]

## 2 Typical Features of Temperature-Dependence Relaxation

As shown in Fig. 3, the loss modulus curve of $Al_{85}La_{10}Ni_5$ MG has three distinct peaks/humps, namely α relaxation at 550 K, β relaxation hump at 470 K, and obvious fast β relaxation peak[25]. The α relaxation at 550 K indicates the glass transition; the β relaxation hump at 470 K suggests the fast and localized motion; the fast β relaxation peak infers that some atoms present more obvious localized motions than those in the slow β relaxation do. The results obtained by simulation method are similar to those by experiments. Fig. 4 shows typical DMS results calculated by simulation method[35]. Fast β relaxation behavior cannot be observed in the ordinary systems because of the immature potential functions. Furthermore, the β relaxation peak can only be detected with prolonging the observation time to the order of microseconds or more[36]. Fast β relaxation can be observed in

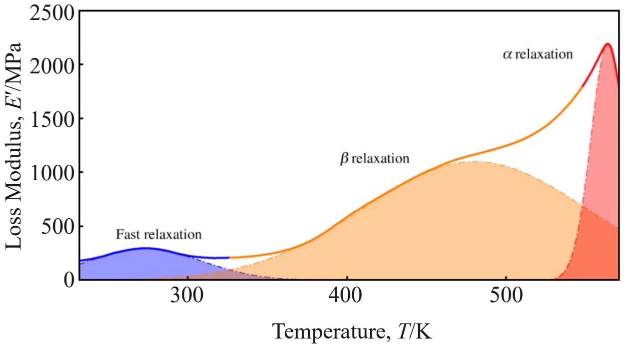

Fig.3 Loss modulus of $Al_{85}La_{10}Ni_5$ MG at frequency of 1 Hz[25]

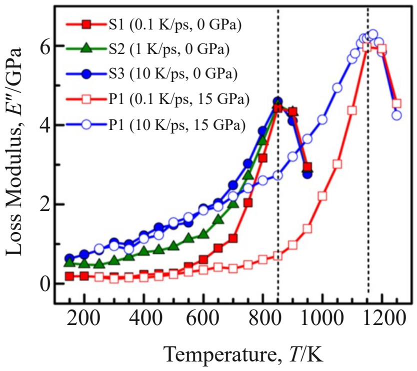

Fig.4 Simulated loss modulus of MGs at different cooling rates[35]

one special system to investigate the mechanism of low temperature relaxation peak. However, in this system, the slow $\beta$ relaxation peak cannot be observed[33]. Generally, glass materials show different $\beta$ relaxation behavior[37–40]: in some glass materials, $\beta$ relaxation presents obvious hump; in other glass materials, the $\beta$ relaxation separates from $\alpha$ relaxation, presenting the excess wing[38]. The fast $\beta$ relaxation also has different behavior: an obvious peak or hump, even just a wing[41–43]. According to the simulation results, most MGs show the excess wing or hump of $\beta$ relaxation and the excess wing of fast $\beta$ relaxation. This is caused by the immature potential function of complex MGs and the short observation duration compared with those in experiments. Only in some specific systems[33,44], the slow $\beta$ relaxation peak or the fast $\beta$ relaxation peak appears.

## 3 Physical Meaning Behind α Relaxation in MGs by Simulation Method

Glass can be formed by the cooling process of non-crystallizing glass forming liquid. The transition from solid-like (liquid-like) material to liquid-like (solid-like) material can be termed as glass transition ($\alpha$ relaxation), which is characterized by $T_g$ with the viscosity of $10^{13}$ Pa·s[45–46]. However, the nature of glass transition is still obscure in solid state theory[45]. Gao et al[47] reported that the observation time is a key parameter for the glass transition in phenomenological perspective. 3D schematic diagram for MGs shows the relationship among temperature, stress, and the observation time[47], as shown in Fig. 5a. Glass transition can be achieved by the variation of temperature, observation time, and/or stress. Without stress, the glass behaves as flow when the observation time is sufficiently long. Guan et al[50] confirmed the link between the stress-induced mechanical flow and temperature-induced glass-to-liquid transition by simulation method.

