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A Free-Volume Model for Thermal Expansion of Metallic Glass

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Many mechanical, thermal and transport behaviors of polymers and metallic glasses are interpreted by the free-volume model, whereas their applications on thermal expansion behaviors of glasses is rarely seen. Metallic glass has a range of glassy states depending on cooling rate, making their coefficients of thermal expansion vary with the glassy states. Anharmonicity in the interatomic potential is often used to explain different coefficients of thermal expansion in crystalline metals or in different metallic-glass compositions. However, it is unclear how to quantify the change of anharmonicity in the various states of metallic glass of the same composition and to connect it with coefficient of thermal expansion. In the present work, isothermal annealing is applied, and the dimensional changes are measured for $La_{62}Al_{14}Cu_{11.7}Ag_{2.3}Ni_5Co_5$ and $Zr_{52.5}Cu_{17.9}Ni_{14.6}Al_{10}Ti_5$ metallic glasses, from which changes in density and the coefficients of thermal expansion of the specimens are both recorded. The coefficients of thermal expansion linearly decrease with densification reflecting the role of free volume in thermal expansion. Free volume is found to have not only volume but also entity with an effective coefficient of thermal expansion similar to that of gases. Therefore, the local regions containing free volume inside the metallic glass are gas-like instead of liquid-like in terms of thermal expansion behaviors.

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Free volume, defined as the volume surrounding an atom that can be exchanged with neighboring atoms without any expenditure of energy,[1] is a conceptual variable that is frequently used to explain the thermal and mechanical behaviors of metallic glasses (MGs), including shear transformation,[2,3] structural relaxation[2] and glass transition.[4,5] Free volume is often quantified by density: the relative change in density after thermo-mechanical treatment reflects the amount of free volume.[6] Linear relationship has been found between free volume and enthalpy change of an MG at its glassy state,[6] and rejuvenation, indicating increases in the free volume and enthalpy, leads to improved room-temperature plasticity of the MG.[7] Wang *et al.* pointed out an ubiquitous form of $M = \frac{M_\infty}{1+X}$, which connects flow units, i.e., the atomic clusters containing free volume, with many properties or behaviors of MGs, including elastic moduli and stored enthalpy at the glassy state.[8] Here, M stands for a material property, M_∞ the material's property after infinitely long-time annealing, and X the concentration of flow units.

Up to data, many physical properties have been evaluated by the free-volume model. However, no one has ever studied the coefficient of thermal expansion (CTE) using the free-volume model. It is known that CTE measures the relative dimensional change of a material per unit temperature. In crystalline metals, thermal expansion can be explained by anharmonic vibration of atoms.[9] The asymmetric shape of the interatomic potential well reflects the anharmonicity,[10] whose variation explains why different elements have different CTEs. The same argument can be applied to MGs with different compositions, too, but fails to answer why MGs of the same composition can have varied CTEs. Unlike crystalline metals, MGs have a range of glassy states depending on the cooling rate even if their compositions are the same.[11] Although researchers argued that the theory of anharmonicity can explain thermal expansion of MGs,[10,12–14] one would expect the anharmonicity and CTE to be unchanged in the same composition because the interatomic potentials are fixed. However, CTE varies at different glassy states of an MG in reality. For example, CTEs of the $Pd_{40}Cu_{30}Ni_{10}P_{20}$ and $Cu_{55}Hf_{25}Ti_{15}Pd_5$ MGs decrease[15,16] whereas CTE of a Pr-based MG increases after thermal annealing.[17] Gangopadhyay *et al.* proposed that cooperativity of atomic clusters apart from anharmonicity of the interatomic potential must be considered to interpret thermal expansion of MGs.[14] Therefore, thermal expansion of MGs requires a new theory beyond anharmonicity of interatomic potentials.

