Identifying packing features of atoms with distinct dynamic behaviors in metallic glass by machine-learning method

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In crystalline solids, plastic deformation is determined by the motion of structural defects, particularly dislocations. As for glassy liquids and disordered solids, it has long been assumed that localized structural rearrangements induced by mechanical load or thermal stimulus also occur at localized defects [1–3]. Metallic glasses have many promising applications as structural materials due to the unique long-range disordered atomic structure [4]. However, such structural disorder makes it overwhelmingly difficult to build a causal link between structure and plastic rearrangements [5–7]. The most promising structural indicators acting as structural defects are soft spots based on the soft vibrational modes [8,9], and volume flexibility [10]. Nevertheless, these indicators are based on the measurement of specific physical quantities and require detailed knowledge of interparticle interactions. Geometrically unfavored motifs (GUMs) and local fivefold symmetry (LFFS) [6,7,11,12], as purely structural indicators, can partially predict the nature of localized atomic rearrangements. However, metallic liquids or glasses have diverse atomic clusters, and thus it is not easy to distinguish which GUMs would be the ones that actually facilitate relaxation events. Recent work showed that such simple short-range order parameter as LFFS is not a sound structural fingerprint of dynamics of glasses because the spatial autocorrelation length of LFFS is only 1.2 Å, much shorter than the common spatial correlation range of approximately 2.2 Å [13]. Very recently, Cubuk *et al.* [14–20] successfully proposed a purely structural parameter, softness, by combining symmetry functions as structural representa-

tions with machine learning (ML) to capture the plasticity and dynamics in simple disorder systems with Lennard-Jones interaction. However, in metallic glassy systems with many-body interaction and composition-sensitive properties, the purely structural descriptor of dynamics still remains a mystery. Thus, it is of particular interest to investigate the structure-dynamics correlation in metallic glasses by ML methods.

In this work, we employ the ML method to build a predictive model in a simulated Cu₅₀Zr₅₀ metallic glass. The atomic softness defined by this predictive model is found to be strongly correlated with the propensity for structural rearrangements. The atoms predicted with positive or negative softness can be classified as “liquid-like” or “solid-like”, respectively. By systematically analyzing the structure of atoms with distinct softness, we observe that the structural difference between these two classes of atoms is dominated by the short-range structure within the first-neighbor shell, associated with non-negligible structure in the medium-range. Moreover, a characteristic distance can be extracted to distinguish the short-range packing features of the two kinds of atoms. Compared with the “solid-like” atoms, the “liquid-like” ones present more dense packing inside the characteristic distance but more loose packing beyond the characteristic distance. It indicates more anisotropic local geometrical packing feature of the “liquid-like” atoms, and provides useful hints about the structure-dynamics correlation in metallic glasses.

A prototypical binary system Cu₅₀Zr₅₀ with the embedded atom method (EAM) potential is employed in this

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work [21], which is selected for its superior glass-forming ability and simple constituents. The system consists of $N = 4000$ atoms. The sample is first equilibrated at 2000 K for 2 ns, and then quenched with a cooling rate of 10^{10} K s^{-1} , during which the external pressure is adjusted to zero within the constant number, pressure and temperature (NPT) ensemble. The glass transition temperature T_g is around 750 K. Simulations are done using LAMMPS [22] with a Nose-Hoove thermostat [23] and a time step of $\delta t = 0.002 \text{ ps}$. The glassy liquid at 800 K is first equilibrated in the NPT ensemble for 1 ns, and the configurations are then collected with a time interval $\Delta t = 1 \text{ ps}$ in the constant number, volume and temperature (NVT) ensemble for structure and dynamics analyses.