It is also demonstrated that the subtle structural change appears during the $\alpha$ relaxation induced by temperature or stress[51]. Indeed, the glass transition is the phenomenon of flow or sluggish dynamics, but the occurrence of glass transition in spite of the subtle change of the structures requires further investigations. Although subtle change exists in pair distribution function (PDF) during the glass transition or $\alpha$ relaxation, Hu et al[48] found the universal structural indicator in MGs: the average degree of five-fold local symmetry $W$, which could characterize the underlying structural mechanism during the dynamic arrested process. A simple relationship $\tau_\alpha = \tau_0 \exp[D/(1-W^\delta)]$ exists between structure and dynamics, suggesting the structural heterogeneity accompanied with the dynamic heterogeneity, where $\tau_\alpha$ exhibits $\alpha$ relaxation time; $\tau_0$ is the relaxation time at infinite liquidus temperature; $D$ and $\delta$ are fitting parameters. This relationship supplies the structural mechanism or atomic structural perspective behind the dynamics arrest during the $\alpha$ relaxation, and the five-fold symmetry is responsible for the dramatic dynamic slowdown. Besides, Yu et al[49] found that the $\alpha$ relaxation always appears when the most probable atomic displacement achieves the critical value (20%) of the average interatomic distance, regardless of the temperature-induced relaxation or stress-induced relaxation. The average interatomic displacement can be calculated by the ratio of the peak of probability density function $p(u)$ to the first peak of PDF ($u_p/r_p$), as shown in Fig. 5d. Lindeman-like criterion can be used to determine the $\alpha$ relaxation. Initially, the Lindeman criterion is used to characterize the melting of crystalline solid. Herein, this criterion is appropriate for $\alpha$ relaxation dynamics induced by temperature or stress. It is worth noting that the Lindeman criterion can present the structure instability, so it can also reveal the structural mechanism of $\alpha$ relaxation in perspective of Lindemann criterion or instability of structures[7,52]. By extensive simulations, Tanaka et al[53] found the structural origin of $\alpha$ relaxation, indicated by the link between drastic slowdown dynamics and critical-like fluctuations of static structural orders. From the dynamical perspective, Yu et al[54] found the relationship between atomic rearrangement and viscoelastic moduli in the $\alpha$ relaxation range. Conrad et al[55] reported that only the slow-moving particles affect the dynamic shear moduli, and the viscoelasticity in MGs is the consequence of all collective rearrangements in the whole system. However, the fast moving atoms are liquid-like and cannot bear the stress. Thus, these atoms cannot support the increase in viscoelastic modulus. This is consistent with the previous report that $\alpha$