The CTEs of MGs have been measured through

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two approaches. The first method is dilatometer that characterizes the macroscopic change of sample dimensions in *in situ* heating or cooling.[17,18] In this case, specimens as long as a few millimeters or centimeters are required to enhance the accuracy of the measurement. For example, linear CTE can be obtained using the expression $\frac{dl}{l_0 dT}$ from experimental measurement, here l_0 is the original length of the sample at temperature T_0, l is the length of the sample at temperature T, $dl = l - l_0$ and $dT = T - T_0$. The second method is synchrotron x-ray scattering that records the microscopic-structure change of the sample on *in situ* heating or cooling.[9,14,16] Positions of the peak maxima in the structural factor $S(q)$ and the radial distribution function $g(r)$ are analyzed to calculate CTEs. Here q is the scattering vector, and r is the distance from the origin. According to the Ehrenfest relation,[19] $q_1 = \frac{1.23\times 2\pi}{r_1}$, where q_1 stands for the position of the first-peak maxima of $S(q)$, and r the equilibrium interatomic distance. Thus, $-\frac{dq_1}{q_1 dT}$ is considered as the microscopic CTE of MG because it equals $\frac{dr}{rdT}$. Experimental evidence shows that this type of microscopic CTE agrees well with the macroscopic CTE of many MGs,[15,16] except for a Zr-based MG.[9] On the other hand, discrepancies are found when using r_1, the position of the first-peak maxima of $g(r)$, to calculate the microscopic CTE. The $\frac{dr_1}{r_1 dT}$ is always found to be much smaller than the macroscopic CTE, e.g., $\frac{dr_1}{r_1 dT}$ is 9% of the macroscopic CTE for the $Cu_{50}Zr_{50}$ MG[20] or negative for the $Pd_{62.1}Al_{27.3}Y_{4.2}Ni_{6.4}$ and $La_{62}Al_{14}Cu_{11.7}Ag_{2.3}Ni_5Co_5$ MGs[21,22] when the specimens are thermally expanded. The position shift of the peak maximum agrees with the macroscopic CTE only when the interatomic spacing is beyond the 4^{th} nearest neighboring atomic shell.[20,23] The discrepancies existing in the microscopic and macroscopic CTEs suggest that the thermal expansion of MGs varies at different length scales.

For crystalline metals, the macroscopic CTE is closely connected to heat capacity.[24] However, the difference between the microscopic CTE (measured by shifts in the diffraction peaks) and the macroscopic CTE (measured by dilatometer) indicates the role of vacancies.[25] This method works because x-ray is only scattered by atoms but *not* by vacancies. Yavari *et al.*, adopted the idea, conducted the same experiment on MGs, and wished to measure free-volume from such discrepancy.[16] However, they failed with this approach as they observed that $-\frac{dq_1}{q_1 dT}$ is the same as the macroscopic CTE, meaning that unlike vacancies in crystal, free volume contributes to the diffraction of the MG. This argument is further confirmed by the decrease of q_1 as a result of structural relaxation in the subsequent cooling and re-heating runs.[16] It then opens two fundamental questions: Is free volume really a volume with no mass (or in vacuum)? Or alternatively, does the free volume has an actual entity that can divert x-ray beam?

In this Letter, we investigate effects of isothermal annealing on the CTEs of $La_{62}Al_{14}Cu_{11.7}Ag_{2.3}Ni_5Co_5$ and $Zr_{52.5}Cu_{17.9}Ni_{14.6}Al_{10}Ti_5$ MGs, and develop a simple semi-empirical model based on free volume, which can answer what entity the free volume is in response to the thermal expansion of MGs. It is found that the free volume has an entity with an effective CTE that is close to half the CTE of the Ar gas. Decrease of CTE in the annealed MG is attributed to the annihilation of free volume.