To explore the correlation between local structure and atomic rearrangement by ML methods, we first need to define the structural rearrangement, thus identifying the rearranging and non-rearranging atoms. In the super-cooled regime, the atom constantly vibrates locally in the cage formed by its neighbors and rarely escapes from the cage with a large displacement. To identify a rearrangement event in the three-dimensional quiescent system, we use a “hop” indicator function, p_{hop} , which was introduced by Candelier *et al.* [24,25]. To define $p_{\text{hop}}(i; t)$ for atom i at time t , we first specify two time intervals $A = [t - t_R/2, t]$ and $B = [t, t + t_R/2]$. The “hop” indicator function then can be written as

$$p_{\text{hop}}(i; t) = \sqrt{\frac{\langle (\mathbf{r}_i - \langle \mathbf{r}_i \rangle_B)^2 \rangle_A \langle (\mathbf{r}_i - \langle \mathbf{r}_i \rangle_A)^2 \rangle_B}{\langle \mathbf{r}_i - \langle \mathbf{r}_i \rangle_A \rangle_B^2}}, \quad (1)$$

where $\langle \rangle_A$ and $\langle \rangle_B$ are averages over the intervals A and B , respectively. If no rearrangement takes place between intervals A and B , then $\langle \mathbf{r}_i \rangle_A$ and $\langle \mathbf{r}_i \rangle_B$ are nearly equal and p_{hop} will be a small value. If a rearrangement does occur, the mean positions will change appreciably and p_{hop} will attain a significantly large value. The hop time parameter, t_R , used in the “hop” indicator function should be approximately the time it takes for the system to complete a rearrangement [15,20,25]. Here we take $t_R = 10 \text{ ps}$ to be at the end of the plateau-like region of the mean square displacement (MSD) data shown in the Supplementary information (Fig. S1). The distance and p_{hop} of an atom as a function of time can be seen in Fig. 1a and b, respectively. In the beginning, the atom locally vibrates within a cage, and the corresponding value of p_{hop} is small. When the atom hops to a new cage with a large displacement, the value of p_{hop} increases accordingly. Therefore, the “hop” indicator function can well describe the atomic rearrangement. We define all rearrangements to be those events with $p_{\text{hop}} > p_c$. The p_c is chosen such that 1% of the atoms from each species have

Figure 1 (a) The distance that an atom has moved from its initial position and (b) the corresponding “hop” indicator p_{hop} over time. Successive rearrangement events can be seen. (c) A schematic of the function $G_i(r)$ for several different values of r . (d) A schematic showing how the local structure of an atom is represented by G_i . We can find a hyperplane (black line) separating rearranging atoms ($y_i = 1$) from stable ones ($y_i = -1$) by SVM. Once the hyperplane is established, the softness S_i can be defined as the distance of atom i embedded into the high-dimensional space to the hyperplane.

gone through a rearrangement, although the specific choice of p_c does not affect our results qualitatively. The p_{hop} distributions of species Cu and Zr atoms differ significantly (see Fig. S2), and thus these two species are treated separately throughout the analysis. In this work, all results here are for the central atoms of species Cu only, but the results also hold for species Zr.

To employ ML methods, characterization of the local structure of each atom is needed. There are a wide variety of methods that can be used [15,26,27]. In order to more easily interpret the ML models and extract physical insights from them, we describe the local structure by the radial symmetry function [16,17]

$$G_i^X(r) = \sum_{j \in X} e^{-\frac{1}{2\delta^2}(r-R_{ij})^2}, \quad (2)$$

where R_{ij} is the distance between atoms i and j , and $X \in \{\text{Cu}, \text{Zr}\}$ refers to the species of atoms near atom i within $R_{ij} < R_c = 10 \text{ Å}$. As shown in Fig. 1c, $G_i^X(r)$ essentially reveals the Gaussian-smeared radial density of

species X at each r . In practice, we discretize the set of radii into $r_n = r_0 + n\delta$ and consider the vector

$$\mathbf{G}_i = (G_i^{\text{Cu}}(r_1), \dots, G_i^{\text{Cu}}(r_N), G_i^{\text{Zr}}(r_1), \dots, G_i^{\text{Zr}}(r_N)). \quad (3)$$

In this work, we keep $\delta = 0.1 \text{ \AA}$, $r_0 = 2 \text{ \AA}$, and $N = 80$ fixed. Therefore, we characterize the local structure around the target atom i by 160 structural descriptors $G_{i,\alpha}$ (where α indexes 1, 2, ..., 160). We note that the different choices of δ and N only bring trifling impact on the results so long as r_n is large enough to include several neighbor shells. $\mathbf{G}_i$ of an atom contains details of local geometrical structure across several shells, as well as chemical features. Thus, we expect that $\mathbf{G}_i$ can sufficiently capture the local structure of individual atom.

