Existence of fractal packing in metallic glasses: Molecular dynamics simulations of Cu$_{46}$Zr$_{54}$

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The recently advocated power-law scaling for fractal packing in amorphous metals is examined in a metallic glass under hydrostatic pressure. We show that the scaling relation $v_a \sim q_1^{-\zeta}$ between the sample molar volume $v_a$ and the first peak position $q_1$ in the scattering function exhibits a varying exponent $\zeta$ from 2.77 to 3.72 in different stages of compression, rather than a constant as the universal fractal dimensionality. Fractal packing of short- and medium-range icosahedral clusters is found to exist but undetectable with high angle scattering. Therefore, the substructure of the metallic glass does not contribute to the power-law exponent. Moreover, we show that the space filling contributed from different alloy components with varying atomic sizes is overlooked in the scaling relation that gives rise to the so-called fractal dimension. The amorphous packing of metallic glasses is actually compact with dimension 3.

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I. INTRODUCTION

The experimental data of the mean atomic volume $v_a$ and the first peak position $q_1$ in the scattering function $S(q)$ in several dozens of multicomponent metallic glasses were compiled and a power-law scaling relation $v_a \sim q_1^{-\zeta}$ was observed, where the exponent $\zeta = 2.31$ [1]. It was argued that since $q_1$ corresponds to the inverse of the first-nearest-neighbor atomic distance $r_1$, i.e., $q_1 \propto r_1^{-1}$, the scaling relation $v_a \sim q_1^{-\zeta}$ becomes $v_a \sim r_1^\zeta$, which implies that the dimensionality of the metallic glasses $d$ equals to $\zeta$. On the other hand, from a space-filling point of view, $v_a$ should scale with $r_1^d$, where $r_1$ is in general the basic unit for atomic packing. For instance, $r_1$ is the size of the unit cell in crystalline materials and the size of the Voronoi cell of each atom in noncrystalline amorphous solids. If $d = 3$, the packing is compact with atoms filling up the space; otherwise, if $d < 3$, the packing is fractal with pores left inside. Compared to other truly fractal objects [2], the reported exponent $\zeta$ less than 3 in the metallic glasses indicates a fractal packing in the amorphous structures. The fractal atomic packing is speculated as by stacking up the structural units made of the (icosahedral) clusters characterized by the cluster size, i.e., the first atomic neighbor distance $r_1$ in the clusters.

The same argument was extended later in a few more multicomponent metallic glasses [3,4] that are under increasing hydrostatic pressure. From synchrotron scattering, a range of $q_1$ values are measured in the pressured samples, along with the mean sample volume $v_a$. The same relation $v_a \sim q_1^{-\zeta}$ was used for scaling [3,4], which gives a fixed value for $\zeta$ at 2.50, leading to the claim that the amorphous packing in the multicomponent metallic glasses has fractal structure with a “general 2.5 power law” [3,4]. Similar to the early work [1], the concrete atomic structure is inferred from this scaling exponent as the icosahedral clusters with fractal packing [3,4].

While intriguing, the power-law scaling and the inferred underlying fractal packing for amorphous structure are subject to several questions, some technical and others fundamental. Due to the lack of detailed experimental data on atomic structure in real space and careful theoretical analysis, these questions can be easily overlooked, which may undermine the scaling argument in Refs. [1,3,4].

The first technical question is about the relationship between $r_1$ and $q_1$. The first peak position $q_1$ in the scattering function is known to be different from $r_1$ except in simple crystals [5]. In general, $r_1$ and $1/q_1$ do not follow a linear relation, which is crucial in performing power-law scaling in the previous works. In fact, it is $r_1$ rather than $q_1$ that should be considered first in the fractal scaling argument for space filling. If $q_1$ and $r_1$ do not follow the simple inverse relation, the entire assumption that the relation $v_a \sim q_1^{-\zeta}$ equals $v_a \sim r_1^\zeta$ with $d$ being the fractal dimensionality would fail. For simplicity, let us assume that $q_1$ and $r_1$ themselves follow a power-law relation, such as $r_1 \sim q_1^{-\zeta}$, where $x$ is a new exponent. Of course, the relation could be much complicated as we show below. In this simple case, the relation $v_a \sim q_1^{-\zeta}$ leads to $\zeta = dx$, where $d$ is the dimensionality from the space-filling relation $v_a \sim r_1^d$. For $x \neq 1$, the exponent $\zeta$ no longer equals the (fractal) dimensionality $d$ and thus, the scaling scheme using $q_1$ does not hold.

