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# Non-monotonic temperature evolution of nonlocal structure–dynamics correlation in CuZr glass-forming liquids\*

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The structure–dynamics correlations in a nonlocal manner were investigated in CuZr metallic glass-forming liquids via classical molecular dynamics simulations. A spatial coarse-graining approach was employed to incorporate the nonlocal structural information of given structural order parameters in the structure–dynamics relationship. It is found that the correlation between structure order parameters and dynamics increases with increasing coarse-graining length and has a characteristic length scale. Moreover, the characteristic correlation length exhibits a non-monotonic temperature evolution as temperature approaches glass transition temperature, which is not sensitive to the considered structure order parameters. Our results unveil a striking change in the structure–dynamics correlation, which involves no fitting theoretical interpretation. These findings provide new insight into the structure–dynamics correlation in glass transition.

**Keywords:** metallic glass-forming liquid, structure–dynamics correlation, molecular dynamics simulation**PACS:** 61.43.Dq, 64.70.pe**DOI:** 10.1088/1674-1056/abf113

## 1. Introduction

Glass transition is one of fundamental problems in condensed matter physics.<sup>[1–3]</sup> As liquid is supercooled, the dynamics is drastically slowed down and becomes spatially heterogeneous.<sup>[4–6]</sup> However, it is not accompanied by any obvious structural changes.<sup>[7,8]</sup> The subtle change in the liquid structure and its effect on the dynamic slowdown have been extensively explored, but still remain elusive.<sup>[8,9]</sup>

Inspired by Frank's hypothesis that liquid may be composed of densely packed icosahedral short-range order building blocks,<sup>[10]</sup> numerous studies have shown that the atomic structures of metallic liquids and glasses can be characterized by a variety of atomic clusters.<sup>[8,11–14]</sup> Based on the atomic cluster model, the subtle changes in the liquid structure in cooling process can be well illustrated by the population of various atomic clusters as a function of temperature.<sup>[8]</sup> Furthermore, the structure–property relationship can be also explored by the atomic cluster model.<sup>[8,9]</sup> For example, the population of the icosahedral clusters and the temperature evolution have been found to be intimately correlated with dynamic slowdown, glass transition, and glass-forming ability in metallic glass-forming liquids, providing useful understanding for the underlying structure basis of dynamic slowdown and glass transition.<sup>[8,9]</sup>

Although the population of the local atomic clusters shows some correlation with dynamics in glass-forming liquids, such correlations are not general for different systems.<sup>[8,15]</sup> So far, more and more studies have demonstrated that the structures beyond the atomic level play more

important roles in determining dynamics in glass-forming liquids.<sup>[16–26]</sup> For example, numerical simulations of 2D glass-forming liquids show that there is an intrinsic link between medium-range crystalline order and slow dynamics as well as dynamical heterogeneity in glass transition.<sup>[16]</sup> It is also found that icosahedral clusters tend to connect with each other and form large clusters, which may naturally lead to slow dynamics and non-exponential relaxation characterized in glass transition.<sup>[16–18]</sup> Furthermore, by introducing graph theory, the medium-range structures formed by connected icosahedral clusters were quantitatively analyzed.<sup>[19,22]</sup> It is found that the microscopic relaxation times increase exponentially with the connectivity of icosahedral clusters.<sup>[19]</sup> In addition, some new physical phenomena were revealed based on the concept of local connectivity, which provides more insights into the dynamics in metallic glass-forming liquids.<sup>[21–25]</sup> It is also found that the number of locally preferred structures in a certain range can predict the dynamics more accurately in the Wahnström system.<sup>[26]</sup> Recently, the spatial coarse-graining of a structure order parameter was developed to incorporate the nonlocal structural information in structure–dynamics relation, showing that a characteristic static correlation length of the underlying structure exists between the microscopic relaxation time and structural order.<sup>[27]</sup> Therefore, an in-depth study of the effect of non-local structure correlation on dynamics is important to understand the dynamic slowdown and glass transition.

In this work, we quantitatively analyze the correlation between the nonlocal structure and the dynamics in metal-

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lic glass-forming liquids. We show that there exists a temperature-dependent characteristic length in supercooled liquids. Our results show that the temperature dependence of the characteristic length scale is non-monotonic, which may be general for different structural order parameters. These findings may provide new insight into the structure–dynamics correlation in glass-forming liquids during supercooling.