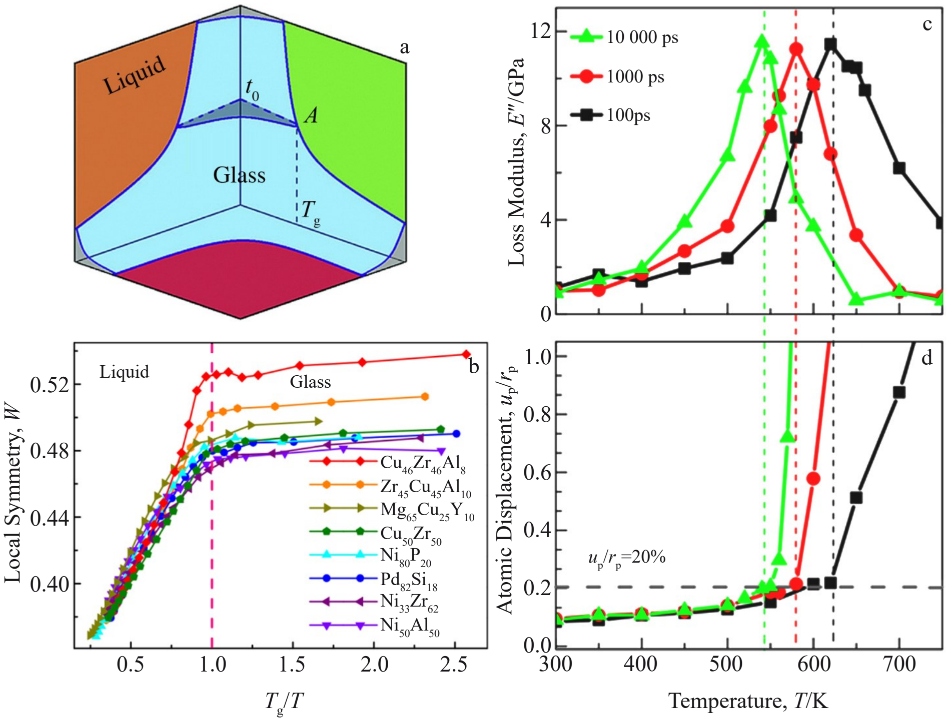

Fig.5 Features and mechanism of $\alpha$ relaxation: (a) schematic diagram of influence factors of observation time $t$, stress $\sigma$, temperature $T$ in $\alpha$ relaxation[47]; (b) five-fold local symmetry $W$ during quenching process[48]; (c) simulated loss modulus[49]; (d) the most probable atomic displacement $u_p/r_p$ at different temperatures[49]

relaxation corresponds to the irreversible non-local atomic rearrangement, which is also the collective rearrangement in the whole systems[56].

## 4 Mechanism of Slow β Relaxation Behavior by Simulation Method

Originally, the slow $\beta$ relaxation was discovered in polymer glasses, which is assumed as the consequence of the motion of side chains or function groups[57]. Afterwards, Johari et al[58] detected the $\beta$ relaxation in glasses of rigid molecule, which changes the relaxation origination from intramolecular degree of freedom to the motion of entire molecule. Therefore, the slow $\beta$ relaxation is regarded as J-G relaxation to be distinguished from other secondary relaxations[58]. Glassy materials with pronounced $\beta$ relaxation usually have good ductility and tensile plasticity[21], and therefore can be regarded as the potential mechanical application materials. Glassy medicines can be recrystallized, whereas the $\beta$ relaxation is not desirable and unstable. Therefore, the crystal counterparts are more ideal for medicines[59]. The $\beta$ relaxation correlates with many properties even in MGs, such as glass transition, fragility, mechanical properties, and deformation behavior[17–21,59], which is important for the investigation of fundamental issues, such as liquid dynamics, rejuvenation, and physical aging[60–62]. Thus, it is urgent to further study the $\beta$ relaxation and to find the related mechanism.

Generally, there are two mechanisms of $\beta$ relaxation: Dixon et al[63] reported that $\beta$ relaxation is the extension of $\alpha$ relaxation, whereas Schneider et al[64] found that $\beta$ relaxation is an independent relaxation mechanism. Related questions and theories have been proposed based on different perspectives.

(1) Is $\beta$ relaxation composed of cooperative motions or local motions? The initial investigation of $\beta$ relaxation by DMS method[31] reported that the motions contributing to $\beta$ relaxation are observed by pinning method, and the pinned particles only participate in the affine displacement other than non-affine deformation. Therefore, the pinned particles do not contribute to the relaxation dynamics. If the $\beta$ relaxation involves the local motion, a small number of pinned particles do not influence the strength of $\beta$ relaxation dramatically. However, the $\beta$ relaxation is completely suppressed when the pinned particles exceeds 2.5at% , which indicates that the motion of $\beta$ relaxation is cooperative[31]. The cooperative motion is regarded as a recoil motion of free particle colliding with a pinned particle, which is derived from the self-part of the intermediate scattering function of systems with different contents of pinned particles[31].

(2) Do all atoms or some specific atoms involve in the $\beta$ relaxation? Is there any dynamic parameter dominating the $\beta$ relaxation process? Yu et al[65] investigated the relaxation behavior through the relationship between mechanical loading time ($T_w$) of DMS method and internal friction ($\delta$). To observe the dynamic information, based on the resultant distribution density function $p(u)$ with different $T_w$, the most probable values of displacement ($u_p$) are basically the same regardless of different $\delta$ at low temperatures. However, the