The relative change of sample volume v, i.e., $\frac{dv}{V_0}$, can be calculated by the relative change of sample length (l) with a first-order approximation, $\frac{dl}{l_0}$, from

$$\frac{dv}{V_0} = 3 \times \frac{dl}{l_0}, \tag{1}$$

where V_0 and l_0 are the volume and length, respectively. The volumetric thermal expansion coefficient α and the linear thermal expansion coefficient β are defined as $\alpha = \frac{dv}{V_0 dT}$, $\beta = \frac{dl}{l_0 dT}$, respectively, where T stands for temperature. Based on Eq. (1), the following relation exists:

$$\alpha = 3\beta. \tag{2}$$

We now consider the MG sample as a composite of matrix and free volume, it then results in

$$dv = dv_{\text{m}} + dv_{\text{f}} = \alpha_{\text{m}} v_{\text{m}} dT + \alpha_{\text{f}} v_{\text{f}} dT,$$

$$\alpha = \frac{dv}{vdT} = \alpha_{\text{m}} \frac{v_{\text{m}}}{v} + \alpha_{\text{f}} \frac{v_{\text{f}}}{v} = \alpha_{\text{m}}(1-x) + \alpha_{\text{f}} x, \tag{3}$$

where α_{m} and α_{f} are the CTEs of MG matrix and free volume, respectively, α is the complex CTE of metallic glass, v_{f} is free volume in the MG, and $x = \frac{v_{\text{f}}}{v}$ for the volume fraction of free volume inside the MG. One should notice that if $x \ll 1$, $x \to 0$ and $1 - x \to \frac{1}{1+x}$, Eq. (3) has the exact form of the ubiquitous relationship proposed by Wang *et al.*[8] When $t = 0$, we have $\alpha = \alpha_0$, $v = V_0$, and $x = x_0$; when $t \to \infty$, we have $\alpha \to \alpha_{\text{m}}$, $v_{\text{f}} \to 0$, $x \to 0$, and v reaches its minimum as $V_0 - \Delta V$. Here, we define ΔV as the maximum volumetric change of the MG by annealing at $t \to \infty$.

From Eq. (3), the difference between the two states is

$$\Delta\alpha = (\alpha_{\text{f}} - \alpha_{\text{m}})\Delta x, \tag{4}$$

where $\Delta\alpha = \alpha_0 - \alpha_{\text{m}}$, $\Delta x = x_0 = \frac{\Delta V}{V_0}$. Then, based on Eq. (4),

$$\alpha_{\text{f}} = \alpha_{\text{m}} + (\alpha_0 - \alpha_{\text{m}}) \frac{V_0}{\Delta V}. \tag{5}$$

To resolve α_{f}, four variables, i.e., α_{m}, α_0, V_0, ΔV, need to be determined.

On the other hand, x at any given t is

$$x = \frac{\Delta V - dv}{V_0}, \tag{6}$$

where $dv = V_0 - v$.

Two MGs, $La_{62}Al_{14}Cu_{11.7}Ag_{2.3}Ni_5Co_5$ and $Zr_{52.5}Cu_{17.9}Ni_{14.6}Al_{10}Ti_5$ (Vit105) were selected in this work. Elements with a purity of (at least 99.5%) were melted by an electric-arc furnace in an argon atmosphere to make ingots. Suction casting was then performed to cast the ingots into a copper mold in an Ar atmosphere. The final rods were 3.5 mm in diameter (ϕ) and 70 mm in length (l). Cylinder samples with ϕ of 3.0 mm and l of 6.0 mm were machined by Luling precision company in Suzhou. X-ray diffraction tests (XRD D8 Advance, Bruker) and differential scanning calorimetry (DSC 8000, PerkinElmer) were performed. All the specimens were amorphous, and the glass transition temperature (T_g) is 409 K for the La-based MG and 665 K for the Zr-based MG. Helium pycnometer (AccuPyc II 1345, Micrometritics) and electronic weight-balance (XS105, Mettler, with an accuracy of 0.01 mg) were applied to measure the sample density (ρ). Five as-cast cylinders of the same MG composition were inserted in one gas chamber that was 12.2 mm in diameter, 11.3 mm in depth and 0.719 cm^3 in volume, and the accuracy of volume determination reaches 0.001 cm^3; ρ are 6.225 ± 0.001 g/cm^3 and 6.630 ± 0.001 g/cm^3 for the La-based MG and the Zr-based MG at the as-cast state, respectively.