The second technical question is related to the errors in multicomponent alloys caused by using the mean value $r_1$ only. Because different elements have different atomic radii and different nearest-neighbor distances, $r_1$ for the entire sample is an average of all individual nearest-neighbor distances for all pairs of elements which are present in the partial radial distribution functions [6]. Correspondingly, the mean atomic volume $v_a$ in multicomponent alloys is thus the summation of the volumes of each type of atoms that can be well represented by their nearest-neighbor packing with different $r_1$’s. Thus, the total sample volume $v_a$ in multicomponent alloys follows cubic scaling law, i.e., $d = 3$, with respect to the atomic size of each type of atoms. Therefore, using a single value of $r_1$
to approximate the space filling by different atoms can lead to uncertainty in the (fractal) dimensionality scaling.

The last is the fundamental question about the validity in inference to the fractal packing of a particular substructure, the icosahedral clusters, from \( q_1 \) from high-angle x-ray diffraction [1,3,4]. Icosahedral clusters are indeed found to populate in a large number of multicomponent metallic glass alloys. However, since all atoms in the multicomponent system participate in scattering, \( q_1 \) obtained from the scattering function in the high-angle scattering contains the contributions from all atoms, including those from the icosahedral clusters as well as nonicosahedral clusters. This is fundamentally different from the scattering from true fractal objects where atoms, molecules, particles, or clusters in the fractal packing are the only diffracting objects [4]. Then the immediate question is whether \( q_1 \) as assumed in Refs. [1,3,4] is the unique representation of this particular local icosahedral structure. In other words, if there is a fractal icosahedral cluster packing, is \( q_1 \) faithful in representing the local clusters only? If not, the scaling argument using \( v_a \sim q_1^{-\zeta} \) is no longer valid.

To answer the above questions, we use atomistic simulation. It is perhaps the only approach by far that can give us any quantitative and detailed information about the atomic packing in amorphous alloys that can help us to clarify these issues.

II. METHODS

The sample we used is the binary metallic glass Cu46Zr54. The choice of this model system with different elements allows us to capture the essence in multicomponent systems [1,3,4]. Here we have the mean \( r_1 \) contributed from two different elements, so the dispersion effect from different atomic sizes is present in this simple model system that may lead to a general relation between \( r_1 \) and \( q_1 \). In addition, this class of metallic glass alloys made of Cu and Zr is known for having a large number of icosahedral clusters. Therefore, we can directly look into the relations between the local icosahedral packing and the scaling relations [1,3,4]. In order to have a large range of length-scale change for \( v_a \), \( r_1 \), and \( q_1 \) needed in performing scaling, we subject the sample with hydrostatic pressure. Note that the details of the repulsive potential for the alloy system are not crucial to the results in metallic systems as long as it remains isotropic and has a right proportionality to the core size of the atoms.

CuZr alloys are known for forming the most stable binary bulk glasses, including Cu46Zr54 and Cu64Zr36 [7–9]. The extraordinary thermal stability gives us opportunity to simulate genuine glassy systems within the short simulation time without crystallization and other phase changes such as chemical segregation, especially under hydrostatic pressure. The computational simplicity endowed in the binary system enables us to explore the atomic packing and related properties with current computational capability that is not possible in multicomponent systems.

The semiempirical many-body embedded atom method (EAM) interatomic potentials by Mendeleev [10] are used for Cu46Zr54. The EAM potentials are well tested [10], which guarantees the reliability of the simulated properties of the CuZr metallic glass during the molecular dynamics (MD) simulation [10]. An NPT ensemble MD simulation is used to obtain the glassy sample where the Andersen barostat is employed to control the pressure and the Nose-Hoover thermostat is used for temperature control. Amorphous Cu46Zr54 is obtained by rapidly quenching the liquid from 2200 to 300 K under zero external pressure with the cooling rate at 1012 K/s. The samples are kept at 300 K for 100 ps for relaxation.

Compression is carried out by applying hydrostatic pressure directly to the above-prepared sample at 300 K using the Parrinello-Rahman method, while the system volume is let to adjust freely to the applied pressure. The samples are subject to continuously increasing pressure with the pressure rate of 1011 GPa/s. The metallic glass is stable up to 80 GPa pressure that is sufficient for our purpose to investigate fractal packing in a genuine homogeneous amorphous phase within the time limit in the MD simulation. To check the possible sample size and pressure rate effects, we used several samples with the total number of atoms \( N = 4000, 32000, \) and \( 108000 \), respectively and pressure rates at \( 1 \times 10^3, 4 \times 10^3, \) and \( 10^{11} \) GPa/s. No significant difference is found for the different samples under different pressure rates that could alter our conclusions. The results presented here are mostly from the sample with 108000 atoms and at the pressure rate of 1011 GPa/s.

At each applied pressure \( P \), we can obtain the system volume \( v_a \) directly from the NPT MD simulation cell size. From the atomic configurations at each pressure, we calculate atomic structures through the quantities such as the radial distribution functions (RDFs) and local atomic cluster packing. The nearest-neighbor distance \( r_1 \) is obtained from fitting the first peak in the total RDFs and \( q_1 \) is acquired from the scattering function \( S(q) \) of the system.