tail of $p(u)$ curve is obviously different, indicating that not all atoms dominate the $\beta$ relaxation behavior. The atoms with displacement larger than $u_p$ are faster atoms, which are the underlying mechanism of internal friction $\delta$, as shown in Fig. 6a[65]. Wang et al[35] systematically investigated the effect of cooling rate and pressure on low temperature relaxation behavior to find the dominant dynamic parameter of $\beta$ relaxation process. After analyzing the spatial distribution of fast atoms, the intrinsic dynamic heterogeneity is the key parameter, which dominates the low temperature relaxation, as shown in Fig. 6b[35]. Additionally, the local relaxation involves less than 30 atoms, and its size is independent of cooling history[53]. These phenomena verify the role of fast atoms in the $\beta$ relaxation, and the intrinsic dynamic heterogeneity is the dynamic mechanism of $\beta$ relaxation.

(3) However, which cooperative motion of fast atoms dominates the $\beta$ relaxation? It is demonstrated that the $\beta$ relaxation can be detected when the observation time is at microsecond level[36]. However, due to the limit of the simulation time, the $\beta$ relaxation exhibits excess wings or humps even in the La-based systems, whereas the obvious peak appears in experiment[67]. Yu et al[44] overcame the difficulties of time scale in simulation and observed the peak of $\beta$ relaxation in $Ni_{80}P_{20}$ system. It is found that most fast atoms have string-like motions, implying that the string-like motions dominate the structural arrangement and relaxation behavior at low temperatures. The most probable time of strings $\tau_{str}$ can be measured by the peak number of atoms involved in strings over the number of fast atoms. As shown in Fig. 6c, the $\tau_{str}$ departures from the time of $\alpha$ relaxation, which can be fitted by the equation $\tau_{str}=\tau_0{}^{n}\tau_\alpha{}^{1-n}$. The coupling model[68] can be used to describe the relationship between $\alpha$ and $\beta$ relaxations. Additionally, the overlap between $\tau_{str}$ and $\tau_\beta$ confirms the correlation between string-like motions and $\beta$ relaxation[44]. Moreover, the relaxation behavior of $Ni_{80}P_{20}$ and $Y_{65}Cu_{35}$ alloys is compared, which presents the peak and excess wing, respectively. It is found that $Ni_{80}P_{20}$ alloy has more sting-like configurations than $Yi_{65}Cu_{35}$ alloy does, and the strings are longer in $Ni_{80}P_{20}$ alloy[66]. The cage-breaking fraction $C(T,\ t=\delta t)=N_{lost}/N_{nb}$ ($N_{nb}$ means the number of neighboring atoms and $N_{lost}$ is the number of lost atoms previously resided in the neighboring regions) at temperature $T$ and time $\delta t$ shows that the cages of $Ni_{80}P_{20}$ alloy are more prone to break, as shown in Fig.6d[66]. This result suggests that cage properties can affect the string-like motions and thereby the $\beta$ relaxation.

(4) Which local structure dominates the slow $\beta$ relaxation? Voronoi analysis is commonly employed to investigate the