## 2. Model and method

The classical molecular dynamics (MD) simulations were performed for the model system of Cu<sub>50</sub>Zr<sub>50</sub> metallic alloy by using LAMMPS package,<sup>[28]</sup> in which the interatomic interactions for CuZr alloy are described by the realistic embedded-atom model (EAM) potential.<sup>[29]</sup> The system contains  $N = 40000$  atoms in a cubic box with periodic boundary conditions applied in three directions. In the process of sample preparation, it was first melted and equilibrated at  $T = 2000$  K for 1000000 MD steps, then cooled down to 300 K with a cooling rate of  $10^{12}$  K/s in NPT ensemble in which the sample size was adjusted to give zero pressure. The glass transition temperature in this glass-forming liquid  $T_g$  is about 720 K. During cooling, structural configurations at different temperatures were collected. After adequate relaxation at each temperature of interest, the ensemble was switched to NVT, and each configuration was then relaxed for 2 ns and 50 atomic configurations were collected as the initial configurations. In order to achieve a meaningful measurement of microscopic relaxation, we performed simulations in the isoconfigurational ensemble (see Ref. [30] for more details). For each initial configuration, 100 trajectories were simulated with different momenta assigned randomly from the appropriate Maxwell–Boltzmann distribution. In all simulations, the time step used to integrate the equations of motion was chosen as 2fs and the temperature was controlled by the Nose–Hoover thermostat.

To characterize the atomic mobility in the glass-forming liquids at different temperatures, the dynamical propensity of atom  $i$  was defined as  $\mu_i(t) = \langle |r_i(t) - r_i(0)|^2 \rangle_{\text{iso}}$ , where  $r_i(t)$  is the atomic position at time  $t$ , and the isoconfigurational average is calculated over many independent simulations. At each temperature,  $\mu_i(t)$  was calculated in the time scale of  $\alpha$ -relaxation time  $\tau_\alpha$ , which is defined as the time scale when the self-intermediate scattering function decays to  $e^{-1}$ .<sup>[8]</sup>

To incorporate the nonlocal structure information in the structure–dynamics relation, a systematic spatial coarse-graining approach was employed for a structure order parameter denoted as  $X$  to detect the correlated nature of structural ordering,<sup>[27]</sup> that is,  $X_i$  for atom  $i$  can be coarse-grained by taking its average over all atoms  $j$  within a coarse-graining distance  $L$ ,

$$\bar{X}_i(L) = \sum_j X_j P(|r_j - r_i|) / \sum_j P(|r_j - r_i|). \quad (1)$$

Here an exponential core  $P(x) = \exp(-x/L)$  was employed by assuming that the effect of the local structure on the dynamics decays exponentially in space. Thus, by coarse-graining of a structure order parameter in this way, one can evaluate how structure affects atomic dynamics at different spatial scales.<sup>[27]</sup>

To characterize the correlation between the atomic mobility and structure order parameter, the Spearman rank correlation coefficient was used, which is given by<sup>[27,31]</sup>

$$C_r = 1 - 6 \sum_i (R_i^c - R_i^d)^2 / N(N^2 - 1). \quad (2)$$

To calculate  $C_r$ , we first sorted atoms in terms of the atomic mobility and the structure order parameter in descending order, respectively, and assigned corresponding ranks to each atom  $i$ . Here  $R_i^d$  and  $R_i^c$  represent the ranking of structural order parameter and atomic mobility of atom  $i$ , respectively.  $C_r$  is 1 if two quantities are related by a monotonically increasing function and  $-1$  if by a decreasing one, whereas  $C_r = 0$  means the absence of the correlation.<sup>[27]</sup>

