DISTINCT RELAXATION DYNAMICS AT ROOM TEMPERATURE IN METALLIC GLASS

by

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In this article we suggest the equations for the distinct relation processes at room temperature in metallic glass for the first time. We consider the Kohlrausch-Williams-Watts decay laws with the stretching exponents values of $\ell = 3/5$ and $\ell = 3/7$. It provides a new insight to the comprehensive understanding of the stretched exponential decay law at room temperature in metallic glass.

Key words: *distinct dynamics, distinct relation processes, relaxation equations, room temperature, Kohlrausch-Williams-Watts decay law, metallic glass*

Introduction

The experiments and numerical simulations studies of the relaxation dynamics at room temperature in metallic glasses (MG) have continuously attracted increasingly interest across the physics and materials science [1]. The relaxation processes at room temperature in MG can be considered as the relaxation dynamics at low temperature in molecular and electronic glasses [2, 3] because there exists such evidence for the non-exponential relaxation [4] due to the time-scale behaviors [5]. The time scale for the aging in MG was considered as the atomic-scale arising in atomic-scale relaxation dynamics in MG [6]. The anelastic relaxation of MG [7-10] can be expressed by the Kohlrausch-Williams-Watts (KWW) function (or stretched exponential function) [11-13]. The KWW decay law (or stretched exponential decay law) was considered in the glasses at low temperature [14]. The KWW decay law for the MG at low temperature was reported in [15]. The important result for the KWW decay law for the high-entropy MG was discovered in [16]. The relaxation dynamics at low temperature in molecular and electronic glasses was described by the KWW relation function [1, 3-5, 8]:

$$\Phi\left(t\right)=\exp\left(-\alpha t^{\ell}\right) \tag{1}$$

where $\alpha = 1/\mu^{\ell}$ is the relaxation constant with the relaxation time ($\mu > 0$) and the stretching exponent ($1 > \ell > 0$). In fact, the series expression of the KWW function is given by [13]:

$$\exp\left(-t^{\ell}\right)=\sum_{i=0}^{\infty}\frac{\left(-1\right)^{i}t^{\ell i}}{i!}$$

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In the experimental measures for MG, there exist the stretching exponent values of $\ell = 3/5$ [7] and $\ell = 3/7$ [1]. The modified KWW relation process for the glasses was also discovered in [17]. Let ρ be the fractal dimensionality of the relaxation pathways in the phase space [18]. With use of the Phillips model [3], it is known that the stretching exponent ℓ $(1 > \ell > 0)$ is expressed as $\ell = \rho/(\rho + 2)$ [3, 18]. The KWW decay law of MG at room temperature with the value of $\ell = 3/5$ is modeled by [2, 7]:

$$\Phi_{3/5}(t) = \exp\left[-\left(\frac{t}{\mu}\right)^{3/5}\right] \tag{2}$$

where eq. (2) was used to present the relaxation for realistic alkali aluminosilicate glasses [7]. It is easily observed that the value of the dimensionality of the relaxation pathways in the phase space is equal to 3 [18]. When $\ell = 3/5$ and $\rho = 3$, the relaxation channel for MG at room temperature goes into the short-range contribution. The KWW decay law of MG at room temperature with the value of $\ell = 3/7$ was expressed by [1, 2]:

$$\Phi_{3/7}(t) = \exp\left[-\left(\frac{t}{\mu}\right)^{3/7}\right] \tag{3}$$

Here, eq.(3) was considered as the relaxation in Corning Gorilla Glass at room temperature [1, 2]. It is clearly seen that the value of the dimensionality of the relaxation pathways in the phase space is equal to 3/2 [18]. When $\ell = 3/7$ and $\rho = 3/2$, the relaxation channel for MG at room temperature goes into the long-range contribution.

Both experimental and simulation studies for the relaxation dynamics in MG at room temperature are still great and important challenge issue [2]. The target for this work is to show the relation equation for the KWW decay law of MG at room temperature with the stretching exponent values of $\ell = 3/5$ and $\ell = 3/7$. The results are used to give the comprehensive understanding of the KWW decay law at room temperature in MG. It may make an important breakthrough for the theoretical framework of the relation dynamics at room temperature in MG.