Having defined rearranging and non-rearranging atoms through p_{hop} and characterized local structure of each atom through $\mathbf{G}_i$, we now use an ML method called support vector machine (SVM) [28] to find function of features (in this case about $\mathbf{G}_i$) that optimally separates points in different classes (in this case about rearranging and non-rearranging atoms). The SVM algorithm is implemented using the LIBSVM package [29]. Firstly, we select a training set with N atoms that are about to rearrange in the next 1 ps, each labeled as $y_i = 1$, and equal atoms that will not rearrange, each labeled as $y_i = -1$. Therefore, a training set of $2N$ atoms can be written as $\{(\mathbf{G}_1, y_1), \dots, (\mathbf{G}_{2N}, y_{2N})\}$. We next use SVM with a linear kernel to construct a hyperplane defined by the hyperplane's normal $\mathbf{w}$ and the bias b , that best divides atoms with $y_i = 1$ from those with $y_i = -1$ in the training set. Once the hyperplane has been constructed, we then employ this hyperplane on the test set. For atom i in the test set, its local structure can be described by $\mathbf{G}_i$, the softness S_i is then defined as $S_i = \mathbf{w} \cdot \mathbf{G}_i + b$ [15], which is shown schematically in Fig. 1d. The atom will be classified as "liquid-like" (prone to rearrangement) if $S_i > 0$, and as "solid-like" (resistant to rearrangement) if $S_i < 0$.

We choose the training set with 10,000 rearranging atoms, each labeled as $y_i = 1$, and equal non-rearranging atoms, each labeled as $y_i = -1$. After the ML training, the hyperplane, acting as the ML model, is constructed. The hyperplane normal $\omega(r)$ for Cu-Cu and Cu-Zr pairs obtained from the SVM is shown in Fig. 2a and b, respectively. Since the softness is defined as integrating the local structure of $G_i(r)$ weighted by $\omega(r)$, a large absolute value of $\omega(r)$ within short-range indicates the short-range order will impose a great effect on softness. Moreover, $\omega(r)$ beyond short-range distance is nontrivial, especially for Cu-Cu pairs, which implies that the medium-range structures play a nonnegligible role in determining soft-

ness. We then construct a test set of 2×10^6 atoms. These atoms are aggregated over every snapshot of the simulation, and the softness of all atoms in the test set is calculated using the machine-learned hyperplane.

To investigate the effectiveness of softness at predicting rearrangements, we first check the relation between softness and p_{hop} . In Fig. 2c, we plot the average softness with p_{hop} . There is a clear trend that the higher the softness, the larger the p_{hop} . Furthermore, we investigate the probability, P_R , that atoms will rearrange as a function of softness. P_R is calculated as the fraction of atoms with a softness that will undergo rearrangements. As shown in Fig. 2d, the probability of rearrangement of high-softness atoms is nearly two orders of magnitude larger than their low-softness counterparts, indicating the robustness of the softness in predicting rearrangements. In Fig. 2e, the contoured map illustrates the spatial distribution of the softness on a slice with a thickness of 10 Å. The locations of the white spots superimposed on the contour denote the spatial information of rearranging atoms. Obviously, the rearrangements have a high propensity to originate from those "liquid-like" regions with $S > 0$. Since atoms with higher softness are more prone to rearrangement, it is necessary to check whether the size of rearrangements is limited by the spatial extent of high-softness regions. Therefore, we first investigate the spatial correlation function of the softness field [19]

$$C(r) = \langle \delta S(0) \delta S(r) \rangle = \frac{\langle S(0)S(r) \rangle - \langle S(0) \rangle^2}{\langle S^2(0) \rangle - \langle S(0) \rangle^2}. \quad (4)$$