III. RESULTS AND DISCUSSION

Figure 1 is the equation of state relating \( v_a \) to applied pressure \( P \) up to 80 GPa. As shown by the RDFs [see Fig. 2(a)], under such a large range of pressure the amorphous structure remains stable. About 31.1% total volume reduction...
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FIG. 2. (a) The RDFs and (b) the $S(q)$ for Cu$_{46}$Zr$_{54}$ sample, perfect icosahedral, and non-ICO clusters at various external pressures. (c) The $r_1$ (top) and $q_1$ (middle) for the entire sample, Cu-Cu, Zr-Zr, and perfect ICO and non-ICO clusters at various external pressures, and their relations between the corresponding $r_1$ and $1/q_1$ (bottom) where the log-log fitting is used for the relations between $r_1$ and $1/q_1$.

is achieved at 80 GPa, which is comparable to that found in experiment [3,4]. $v_a$ is obtained directly from the sample volume in simulation; it can also be obtained from the first peak position $r_1$ in the total RDF as done in many experiments, but the obtained volume is an approximation to the true volume [see Fig. 1]. In this work, we shall use the former. For later analysis, we also obtain the molecular volumes for icosahedral (ICO) and nonicosahedral (non-ICO) clusters in the sample (see detailed explanation below) which are plotted in the inset in Fig. 1.

Corresponding to the RDFs [Fig. 2(a)], the scattering functions $S(q)$ at different pressures are obtained for the entire sample. We also obtain the partial RDFs and $S(q)$ for the samples that contain only icosahedral and nonicosahedral clusters [Fig. 2(b)]. The technical details will be given later. By using Gaussian fitting of the first peaks in both the RDFs [Fig. 2(a)] and $S(q)$ [Fig. 2(b)], we obtain $r_1$ and $q_1$ at different pressures [top and middle panels in Fig. 2(c)] for the entire sample and for each pair of atoms, Cu-Cu, Cu-Zr, and Zr-Zr, from the partial RDFs. We also perform the same fitting procedure to obtain $r_1$ and $q_1$ from the samples that contain icosahedral and nonicosahedral clusters. As shown in the lower panel in Fig. 2(c), for the entire sample as well as the samples containing only icosahedral and nonicosahedral clusters, their corresponding $r_1$ and $1/q_1$ do not exhibit a linear relation.

Using the mean atomic volume $v_a$ and $q_1$ for the entire sample between zero and 80 GPa in the scaling relation $v_a \sim q_1^{-\zeta}$, we obtain $\zeta = 2.880 \pm 0.030$ [Fig. 3(a)], while the early result is 2.31 and a “general” result is 2.5, respectively [1,3,4]. With the value of the scaling exponent $\zeta$ less than 3, at first glance the amorphous packing may be thought as having fractal packing. In the following, we shall show that $\zeta$ obtained this way is not the true fractal dimensionality $d$.

From Fig. 2(c), we notice that $r_1$ and $q_1$ do not show a linear relation with respect to pressure. The relation between $r_1$ and $1/q_1$ are also nonlinear with respect to each other [lower panel in Fig. 2(c)]. This nonlinearity means that we may get different scaling exponents $x (\neq 1)$ for $r_1 \sim q_1^{-x}$. From the data in the lower panel in Fig. 2(c), we have the exponent $x \approx 0.870 \pm 0.028$ approximately [Fig. 3(b)]. Therefore, the true dimensionality $d = \zeta / x \approx 3.310 \pm 0.146$. As discussed above, we can also use directly the scaling relation $v_a \sim r_1^d$ for spacing filling, rather than $v_a \sim q_1^{-\zeta}$, where the data for $r_1$ are from Fig. 2(c). In this case, the best fitting gives $d = 3.270 \pm 0.081$ [Fig. 3(c)], showing that the exponent $\zeta$ does not equal to the fractal dimension $d$ as it is corrupted by $x$. As we will discuss below, the dimensionality $d$ obtained using the scaling relation $v_a \sim r_1^d$ does not approach 3 exactly because $r_1$ used in this relation is still an approximation which contributes uncertainty from the atomic size dispersity in multicomponent alloys.
FIG. 3. The log-log plot of the relations: (a) \( v_\alpha \sim q_1^{-\zeta} \), (b) \( r_1 \) and \( 1/q_1 \), and (c) \( v_\alpha \sim r_1^{\zeta} \) for the data between zero and 80 GPa. The insets in (c) are for low- and high-pressure data and the fitting in the two regimes.

In Refs. [1,3,4], the atomic structure behind the inferred fractal packing is the short-range clusters and their spatial distribution that form percolating clusters [1,3,4]. The icosahedral clusters are considered as dominating the atomic packing and as a result, contribute to fractal dimensionality via \( q_1 \).