Methods

To get the equation of the KWW decay law at room temperature, we start with the exponential relaxation for the relaxation dynamics with the relation time $\vartheta > 0$. The relaxation function $\Phi_C(t)$ for the exponential relaxation process reads [1, 3]:

$$\Phi_C(t) = \exp\left(-\frac{t}{\vartheta}\right) \tag{4}$$

where t is the time. The equation for the exponential relaxation process with eq. (4) can be expressed as [1, 3]:

$$\Phi_C^{(1)}(t) + \frac{1}{\vartheta}\Phi_C(t) = 0 \tag{5}$$

The initial value condition for the exponential relaxation process at the point $t = 0$ is suggested [1, 3]:

$$\Phi_C(0) = 1$$

By taking $t = g(x)$ and $\vartheta = \varpi > 0$ in eq. (4), where $g^{(1)}(x) > 0$ it is very easy to see:

$$\Phi_g(x) = \exp\left(\frac{g(x)}{\varpi}\right) \tag{7}$$

which yield that:

$$\frac{1}{g^{(1)}(x)}\frac{\mathrm{d}\Phi_g(x)}{\mathrm{d}x}+\frac{1}{\varpi}\Phi_g(x)=0 \tag{8}$$

where the initial value condition at the point $t = 0$ reads $\Phi_g(0) = \exp(-g(0)/\varpi)$. When we take $\varpi = 1$ in eq. (8), we can get:

$$\frac{1}{g^{(1)}(x)}\frac{\mathrm{d}\Phi_g(x)}{\mathrm{d}x}+\Phi_g(x)=0 \tag{9}$$

which is in agreement with the reported result [13] under the initial value condition of eq. (9). Making use of the aforementioned results, we now derive the relation equations for the distinct relation processes at room temperature in MG. Taking $g(x) = t^\ell$ and $\varpi = \alpha$ in eq. (7), we present the relation function for the KWW decay law:

$$\Phi(t)=\exp\left[-\left(\frac{t}{\mu}\right)^{\ell}\right] \tag{10}$$

Substituting $g(x) = t^\ell$ and $\varpi = \alpha$ into eq. (8), the relation equation of the KWW decay law (10) can be given:

$$\ell^{-1}t^{1-\ell}\frac{\mathrm{d}\Phi(t)}{\mathrm{d}t}+\frac{1}{\mu^{\ell}}\Phi(t)=0 \tag{11}$$

Appling $g(x) = t^\ell$ and taking $t = 0$ in eq. (9), the initial value condition for the relation eq. (11) at the point $t = 0$ is given by $\Phi(0) = 1$. Theoretically, eq. (11) may be used to describe the theory of the relaxation dynamics at low temperature in molecular and electronic glasses [3] for the different stretching exponents and dynamical heterogeneities [19]. When the stretching exponent value ℓ is equal to 1, the process becomes the exponential relaxation process for the relation function (4) [1].

Results

We now consider the KWW decay law of glasses at room temperature with the stretching exponent values of $\ell = 3/5$ and $\ell = 3/7$. When the value of the stretching exponent for the KWW decay law of the metallic glasses at room temperature is $\ell = 3/5$, it is seen from eq. (11) that the relation equation for the KWW decay law of MG at room temperature can be written:

$$\frac{5}{3}t^{2/5}\frac{\mathrm{d}\Phi_{3/5}(t)}{\mathrm{d}t}+\mu^{-3/5}\Phi_{3/5}(t)=0 \tag{12}$$

with the initial condition of $\Phi_{3/5}(0) = 1$.

In a similar way, making use of eq. (11), the relation equation for MG at room temperature for the value of $\ell = 3/7$ is given:

$$\frac{7}{3}t^{4/7}\frac{\mathrm{d}\Phi_{3/7}(t)}{\mathrm{d}t}+\mu^{-3/7}\Phi_{3/7}(t)=0 \tag{13}$$

with the initial value condition of $\Phi_{3/7}(0) = 1$.

As shown in tab. 1, by taking $\ell = 3/5$ in eq. (10), eq. (13) is the relaxation equation for the relaxation channel for MG at room temperature in the short-range contribution with $\ell = 3/5$ and $\rho = 3$ and eq. (2) is the relation function for MG at room temperature with $\ell = 3/5$. There exists a typical example for the KWW decay law with the distinct relation process, given by eq. (13), which is the relaxation behavior for realistic alkali aluminosilicate glasses [7]. Compared with the exponential relaxation process (4), the distinct relation process with $\ell = 3/5$ and $\rho = 3$ needs to care about the power-law term of $\alpha(t) = 5t^{2/5}/3$ and the relaxation constant changes from $1/\vartheta$ into $\mu^{-3/5}$.

Table 1. The mathematical and physical processes for the distinct relaxation dynamics at room temperature in MG

Stretching exponents values	Dimensionalities of the relaxation pathways	Distinct relation processes	Initial value conditions	KWW decay laws	Physical processes
$\ell = 3/5$ [2]	$\rho = 3$ [3]	(12)	$\Phi_{3/5}(0) = 1$	(2) [7]	The short-range contribution [18]
$\ell = 3/7$ [2]	$\rho = 3/2$ [3]	(13)	$\Phi_{3/7}(0) = 1$	(3) [1]	The long-range contribution [18]