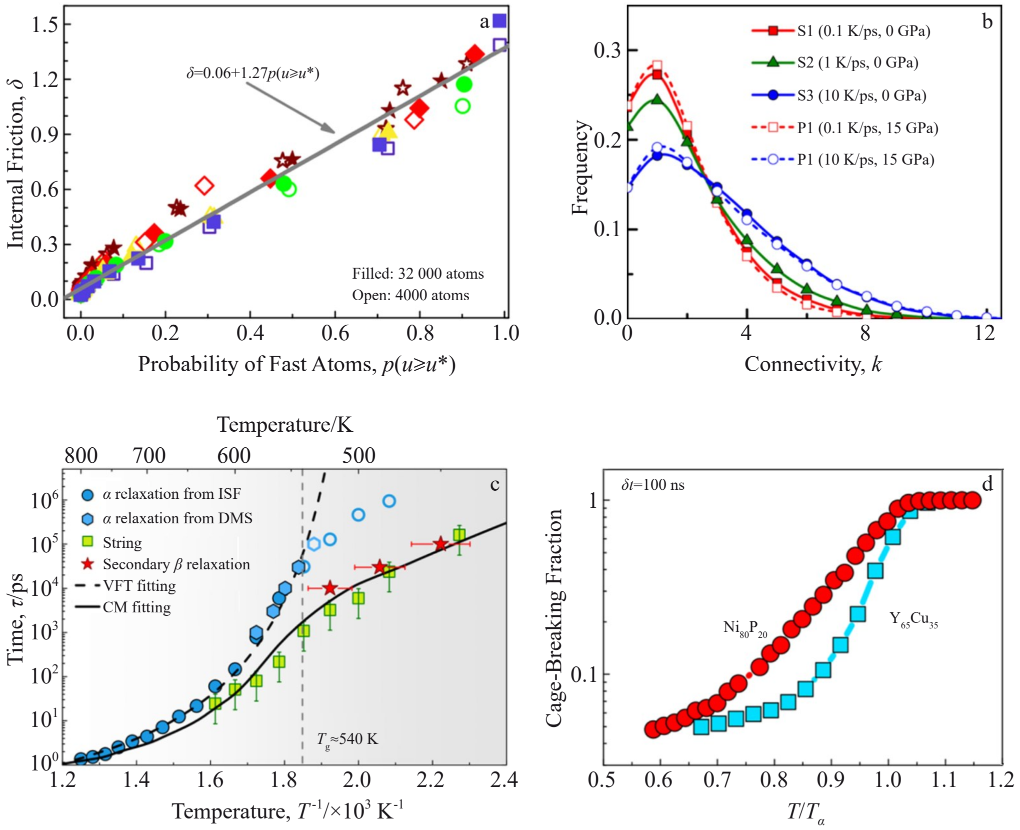

Fig.6 Mechanism of slow $\beta$ relaxation: (a) relationship between internal friction $\delta$ and probability of fast atoms $p(u>u^*)$[65]; (b) connectivity distribution of fast atoms reflecting the dynamic heterogeneity information[35]; (c) relationships between temperature and time of $\alpha$ relaxation, $\beta$ relaxation, and string motions as well as Vogel-Fulcher-Tammann (VFT) fitting and coupling model (CM) fitting results[44]; (d) relationship between cage-breaking fraction and scaled temperature in $Ni_{80}P_{20}$ and $Y_{65}Cu_{35}$ alloy[66]

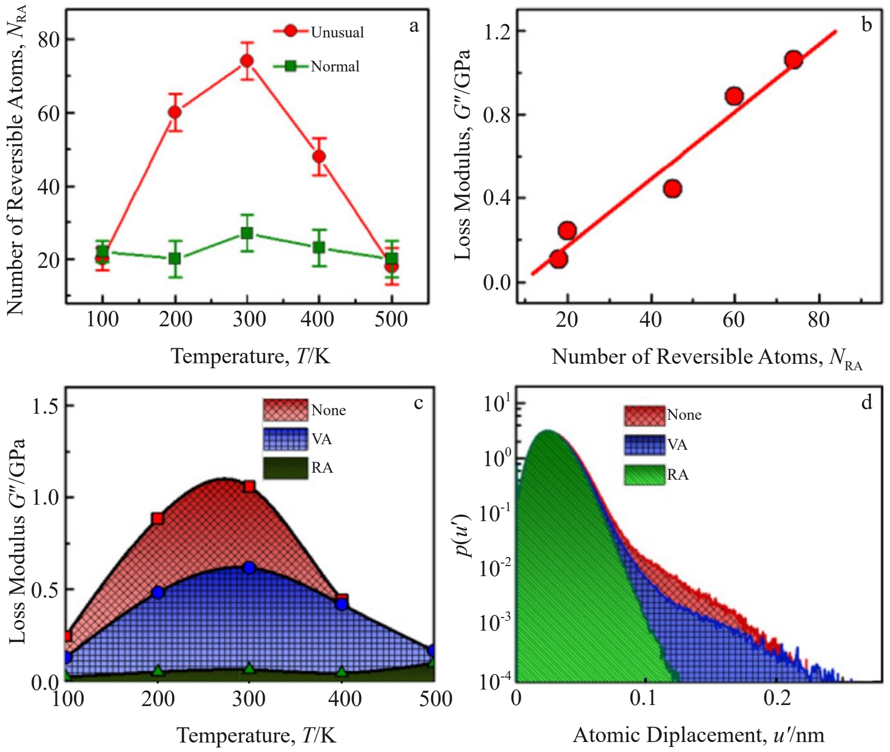

Fig.7 Mechanism of ultra-low temperature relaxation peak[33]: (a) relationship between the number of reversible atoms and temperature; (b) linear relationship between loss modulus and the number of reversible atoms; (c) relationship between loss modulus and temperature; (d) relationship between $p(u')$ and atomic displacement $u'$ (none: no motion; VA: vibrational atoms; RA: reversible atoms)