## 3. Results and discussion

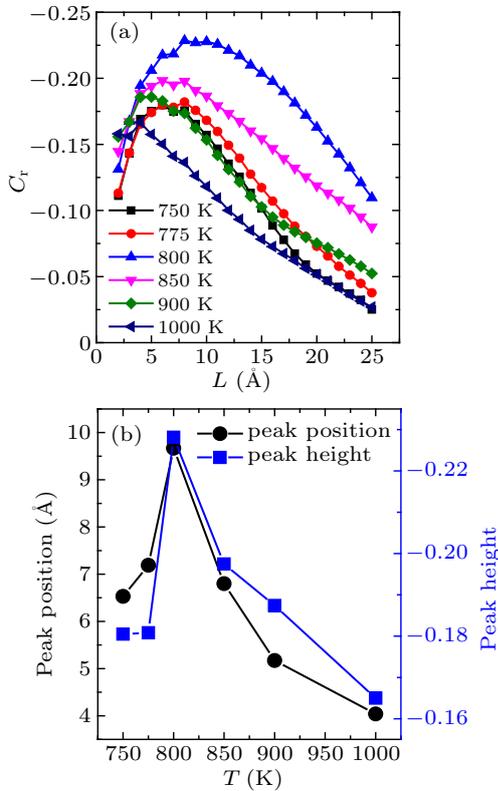
Figure 1(a) shows the correlation between the atomic mobility and structure order parameter of the five-fold local symmetry (FFLS) as a function of coarse-graining length  $L$  in CuZr metallic glass-forming liquids at different temperatures. Here FFLS was chosen to be the structure order parameter of atom  $i$ , which can be defined as

$$f_i^5 = n_i^5 / \sum_{k=3,4,5,6} n_i^k, \quad (3)$$

where  $n_i^k$  ( $k = 3, 4, 5, 6$ ) represents the number of  $k$ -edged polygon in the Voronoi polyhedron of atom  $i$  denoted as  $\langle n_i^3, n_i^4, n_i^5, n_i^6 \rangle$  by the Voronoi tessellation.<sup>[32–34]</sup> Thus, the average FFLS in a glass-forming liquid can be expressed as  $f_5 = \sum_i f_i^5 / N$ .<sup>[33,34]</sup> It should be noted that negative correlation was obtained between  $\mu_i$  and  $f_i^5$ , which means that larger FFLS may slow down the dynamics of atoms in glass-forming liquids.

As shown in Fig. 1(a), the first point at each temperature, since only the central atoms were included in coarse graining, shows the correlation between local structure and dynamics. As temperature decreases from 1000 K to 750 K, the correlation decreases gradually. Moreover, the correlation value at different temperatures is relatively small, which indicates that the local atomic structure has only weak correlation with dynamics in glass-forming liquids. As the coarse-graining length  $L$  increases, the correlation at all temperatures increases and shows a peak, which is consistent with the results of previous studies.<sup>[27]</sup> The peak of the correlation is a natural consequence of the fact that coarse-graining can incorporate the effect of atomic structure on dynamics in greater distances.

It is concluded that there is a relatively significant relationship between structure and dynamics at these length scales i.e., peak positions as shown in Fig. 1(a). Meanwhile, the peak height and position change significantly with temperature. At 1000 K, the highest temperature we examined, the correlation only shows a small peak at a very small coarse-graining length  $L$ , and then decays rapidly. With the decrease of temperature, the peak height increases rapidly, and the peak position also shifts to larger length  $L$ , reaching the maximum values around 800 K. Instead of further increase, the peak height becomes lower and the peak position shifts back to smaller length  $L$ , as temperature further decreases closer to  $T_g$ . Such non-monotonic temperature evolution of the structure-dynamics correlation has not been observed in previous studies. To get more detailed temperature-dependent behavior of the correlation between coarse-grained FFLS and atomic mobility, we extracted the peak height and position of the correlation at various temperatures. Figure 1(b) clearly shows the non-monotonic change of the peak height and position as temperature decreases toward  $T_g$  in metallic glass-forming liquids. The simultaneous decrease of peak height and peak position indicates that the decrease of correlation is not only the reduction of the influence range of the local structure, but also the weakening of the influential ability.



**Fig. 1.** (a) Correlation between five-fold local symmetry and atomic mobility as functions of coarse graining length  $L$  at various temperatures in metallic glass-forming liquids. (b) Temperature dependence of peak height and position in the structure-dynamics correlation shown in (a).

In order to investigate whether this non-monotonic temperature evolution of the correlation between atomic mobil-

ity and coarse-grained FFLS is general behavior in metallic glass-forming liquids or structure order parameter dependent, we employed another structural order parameter of local packing capability  $\Omega$  proposed by Tong and Tanaka.<sup>[27]</sup> It is designed to measure the deviation between a local packing and the perfect arrangement of the most efficient packing of neighboring particles around the central particle in hard-sphere-like model glass formers.<sup>[27]</sup> Metallic glass-forming liquids can be regarded as dense random packing of hard spheres, and the nearest-neighbors of each atom can be determined by the Voronoi tessellation.<sup>[8]</sup> The central atom  $i$  and three of the neighbors next to each other,  $j$ ,  $k$ , and  $l$  can form a tetrahedron. Such tetrahedra of four neighboring atoms are the fundamental structural units in 3-dimensional metallic liquids and glasses. Here the corresponding reference tetrahedrons in metallic glass-formers can be defined if the edge lengths are just the respective minimum distances of the four atoms with each other, that is, the first non-zero distances in partial pair correlation functions, which is different from the reference tetrahedron in hard-sphere systems that the four particles are perfectly just in touch.<sup>[27]</sup> Thus, the imperfection of a tetrahedron can be quantified as