By applying $\ell = 3/7$ in eq. (10), eq. (14) is the relaxation equation for the relaxation channel for MG at room temperature in the long-range contribution with $\ell = 3/7$ and $\rho = 3/2$ based on the Phillips diffusion-trap theory [3, 18], and eq. (3) is the relation function for MG at room temperature with $\ell = 3/7$. It has been observed that the typical example for the KWW decay law with the distinct relation process, given by eq. (14), which is the room temperature relaxation behavior for Corning Gorilla Glass at room temperature. In fact, the special conditions for the relaxation behavior were presented in [1]. Compared with the exponential relaxation process (4), the distinct relation process with $\ell = 3/7$ and $\rho = 3/2$ needs to care about the power-law term of $\beta(t) = 7t^{4/7}/3$ and the relaxation constant changes from $1/\vartheta$ into $\mu^{-3/5}$.

Conclusion

In the work we have presented the equations for KWW decay laws at room temperature in MG. They have been applied to illustrate two experiment evidences for the distinct relaxation dynamics. The result is a positive reply for the important challenge for KWW decay laws.

Contribution

Contribute to the work in Honor of Professor Feng Gao's 60th Birthday.

Nomenclature

ℓ – stretching exponent, [–]
t – time, [s]

Greek symbol

μ – relaxation time, [s]

References

[1] Welch, R. C., *et al*., Dynamics of Glass Relaxation at Room Temperature, *Physical Review Letters*, *110* (2013), 26, ID265901
[2] Sun, Y. T., *et al*., Distinct Relaxation Mechanism at Room Temperature in Metallic Glass, *Nature Communications*, *14* (2023), 1, ID540
[3] Phillips, J. C., Stretched Exponential Relaxation in Molecular and Electronic Glasses, *Reports on Progress in Physics*, *59* (1996), 9, ID1133
[4] Sastry, S., *et al*., Signatures of Distinct Dynamical Regimes in the Energy Landscape of a Glass-Forming Liquid, *Nature*, *393* (1998), June, pp. 554-557
[5] Rabani, E., *et al*., Direct Observation of Stretched-Exponential Relaxation in Low-Temperature Lennard-Jones Systems Using the Cage Correlation Function, *Physical Review Letters*, *82* (1999), 18, ID3649
[6] Ruta, B., *et al*., Atomic-Scale Relaxation Dynamics and Aging in a Metallic Glass Probed by X-Ray Photon Correlation Spectroscopy, *Physical Review Letters*, *109* (2012),16, ID165701
[7] Yu, Y., *et al*., Stretched Exponential Relaxation of Glasses at Low Temperature, *Physical Review Letters*, *115* (2015), 16, ID165901

[8] Zhang, X., *et al*., Pressure-Induced Non-monotonic Cross-Over of Steady Relaxation Dynamics in a Metallic Glass, *Proceedings of the National Academy of Sciences*, *120* (2023), 24, IDe2302281120
[9] Zhu, F., *et al*., Intrinsic Correlation between β-Relaxation and Spatial Heterogeneity in a Metallic Glass, *Nature Communications*, *7* (2016), 1, ID11516
[10] Yang, Q., *et al*., Structural Length-Scale of β Relaxation in Metallic Glass, *The Journal of Chemical Physics*, *157* (2022), 18, 184504
[11] Kohlrausch, R., Theorie des Elektrischen Rückstandes in der Leidener Flasche, *Annalen der Physik*, *167* (1854), 2, pp.179-214
[12] Williams, G., Watts, D. C., Non-Symmetrical Dielectric Relaxation Behaviour Arising from a Simple Empirical Decay Function, *Transactions of the Faraday Society*, *66* (1970), June, pp.80-85
[13] Yang, X. J., *Theory and Applications of Special Functions for Scientists and Engineers*, Springer Nature, Singapore, Singapore, 2022
[14] Yu, Y., *et al*., Stretched Exponential Relaxation of Glasses at Low Temperature, *Physical Review Letters*, *115* (2015), 16, ID165901
[15] Luo, P., *et al.*, Relaxation Decoupling in Metallic Glasses at Low Temperatures, *Physical Review Letters*, *118* (2017), 22, ID225901
[16] Duan, Y. J., *et al*., Connection between Mechanical Relaxation and Equilibration Kinetics in a High-Entropy Metallic Glass, *Physical Review Letters*, *132* (2024), 5, ID056101
[17] Sen Gupta, B., Das, S. P., Glassy Aging with Modified Kohlrausch-Williams-Watts Form, *Physical Review E*, *76* (2007), 6, ID061502
[18] Mauro, J. C., Mauro, Y. Z., On the Prony Series Representation of Stretched Exponential Relaxation, *Physica A*, *506* (2018), Sept., pp. 75-87
[19] Simdyankin, S. I., Mousseau, N., Relationship between Dynamical Heterogeneities and Stretched Exponential Relaxation, *Physical Review E*, *68* (2003), 4, ID041110

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