features of fast atoms in MGs. Yu et al[65] found that the icosahedral polyhedrons and fast atoms are unrelated. Instead, fast atoms are polyhedrons with complex geometries. However, the accurate relationship between structure and $\beta$ relaxation is still in debate.

## 5 Mechanism of Relaxation Located at Much Lower Temperatures by Simulation Method

Glassy materials are composed of regions with different relaxation time, which correspond to different relaxation modes. MGs have similar characteristics[10]. When the test temperature is very low (173 K, in La-based MG), the fast $\beta$ relaxation can be observed from 200 K to 300 K[41–42]. The strength of this new peak is approximately 1/100 of that of $\alpha$ relaxation, and the activation energy is rather low, which is about half of that of $\beta$ relaxation[41]. Rico et al[69] found the rattling motions constitute the fast processes through annealing method. Furthermore, Wang et al[33] found that a specific MG model has the ultra-low temperature ($0.3T_g$) relaxation peak through DMS method, which is similar to the fast relaxation peak. Different from slow $\beta$ relaxation, no correlations can be found between fast atoms and loss modulus. According to the atomic trajectories, the atomic motions are classified into three types. Type 1: the atoms vibrate smoothly around the initial locations with the displacement less than 0.1 nm. Type 2 and type 3: the atoms have intermittent motions: vibrations→rapid reversible motions→irreversible jumps. The atoms of type 2 exhibit reversible properties, whereas the atoms of type 3 show irreversible motions. The reversible atoms (type 2) show good linear relationship with loss modulus, as shown in Fig. 7b[33], indicating that the low temperature relaxation peak may originate from the reversible atoms. The atomic pinning method is used to confirm the relationship between the reversible atoms and loss modulus, as shown in Fig. 7c – 7d. After pinning the reversible atoms, the loss modulus and the atomic displacements decrease dramatically. This confirms that the fast $\beta$ relaxation peak originates from reversible atoms. Additionally, the atoms contributing to fast $\beta$ relaxation also show string-like motions[25]. The rattling phenomenon of atoms shows that the reversible process has connection with the fast $\beta$ relaxation[69], which requires further research.

## 6 Summary

This review summarizes the recent development of the mechanisms of relaxation behavior by simulation method in metallic glasses (MGs), which reveals the nature of glass and provides information for property modification, such as deformation behavior and crystallization. However, the physical mechanisms are still obscure, which requires further research.

1) The relationship between structures and relaxation behavior should be further studied through suitable structural parameters.

2) The potential function is the most fundamental and important factor in the simulation. However, the accuracy of

the potential functions needs to be enhanced due to the lack of consideration of electronic structures in current researches. Potential functions are suitable to calculate some specific properties, and more accurate potential functions are required to check the relaxation properties.

3) The mechanism of relaxation behavior in different MGs is complex due to the relationship between relaxations and composition[70]. Some useful potential functions in complicated MGs are required.

4) It is promising that the relaxation modes are crucial for property modification of glassy materials.