Thermal mechanical analysis (TMA 402 F3, Netzsch) was made for thermal expansion measurements. A uniaxial compressive stress of 4.25 kPa was applied on the cylindrical specimens ($\phi = 3.0$ mm and $l = 6.0$ mm) before thermal treatment. The applied stress is less than one in ten thousands of the yield stress of the La-based MG or Zr-based MG, respectively, guaranteeing elastic deformation of the samples below T_g. The Zr-based and La-based specimens were kept at 303 K for 3 min at the beginning of thermal treatment, which stabilized the thermal environment of the machine. Next, they were heated to $0.90T_g$ at a constant rate of 3 K/min, held at $0.90T_g$ for 3 min, and then cooled back to 350 K at a constant rate of −3 K/min and kept for 3 min at this temperature. Similar thermal protocol was conducted by ten more times in the temperature range between 350 K and $0.90T_g$ except that the isothermal annealing interval was extended to 2, 3, 5, 5, 15, 30, 60, 120, 240, 480, 960 min in sequence.

Thermal mechanical analyzer (TMA) records l during *in situ* heating and cooling experiments, from which α can be derived. Take Fig. 1 as an example, $\frac{dl}{l_0}$ increases on heating (red lines) and decreases on cooling (blue lines), implying expansion on heating and contraction on cooling, respectively. In the 1st heating run, $\frac{dl}{l_0}$ linearly increases with the increasing T until 480 K ($= 0.72T_g$) as indicated by the dashed line. The slope of the curve, 1.02×10^{-5} K^{-1}, is taken as β_0, so α_0 is 3.06×10^{-5} K^{-1} according to Eq. (1). Increase of $\frac{dl}{l_0}$ continues at $T > 480$ K, but the curve is inclined below the dashed line, demonstrating a nonlinear thermal expansion. The 480 K coincides with the onset of the pre-T_g exothermic peak in calorimetry and correlated with the structural relaxation of the MG. The 1st heating run stops at 598 K ($= 0.90T_g$), and an isothermal annealing (dotted lines) of 3 min started. In the 1st cooling run, a linear decrease of $\frac{dl}{l_0}$ with the decreasing T was seen in the range of 350–480 K. A linear fit of the data from this range is performed, and the slope ($\frac{dl}{l_0 dT}$) is taken as β, that is, 1.02×10^{-5} K^{-1}. Here, α of 3.06×10^{-5} K^{-1} is directly calculated from β based on Eq. (2). At 532 K ($= 0.80T_g$), a reduction in $\frac{dl}{l_0}$ of 2.7×10^{-4} is detected between the 1st heating and the 2nd heating runs, implying a decrease in $\frac{dv}{V_0}$ of 8.1×10^{-4} based on Eq. (1). The same heating and cooling runs between 350 K and 598 K are repeated 11 times and α is determined from the cooling curves, $\frac{dv}{V_0}$ is determined from the heating curves to $0.80T_g$. Thus, TMA measurements provide information of α, α_0 and $\frac{dv}{V_0}$.

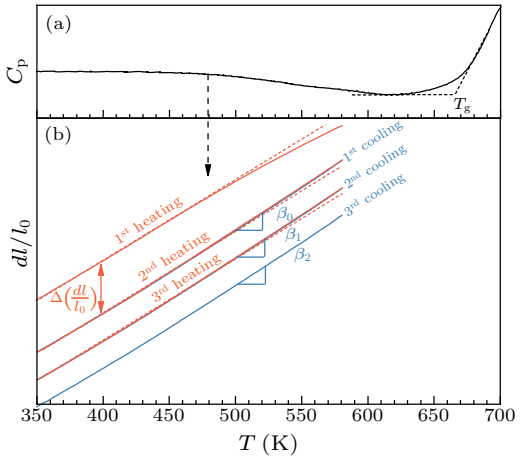

Fig. 1. DSC (a) and TMA (b) curves of a Zr-based MG. Relaxation starts from nearly 480 K ($0.70T_g$). Sample length is l_0, its relative change is $\frac{dl}{l_0}$ and temperature is T. The heating curves are colored in red, and the cooling curves in blue. The dashed line marks the linear response of $\frac{dl}{l_0}$ to T in the 1st heating run to 480 K from 350 K, and the slope of the dashed line is β_0. Between 350 K and 480 K, the slope of the cooling curve is taken as β_n (n = 1–12, and n stands for the nth cooling). At 432 K ($= 0.80T_g$), difference in $\frac{dl}{l_0}$ is recorded as the length change after the nth cooling (n = 1–12). The double-side arrow denotes the length change after the 1st cooling.