$$\omega_{(ijkl)} = \frac{\sum_{\langle ab \rangle} |r_{ab} - \sigma_{ab}|}{\sum_{\langle ab \rangle} \sigma_{ab}}, \quad (4)$$

where  $\langle ab \rangle$  runs over the six edges of the tetrahedron  $\langle ijkl \rangle$ ,  $r_{ab}$  is the edge length of this tetrahedron, and  $\sigma_{ab}$  is the edge length of the reference tetrahedron. Finally, the deviation of the local packing around the central atom  $i$  from the most efficiently packable configuration can be measured as

$$\Omega_i = \frac{1}{N_i^{\text{tetra}}} \sum_{\langle ijkl \rangle} \omega_{(ijkl)}, \quad (5)$$

where  $N_i^{\text{tetra}}$  is the total number of tetrahedra including the central atom  $i$  as a member.<sup>[27]</sup> Larger  $\Omega$  means more deviation and more loosely packed.

Figure 2(a) shows the correlation between the order parameter  $\Omega_i$  and atomic mobility  $\mu_i$  as functions of coarse graining length  $L$  at various temperatures. Here  $C_r$  shows positive values, because larger  $\Omega_i$  means more loosely packed around atom  $i$ , so that atom  $i$  is more mobile. It is shown that  $C_r$  increases and then decreases as coarse graining length  $L$  increases, showing a peak at a certain  $L$ . This is consistent with the correlation between  $\mu_i$  and  $f_i^5$  shown in Fig. 1(a). It is also consistent with that obtained in hard-sphere-like glass-formers.<sup>[27]</sup> Furthermore, the peak height and position also increase as temperature decreases down to 800 K, but decreases as temperature further decreases. Figure 2(b) shows the corresponding peak position and height of the correlation between  $\Omega_i$  and  $\mu_i$  as a function of temperature, which is highly consistent with that between  $f_i^5$  and  $\mu_i$  shown in Fig. 1(b). They both

show a peak at 800 K. Thus, both the structure order parameters of  $f_i^5$  and  $\Omega_i$  produce almost the same structure–dynamics correlation. This indicates that the structural order may affect dynamics in a correlated manner over a characteristic correlation length in metallic glass-forming liquids, and such correlation has non-monotonic temperature dependence which could be general in metallic glass-forming liquids.

To understand the non-monotonic temperature dependence of the structure–dynamics correlation in a characteristic length, we analyzed the distributions of the atomic mobility, FFLS, and  $\Omega_i$  at 1000 K, 800 K, and 750 K, respectively. This is because Spearman rank correlation coefficient we adopted does not care about the actual value of the parameter, but its ranking in the whole population. For the atomic mobility on the time scale of  $\tau_\alpha$  shown in Fig. 3(a), although the atomic mobility is lower with decreasing temperature, the overall increase is due to the rapid growth of  $\tau_\alpha$  in the cooling process at the same time, the wider distribution means that the dynamic heterogeneity increases with the decrease of temperature. It can be seen in Fig. 3(b) that the distribution of FFLS changes gradually but not significantly with temperature. For the structural order parameter of  $\Omega$ , the distribution became narrower and higher, and shifts to smaller value with decreasing temperature, as shown in Fig. 3(c). It can be seen that all the distributions of these variables show consistent change with decreasing temperature. There is no any particular features showing below 800 K which could correspond to the non-monotonic behavior of the correlation length and strength shown in Figs. 1(b) and 2(b). Moreover, due to the generality of the non-monotonic behavior, we tend to associate it with