As shown in Fig. 2f, we find that $\langle \delta S(0) \delta S(r) \rangle$ exhibits approximately exponential decay, and the red dashed line is fitted by $\langle \delta S(0) \delta S(r) \rangle = Ae^{-r/\xi_S}$ with $\xi_S \approx 2.52 \text{ \AA}$. This length scale is commensurate with the spatial correlation length previously identified in metallic glassy systems [13], implying that softness is also a good structural descriptor to predict the dynamic feature of metallic glasses. To measure the spatial extent of rearrangements, we then consider the spatial correlation of p_{hop} . As with softness, we find that the correlation $\langle \delta p_{\text{hop}}(0) \delta p_{\text{hop}}(r) \rangle$ decays exponentially with $\xi_R \approx 2.55 \text{ \AA}$. Thus, we can conclude that the characteristic size of localized rearrangements is encoded in the size of spatial correlation of softness in metallic glassy system. This observation is in excellent agreement with the earlier results in Kob-Andersen model systems [16].

The above results demonstrate that the softness is effective in predicting the rearrangement, indicating that there is a strong structural component to rearrangement.

Figure 2 (a, b) The hyperplane normal $\omega(r)$ for Cu-Cu and Cu-Zr pairs, respectively. The black dashed lines denote the first trough position of the RDF of the system for Cu-Cu and Cu-Zr pairs, respectively. (c) Correlation between the average p_{hop} with softness. Each data point is the average for 5% of all of the atoms, sorted in the order of increasing softness. (d) The probability that atoms will rearrange as a function of their softness. Each data point is the average for 5% of all of the atoms, sorted in the order of increasing softness. (e) The contour map denoting the softness field in the slice of 10 Å thick. The locations of the rearrangements are indicated by the white spots. (f) The spatial correlation functions for softness (red) and rearrangement (blue). The dashed lines are fits to Ae^{-r/ξ_S} with $\xi_S \approx 2.52$ Å for softness and Ae^{-r/ξ_R} with $\xi_R \approx 2.55$ Å for rearrangement.

To illustrate this, we refer to the radial distribution function (RDF) of the “liquid-like” ($S > 0$) and the “solid-like” ($S < 0$) atoms. When the system is isotropic, the structure function $G_i^X(r)$ is related to the RDF [14]

$$g_{A-X}(r) = \lim_{\delta \rightarrow 0} \langle G_i^X(r) \rangle / (4\pi r^2), \quad (5)$$

where A and X are species of the central atom and

neighboring atom, respectively. As shown in Fig. 3a and b, we notice that the “liquid-like” (or “solid-like”) atoms classified by the hyperplane and the rearranging (or non-rearranging) ones have similar RDFs, implying that the hyperplane learned from the SVM can reliably distinguish rearranging atoms from stable ones. Comparing $g(r)$ of the “liquid-like” with the “solid-like” atoms for Cu-Cu

Figure 3 (a, b) The RDFs of Cu-Cu pairs averaged over “liquid-like” atoms with $S > 0$ (red line) versus rearranging atoms with $p_{\text{hop}} > p_c$ (blue dashed line) and “solid-like” atoms with $S < 0$ (red line) versus non-rearranging atoms with $p_{\text{hop}} < p_c$ (blue dashed line), respectively. (c) The difference of coordination number ΔN_c as a function of r_{cutoff} between “liquid-like” and “solid-like” atoms. The green arrow denotes the characteristic length of $r_c = 2.85 \text{ \AA}$. (d) Correlation between the average local configurational anisotropy $|u|$ with softness. Each data point is the average for 5% of all of the atoms, sorted in the order of increasing softness. (e, f) The schematic of local geometry for “liquid-like” (red) and “solid-like” (blue) atoms, respectively. The black dashed circles denote the range of characteristic length r_c . The length of arrows denotes the magnitude of the local configurational anisotropy $|u|$. Atoms inside the circular region of the radius $r < r_c$ are colored as green, while atoms outside the circular region are colored as orange.

pairs, we find that the structural differences between them are beyond the first shell. The obvious splitting of the second peak suggests the enhanced medium-range order for the “solid-like” atoms. The similar results can also be found for $g(r)$ of Cu-Zr pairs shown in Fig. S3.