In our experiment, long-time isothermal annealing at $0.90T_g$ was performed to obtain α_m and Δv with the applied t up to 1.2×10^5 s. As shown in Fig. 2(a), $\frac{dv}{V_0}$ remains nearly unchanged after $t > 4.0 \times 10^4$ s, suggesting that the free volume is depleted or $v_f \to 0$ (and $x \to 0$). Thus, the maximum $\frac{dv}{V_0}$ represents $\frac{\Delta V}{V_0}$. Because $V_0 = \frac{m}{\rho}$ with m being the sample mass, ΔV is calculated as the product of V_0 and maximum $\frac{dv}{V_0}$.

For the La-based MG, ΔV is $3.8 \times 10^{-5}\,\mathrm{cm}^3$; for the Zr-based MG, ΔV is $8.1 \times 10^{-5}\,\mathrm{cm}^3$. Here, $\frac{dv}{V_0}$ can be transferred into x based on Eq. (6). Figure 2(b) exhibits how x changes with t. With the increasing t, x is diminished. On the other hand, α is saturated when $t > 4.0 \times 10^4$ s [Fig. 2(c)]. Since x is zero, the saturated α denotes α_m representing the CTE of the MG matrix. For the La-based MG, α_m is $2.3 \times 10^{-4}\,\mathrm{K}^{-1}$; for the Zr-based MG, α_m is $7.8 \times 10^{-5}\,\mathrm{K}^{-1}$.

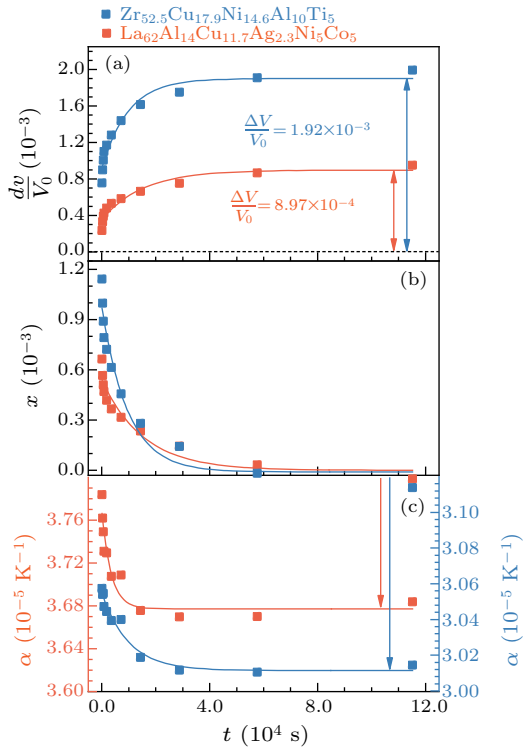

Fig. 2. Effects of annealing on the La-based and Zr-based MGs. (a) The relative volumetric change $\frac{dv}{V_0}$, (b) the volume fraction of free volume in the MG (x), and (c) the volumetric thermal expansion coefficient α with the annealing time t. Saturations with the increasing t are seen for $\frac{dv}{V_0}$, x and α in both MGs. The saturated volumetric change $\frac{\Delta V}{V_0}$ is marked by the double-side arrow, and the matrix's thermal expansion coefficient α_m by the arrow.

The validity of Eqs. (3)–(5) needs the thermal expansion coefficient to be tested to see if α is linearly correlated with x. Figure 3 plots α against x where linear correlations are found for both MGs. The root mean square (R^2) of the linear fit is 0.94 for the La-based MG and 0.96 for the Zr-based MG. Therefore, Eqs. (3)–(5) are valid, and α_f can be obtained from α_m, α_0, V_0, ΔV based on Eq. (5). Table 1 lists the measured α_m, α_0, V_0, ΔV and the calculated α_f of both MGs.