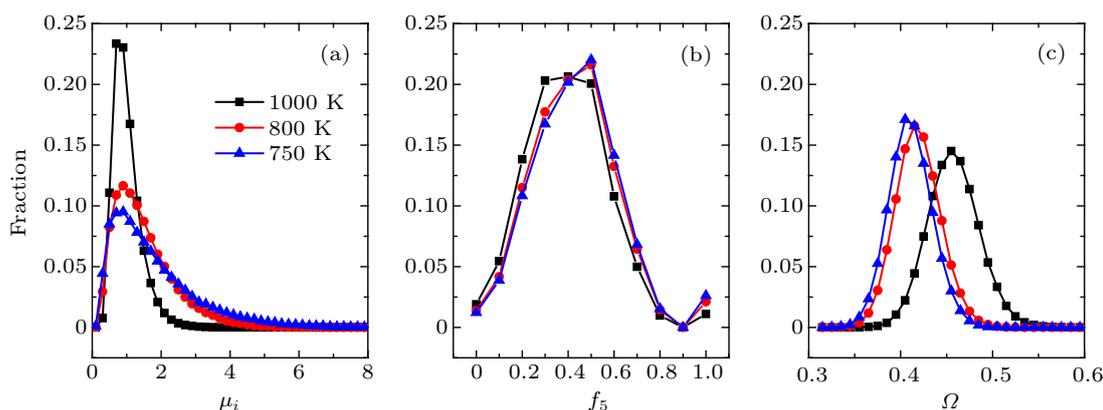


Fig. 3. Distribution of the atomic mobility (a), five-fold local symmetry (b), and  $\Omega$  (c) at 1000 K, 800 K, and 750 K, respectively.

We noticed that in Ref. [27], the nonlocal structure–dynamics correlation has monotonic temperature evolution in 2D and 3D polydisperse and binary mixtures of particles with harmonic potentials, which is in contrast to the non-monotonic temperature evolution observed above. This could be due to the different interatomic interaction potentials. Here, realistic many-body EAM potentials were employed.<sup>[29]</sup> Further stud-

ies need to be done to clarify this issue.

We also investigated the correlation between the atomic mobility and some specific atomic clusters by changing the coarse-graining length for the metallic glass-forming liquids at different temperatures. Here three typical atomic clusters,  $\langle 0, 0, 12, 0 \rangle$ ,  $\langle 0, 2, 8, 2 \rangle$ , and  $\langle 0, 3, 6, 4 \rangle$  were considered, due to relatively high population in metallic glass-forming liquids.

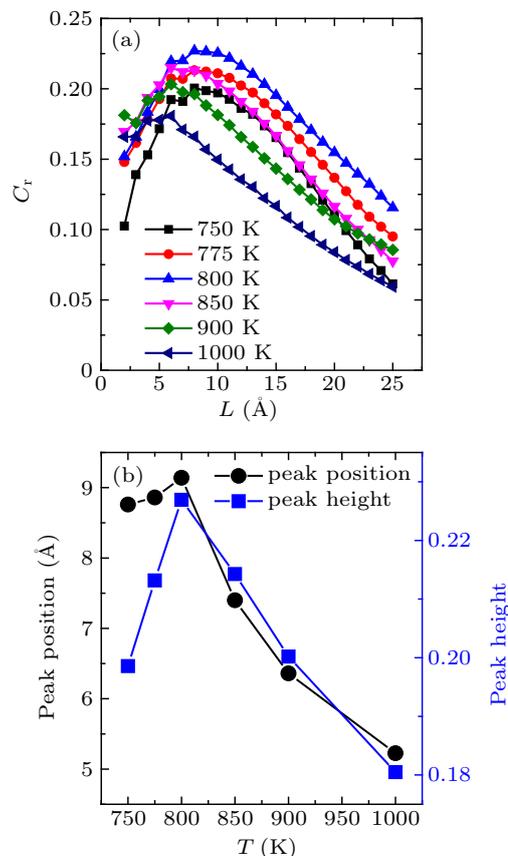
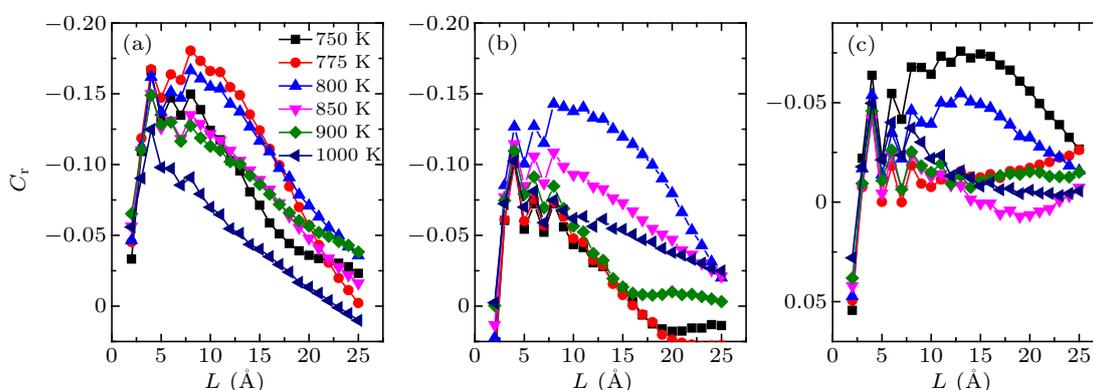