To fully understand the local environment of the “liquid-like” and the “solid-like” atoms, we next calculate

the coordination number, N_c , of these two groups of atoms. The difference of N_c between them, $\Delta N_c = N_c(S > 0, r_{\text{cutoff}}) - N_c(S < 0, r_{\text{cutoff}})$, as a function of r_{cutoff} is shown in Fig. 3c. It shows that there exists a clear characteristic length $r_c = 2.85 \text{ \AA}$ that is approximately equal to the first peak position of the RDF of the system, within the first neighbor shell. The “liquid-like” atoms have more

neighbors when r_{cutoff} is below r_c , while the result is opposite when r_{cutoff} is above r_c , suggesting that the “liquid-like” atoms are tightly packed within r_c but loosely packed beyond r_c . This observation is further confirmed in another metal-metal glass $\text{Ni}_{50}\text{Nb}_{50}$ [30] and a metal-metalloid glass $\text{Ni}_{80}\text{P}_{20}$ [31], indicating the generality of this finding among metallic glasses (see Fig. S4). Furthermore, we analyze the local configurational anisotropy, $|u_i|$, defining the deviation from the center of atom i to the centroid of its corresponding Voronoi cell [32–34]. For atoms in full icosahedra, the center of the atom and the corresponding Voronoi cell centroid coincide and $|u_i|=0$. However, for atoms in distorted polyhedra, the atom’s center deviates from the centroid of corresponding Voronoi polyhedron. Therefore, the local configurational anisotropy signifies the degree of symmetry breaking of atomic environment and thus the propensity for vibrations [32–36]. As shown in Fig. 3d, $|u|$ linearly increases with softness. It implies that the “liquid-like” atoms with larger value of softness have more anisotropic structure and thereby are more likely to rearrange. From the above, we can depict the local geometry of the “liquid-like” and the “solid-like” atoms shown in Fig. 3e and f, respectively. As compared with “solid-like” atoms, “liquid-like” counterparts are closely packed within the characteristic range r_c , but have more local void spaces beyond the characteristic range r_c . Moreover, “liquid-like” atoms present higher degree of distortion in their atomic environment, indicating a high propensity for rearrangements.

In summary, we have presented a novel ML approach to identify the atoms prone to rearrangements in the $\text{Cu}_{50}\text{Zr}_{50}$ metallic glassy system. We find that the “liquid-like” and the “solid-like” atoms classified by machine-learned hyperplane display distinct dynamic features. Moreover, we observe a characteristic length r_c within the first neighbor shell differentiating the short-range packing features of these two classes of atoms. The “liquid-like” atoms present more tight packing within r_c , but more loose packing beyond r_c . In addition, the “liquid-like” atoms have more anisotropic atomic environment, which promotes rearrangements. Our findings provide comprehensive insights into the structure-dynamics relationship of metallic glassy systems.

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Author contributions Bai H and Guan P conceived and led the research; Wu Y conducted the calculations and analyzed the data. Wu Y, Guan P and Bai H wrote the paper with the input from Wang WH. All authors contributed to the general discussion.

Conflict of interest The authors declare that they have no conflict of interest.

Supplementary information Supporting data are available in the online version of the paper.

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机器学习方法识别金属玻璃中不同动力学原子的结构特征

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摘要 直接从无序体系的结构中预测易于发生重排的原子一直是一个挑战。本文以金属玻璃 $\text{Cu}_{50}\text{Zr}_{50}$ 为研究对象, 通过机器学习的方法成功识别出倾向于发生重排的“类液原子”。另外, 我们还观测到在第一壳层以内存在一个临界尺度。在临界尺度以内, “类液原子”的近邻排列更紧密; 然而超过这个临界尺度, 其近邻排列相对疏松。研究表明“类液原子”的各向异性度更大, 这可能是“类液原子”更容易发生重排的结构起源。我们的研究表明机器学习能为理解金属玻璃本征的不均匀性提供一种非传统的方法, 同时揭示了无序材料中不均匀动力学的结构起源。