In this work, the volumetric CTE of the MG matrix, the free volumes of La-based and Zr-based MGs are obtained from Eq. (5). The nonzero α_f of both MGs emphasizes that the free volume cannot be interpreted just as "volume" but should be considered as an entity. Furthermore, α_f is larger than α_m, e.g., about 36× for the La-based MG and 33× for the Zr-based MG. This magnitude of change is significantly larger than that of the elastic moduli as estimated by Sun *et al.*,[26] who found that the flow unit has elastic moduli about one tenth of that of the matrix. Moreover, these flow units containing free volume are often interpreted as liquid-like regions. However, the absolute values of α_f (Table 1) are at least one order of magnitude larger than most metallic liquids (in the order magnitude of 10^{-5}–$10^{-4}\,\mathrm{K}^{-1}$[27]), and are close to half the value of the inert gas. For example, argon has an α of $2.48 \times 10^{-3}\,\mathrm{K}^{-1}$.[28,29] Thus, in terms of CTE, the free volume is more gas-like rather than liquid-like. It is possible that the flow units are so loose that researchers have paid more attention to its volume and ignored its matter. However, evidences from both x-ray scattering[16] and thermal expansion (the present work) emphasize the "entity" of the free volume. Understanding the entity of the free volume may be useful in interpreting the new phenomena of MG nanoparticles,[30] MG nanowires,[31] MG composite,[32] and the MG-forming liquid.[33]

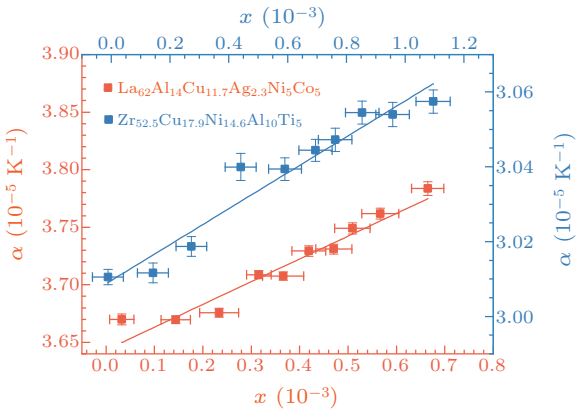

Fig. 3. The volumetric thermal expansion coefficient α vs the free-volume fraction x. Nice linear fits are obtained for both La-based and Zr-based MGs.

Table 1. Parameters V_0, ΔV, α_0, α_m and α_f of the La-based and Zr-based MGs.

Composition	V_0 ($10^{-2}\mathrm{cm}^3$)	ΔV ($10^{-5}\mathrm{cm}^3$)	α_0 ($10^{-5}\mathrm{K}^{-1}$)	α_m ($10^{-5}\mathrm{K}^{-1}$)	α_f ($10^{-5}\mathrm{K}^{-1}$)
$La_{62}Al_{14}Cu_{11.7}Ag_{2.3}Ni_5Co_5$	4.2	3.8	3.8	3.68	137
$Zr_{52.5}Cu_{17.9}Ni_{14.6}Al_{10}Ti_5$	4.2	8.1	3.1	3.01	102

A semi-empirical free-volume model is constructed for metallic glass to explain the change of thermal expansion coefficient in annealing. The volumetric thermal expansion coefficient of metallic glass is found linearly decreased with the increasing free volume inside the metallic-glass matrix. The volumetric thermal ex-

pansion coefficient of free volume is derived from the annealing data. It is found that the volumetric thermal expansion coefficient of free volume is about 33–36 times that of the matrix. The present work suggests that the free volume inside the metallic glass has an entity, which is more gas-like than liquid-like in terms of the volumetric thermal expansion coefficient.