Fig. 2. (a) Correlation between the structural order parameter of  $\Omega$  and atomic mobility as functions of coarse graining length  $L$  at various temperatures in metallic glass-forming liquids. (b) Temperature dependence of peak height and position in the structure–dynamics correlation shown in (a).

To quantify the number of specific clusters associated with a given atom, we counted the number of a specific atomic cluster within a spherical coarse-graining region of radius  $L$  around each atom, which was used as the structural order parameter of atom  $i$  for structure–dynamics correlation similar to the previous study.<sup>[26]</sup> As shown in Fig. 4, for all three clusters, the correlation shows a general increase and decrease behavior with increasing coarse-graining length. However, the correlation shows multiple peaks, which is different from those shown in Figs. 1(a) and 2(a). For a specific cluster, the peak positions are almost identical at different temperatures. This indicates that there are some characteristic length scales of atomic clusters, independent of temperature, which may relate to the atomic packing of a specific cluster in short-to-medium range. For example, icosahedral clusters of  $\langle 0, 0, 12, 0 \rangle$  tend to con-

nect to each other and form a network structure which may have some characteristic lengths.<sup>[17]</sup>

Correlation between the atomic clusters and dynamics also shows non-monotonic temperature evolution, as shown in Fig. 4. However, the increase-to-decrease temperature may be different for different clusters, ranging between 750 K and 800 K. This confirms that the non-monotonic temperature evolution of the non-local structure–dynamic correlations may be general in metallic glass-forming liquids. On the other hand, the absolute value of the correlation varies greatly among the different clusters. The maximum value for  $\langle 0, 0, 12, 0 \rangle$  is around  $-0.15$ , while it is only  $-0.05$  for  $\langle 0, 3, 6, 4 \rangle$ , which indicates that the effect of the non-local structure of  $\langle 0, 3, 6, 4 \rangle$  is almost negligible, consistent with previous studies.<sup>[8,22]</sup>



**Fig. 4.** Correlation between local atomic clusters and atomic mobility as functions of coarse graining length  $L$  at various temperatures in metallic glass-forming liquids. (a)  $\langle 0, 0, 12, 0 \rangle$ , (b)  $\langle 0, 2, 8, 2 \rangle$ , (c)  $\langle 0, 3, 6, 4 \rangle$ .

We noticed that a surprising non-monotonic temperature evolution of dynamic correlations is revealed in glass-forming liquids.<sup>[35]</sup> It is found that the static length scales grow in a steady and monotonic manner with decreasing temperature, while the dynamic length scales obtained by fitting relaxation time show a striking local maximum which has not been observed in previous studies.<sup>[35]</sup> It is argued that this may be an indirect confirmation that the cooperative domain changes shape from an open structure to a more compact structure as temperature crosses the mode-coupling temperature.<sup>[36]</sup> In our work, however, we observed that the nonlocal structure–dynamics correlation exhibits non-monotonic temperature evolution in CuZr metallic glass-forming liquids. The inconsistent temperature evolution of static and dynamic length scales observed in Ref. [35] could imply a non-monotonic temperature evolution of structure–dynamics correlations in glass-forming liquids.

#### 4. Conclusion

The effect of nonlocal structure on dynamics in CuZr metallic glass-forming liquids was investigated via classical molecular dynamics simulations. The structure–dynamics cor-

relation in metallic glass-forming liquids shows a characteristic length scale which exhibits a non-monotonic temperature evolution in glass transition. The striking non-monotonic behavior in structure–dynamics correlation has not been detected in previous studies and implies that the structure–dynamics correlation in glass transition may be far more complicated.

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