## References

1 Dyre J. *Review of Modern Physics*[J], 2006, 78(3): 953

2 Petrie F. *Transactions of the Newcomen Society*[J], 2014, 5(1): 72

3 Lunkenheimer P, Schneider U, Brand R *et al. Contemporary Physics*[J], 2000, 41(1): 15

4 Wang W H, Dong C, Shek C H. *Materials Science & Engineering R: Reports*[J], 2004, 44(2–3): 45

5 Yavari A R. *Nature*[J], 2006, 439(7075): 405

6 Sheng H W, Luo W K, Alamgir F M *et al. Nature*[J], 2006, 439(7075): 419

7 Egami T. *Materials Science and Engineering A*[J], 1997, 226: 261

8 Wang W H. *Advanced Materials*[J], 2009, 21(45): 4524

9 Debenedetti P G, Stillinger F H. *Nature*[J], 2001, 410(6825): 259

10 Angell C A, Ngai K L, McKenna G B *et al. Journal of Applied Physics*[J], 2000, 88(6): 3113

11 Ngai K. *Relaxation and Diffusion in Complex Systems*[M]. Berlin: Springer, 2011

12 Liu X, Xu Y, Hui X *et al. Physical Review Letters*[J], 2010, 105(15): 155501

13 Klement W, Willens R H, Duwez P O L. *Nature Communication*[J], 1960, 187(4740): 869

14 Okumura H, Chen H S, Inoue A *et al. Journal of Applied Physics*[J], 1991, 130(3): 304

15 Peker A, Johnson W L. *Applied Physics Letters*[J], 1993, 63(17): 2342

16 Inoue A. *Acta Materialia*[J], 2000, 48: 279

17 Ediger M D, Harrowell P. *Journal of Chemical Physics*[J], 2012, 137(8): 80901

18 Xing P, Zhuang Y, Wang W *et al. Journal of Applied Physics*[J], 2002, 91(8): 4956

19 Yu H B, Wang Z, Wang W H *et al. Journal of Non-crystal Solids*[J], 2012, 358(4): 869

20 Yu H B, Wang W H, Bai H Y *et al. Physical Review B*[J], 2010, 81(22): 220201

21 Yu H B, Shen X, Wang Z *et al. Physical Review Letters*[J], 2012, 108(1): 15504

22 Yu H B, Wang W H, Samwer K. *Materials Today*[J], 2013, 16(5): 183

23 Zhou Z Y, Sun Y, Gao L *et al. Acta Materialia*[J], 2023, 246: 118701

24 Luo P, Wen P, Bai H Y *et al. Physical Review Letters*[J], 2017, 118(22): 225901

25 Chang C, Zhang H P, Zhao R *et al. Nature Materials*[J], 2022, 21(11): 1240

26 Plimpton S. *Journal of Computational Physics*[J], 1995, 117(1): 1

27 Yu H B, Wang W H, Bai H Y *et al. National Science Review*[J], 2014, 1: 429

28 Qiao J C, Wang Q, Crespo D *et al. Chinese Physics B*[J], 2017, 26: 16402

29 Qiao J C, Zhang L T, Tong Y *et al. Advances in Mechanics*[J], 2022, 52: 117

30 Wen P, Zhao D Q, Pan M X *et al. Applied Physics Letters*[J], 2004, 84(15): 2790

31 Cohen Y, Karmakar S, Procaccia I *et al. Euro Physics Letters*[J], 2012, 100(3): 36003

32 Widmer-Cooper A, Harrowell P, Fynewever H. *Physical Review Letters*[J], 2004, 93(13): 135701

33 Wang B, Wang L J, Shang B S *et al. Acta Materialia*[J], 2020, 195: 611

34 Fan Y, Iwashita T, Egami T. *Physical Review Letters*[J], 2015, 115: 45501

35 Wang B, Shang B S, Gao X Q *et al. Journal of Physical Chemistry Letters*[J], 2016, 7(23): 4945

36 Kudlik A, Tschirwitz C, Benkhof S *et al. Europhysics Letters*[J], 1997, 40(6): 649

37 Wen P, Zhao D Q, Pan M X *et al. Intermetallics*[J], 2004, 12(10–11): 1245

38 Wang W H, Wen P, Liu X F. *Journal of Non-crystal Solids*[J], 2006, 352(42–49): 5103