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References

[1] Murali P and Ramamurty U 2005 *Acta Mater.* **53** 1467
[2] Spaepen F 1977 *Acta Mater.* **25** 407
[3] Spaepen F 2006 *Scr. Mater.* **54** 363
[4] Turnbull D and Cohen M H 1961 *J. Chem. Phys.* **34** 120
[5] Turnbull D and Cohen M H 1970 *J. Chem. Phys.* **52** 3038
[6] Slipenyuk A and Eckert J 2004 *Scr. Mater.* **50** 39
[7] Ketov S V, Sun Y H, Nachum S, Lu Z, Checchi A, Beraldin A R, Bai H Y, Wang W H, Louzguine-Luzgin D V, Carpenter M A and Greer A L 2015 *Nature* **524** 200
[8] Wang D P, Zhu Z G, Xue R J, Ding D W, Bai H Y and Wang W H 2013 *J. Appl. Phys.* **114** 173505
[9] Mattern N, Stoica M, Vaughan G and Eckert J 2012 *Acta Mater.* **60** 517
[10] Kato H, Chen H S and Inoue A 2008 *Scr. Mater.* **58** 1106
[11] Sun Y, Concustell A and Greer A L 2016 *Nat. Rev. Mater.* **1** 16039
[12] Bordat P, Affouard F, Descamps M and Ngai K L 2004 *Phys. Rev. Lett.* **93** 105502
[13] Qu D, Liss K D, Yan K, Reid M, Almer J D, Wang Y, Liao X and Shen J 2011 *Adv. Eng. Mater.* **13** 861
[14] Gangopadhyay A K, Pueblo C E and Kelton K F 2020 *Phys. Rev. Mater.* **4** 095602
[15] Louzguine D V, Yavari A R, Ota K, Vaughan G and Inoue A 2005 *J. Non-Cryst. Solids* **351** 1639
[16] Yavari A R, Le M A, Inoue A, Nishiyama N, Lupu N, Matsubara E, Botta W J, Vaughan G, Di Michiel M and Kvick A 2005 *Acta Mater.* **53** 1611
[17] Meng Q G, Zhang S G, Li J G and Bian X F 2006 *Scr. Mater.* **55** 517
[18] Ota K, Botta W J, Vaughan G and Yavari A R 2005 *J. Alloys Compd.* **388** L1
[19] Ehrenfest P 1915 *Proceedings of the Knoinklijke Akademie van Wetenschappen te Amsterdam* **17** 1184
[20] Zhang Y, Mattern N and Eckert J 2013 *Appl. Phys. Lett.* **102** 081901
[21] Evertz S, Music D, Schnabel V, Bednarcik J and Schneider J M 2017 *Sci. Rep.* **7** 15744
[22] Bednarcik J, Michalik S, Sikorski M, Curfs C, Wang X D, Jiang J Z and Franz H 2011 *J. Phys: Condens. Matter.* **23** 254204
[23] Su Y, Wang X, Cao Q, Zhang D and Jiang J Z 2020 *J. Phys. Chem. C* **124** 19817
[24] Tang M, Pan X, Zhang M and Wen H 2021 *Chin. Phys. Lett.* **38** 026501
[25] Simmons R O and Balluffi R W 1960 *Phys. Rev.* **117** 52
[26] Sun B A, Hu Y C, Wang D P, Zhu Z G, Wen P, Wang W H, Liu C T and Yang Y 2016 *Acta Mater.* **121** 266
[27] Aqra F and Ayyad A 2011 *Appl. Surf. Sci.* **257** 6372
[28] Yaws C L 2001 *Matheson Gas Data Book* 7^{th} edn (New York: McGraw-Hill)
[29] Yaws C L 1999 *Chemical Properties Handbook* (New York: McGraw-Hill)
[30] Zhang S, Wang W and Guan P 2021 *Chin. Phys. Lett.* **38** 016802
[31] Dong J, Feng Y H, Huang Y, Yi J, Wang W H, Bai H Y and Sun B A 2020 *Chin. Phys. Lett.* **37** 017103
[32] Li D M, Chen L S, Yu P, Ding D and Xia L 2020 *Chin. Phys. Lett.* **37** 086401
[33] Cao Q L, Huang D H, Yang J S and Wang F H 2020 *Chin. Phys. Lett.* **37** 076201