39 Zhu Z G, Li Y Z, Wang Z *et al. Journal of Chemical Physics*[J], 2014, 141(8): 84506

40 Yu H B, Samwer K, Wang W H *et al. Nature Communications*[J], 2013, 4(1): 2204

41 Wang Q, Zhang S T, Yang Y *et al. Nature Communications*[J], 2015, 6(1): 7876

42 Küchemann S, Maaß R. *Scripta Materialia*[J], 2017, 137: 5

43 Jiang H Y, Luo P, Wen P *et al. Journal of Applied Physics*[J], 2016, 120(14): 145106

44 Yu H B, Richert R, Samwer K, *Science Advances*[J], 2017, 3: e1701577

45 Angell C A. *Current Opinion Solid State Materials Science*[J], 1996, 1(4): 578

46 Biroli G, Garrahan J P. *Journal of Chemical Physics*[J], 2013, 138(12): 12A301

47 Gao X Q, Wang W H, Bai H Y. *Journal of Materials Science & Technology*[J], 2014, 30(6): 546

48 Hu Y C, Li F X, Li M Z *et al. Nature Communications*[J], 2015, 6(1): 1

49 Yu H B, Richert R, Maass R *et al. Physical Review Letters*[J],

2015, 115(13): 135701

50 Guan P F, Chen M W, Egami T. *Physical Review Letters*[J], 2010, 104(20): 205701

51 Wang L, Xu N. *Physical Review Letters*[J], 2014, 112(5): 55701

52 Samanta A, Tuckerman M E, Yu T Q *et al. Science*[J], 2014, 346(6210): 729

53 Tanaka H, Kawasaki T, Shintani H *et al. Nature Materials*[J], 2010, 9: 324

54 Yu H B, Richert R, Samwer K. *Journal of Physical Chemistry Letters*[J], 2016, 7(19): 3747

55 Conrad J C, Dhillon P P, Weeks E R *et al. Physical Review Letters*[J], 2006, 97(26): 265701

56 Wang B, Wang L J, Wang W H *et al. Journal of Applied Physics*[J], 2017, 121(17): 175106

57 Retting W. *European Polymer Journal*[J], 1970, 6(6): 853

58 Johari G P. *Journal of Chemical Physics*[J], 1970, 53(6): 2372

59 Bhattacharya S, Suryanarayanan R. *Journal of Pharmaceutical Sciences*[J], 2009, 98(9): 2935

60 Qiao J C, Casalini R, Pelletier J M. *Journal of Chemical Physics*[J], 2014, 141(10): 104510

61 Wen P, Zhao Z F, Wang W H. *Science in China Series G: Physics, Mechanics and Astronomy*[J], 2008, 51(4): 356

62 Liang S Y, Zhang L T, Wang B *et al. Intermetallics*[J], 2024, 164: 108115

63 Dixon P K, Wu L, Nagel S R *et al. Physical Review Letters*[J], 1990, 65(9): 1108

64 Schneider U, Brand R, Lunkenheimer P *et al. Physical Review Letters*[J], 2000, 84(24): 5560

65 Yu H B, Samwer K. *Physical Review B*[J], 2014, 90(14): 144201

66 Yu H B, Yang M H, Sun Y *et al. Journal of Physical Chemistry Letters*[J], 2018, 9(19): 5877

67 Zhang H P, Wang F R, Li M Z. *Journal of Physical Chemistry B*[J] 2019, 123(5): 1149

68 Ngai K L, Paluch M. *Journal of Chemical Physics*[J], 2004, 120(2): 857

69 Rico P P, Papageorgiou D, Greer A *et al. Acta Materialia*[J], 2017, 135: 290

70 Duan Y J, Zhang L T, Qiao J C *et al. Physical Review Letters*[J], 2022, 129(17): 175501

# 金属玻璃弛豫行为及其机理的模拟研究进展

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**摘　要：**金属玻璃的弛豫动力学研究非常复杂，极具挑战性。弛豫（$\alpha$弛豫、慢$\beta$弛豫和快$\beta$弛豫）发生在不同的温度下。利用模拟可观测微观原子信息的优势，评述了模拟中3种典型弛豫的特征和机理，并讨论了它们对材料力学性能的影响。讨论了近年来通过模拟方法获得的与弛豫相关的动力学、结构和物理机理方面的研究进展。本综述有助于认识玻璃的本质，建立玻璃材料的动力学-结构-性能关联。

**关键词：**金属玻璃；弛豫行为；动力学；结构；机制

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