FIG. 4. (a) The atomic fraction of the perfect icosahedral (555) clusters and other clusters (433), (544), (444), (666), and (422) at different applied pressure. The inset is an atomic configuration of a perfect icosahedral cluster made of 13 Cu (blue) and Zr (green) atoms. (b) The atomic configurations of perfect icosahedral clusters (left) and nonicosahedral clusters (right) made of Cu (blue) and Zr (green) atoms. (c) The log-log plot of the relations between the total sample volume (total) and the corresponding \( q_1's \), \( v_\alpha \sim q_1^{-\zeta} \), for the samples containing all atoms and the atoms in the perfect icosahedral and nonicosahedral clusters. As a comparison, the same relation relating the volumes of the icosahedral and nonicosahedral clusters and their corresponding \( q_1's \) from the middle panel of Fig. 2(c) are plotted.

To examine this proposal, we mapped out all local clusters in the system, including the perfect icosahedra with fivefold symmetry termed as (555) [Fig. 4(a) and the inset]. This is done by using Honeycutt-Anderson’s common-neighbor analysis [11]. Note that the local cluster packing indexed with the Honeycutt-Anderson method contains neighbor atoms with icosahedral as well as nonicosahedral symmetry [11]. The perfect icosahedral clusters have fivefold symmetry for all 12
neighbor atoms, i.e., (555). As seen, icosahedral packing in the binary metallic glass is the most popular one with the largest fraction of atoms involved, about 20.8% at zero pressure and increases to 54.0% at 80 GPa. The results are very much similar to those found in other binary and multicomponent alloys [12–15]. The nonspacing filling, perfect icosahedral cluster with fivesix symmetry was suggested as the basic structural unit for amorphous alloys [16,17].

In Fig. 4(b), we plotted separately these perfect icosahedral clusters as well as the nonicosahedral clusters in the sample. One can see that these clusters have bicontinuous distribution in space. If viewed separately, each type of the cluster distributions is not space filling, i.e., with holes or pores, visible to our eyes. The spatial distribution of the icosahedral and nonicosahedral clusters gives rise to the perception of "fractal" packing of metallic glasses. However, as we show below, not only is this separation of atoms into the two substructures in the metallic glass artificial but also does not lead to long-range fractal packing as expected.

We have already shown that it is problematic in obtaining $d$ from $\zeta$ from the scaling $v_{\xi} \sim q_1^{-\zeta}$ due to the nonlinear relations between $r_1$ and $q_1$. To delineate the contribution from the icosahedral cluster packing from the rest of the atoms, we perform another test:

1. We remove all atoms that are not in the perfect icosahedral clusters [Fig. 4(b)], including those in the clusters with partial icosahedral symmetry. Therefore, we have an "only perfect icosahedral cluster packed" sample, or ICO sample. Using the same procedure mentioned above, we then calculate the corresponding volume for each atom in the perfect icosahedral clusters from Voronoi analysis, $r_1$ and $q_1$ (Fig. 1), RDFs [Fig. 2(a)] and $S(q)$ [Fig. 2(b)] for the ICO samples.

2. As a comparison, we also created another sample that excludes all atoms with perfect icosahedral symmetry, or non-ICO sample. Thus, we have a complement model to the ICO sample discussed previously.

In addition, we have the sample that contains all atoms, including ICO and non-ICO. Results from these three types of samples would allow us to compare and examine the proposed contributions from icosahedral clusters, and nonicosahedral clusters as well.

The top and middle panels in Fig. 2(c) show that $r_1$ and $q_1$ obtained from theicosahedron-only sample nearly overlap with those from the whole sample containing all atoms, and $r_1$ and $q_1$ follow nonlinear relations in the whole sample as well as the ICO and non-ICO samples [bottom panel in Fig. 2(c)]. As shown in Fig. 4(c), scaling the total sample volume $v_\xi$ versus $q_1$ from the perfect icosahedral clusters yields $\zeta = 3.156 \pm 0.032$ and the nonicosahedral clusters gives $\zeta = 2.852 \pm 0.024$. The exponents are close to 3.

The scaling relations between the volumes of the icosahedral and nonicosahedral clusters and their corresponding $q_1$‘s are also shown [Fig. 4(c)], which gives rise to $\zeta = 2.909 \pm 0.027$ and $\zeta = 2.968 \pm 0.027$, respectively. Once again, the exponents are very close to 3 as in the full space filling. These results show, ironically, that the proposed would-be dominant icosahedral clusters do not contribute to the fractal dimensionality, although they do appear to have fractal-like morphology when viewed by our eyes.

This outcome is not surprising since the high-angle diffraction such as in synchrotron or normal x-ray scattering [1,3,4] is not supposed to selectively pick up the diffraction from only the atoms with icosahedral packing in the short- and medium-range scales. All atoms participate in scattering. In other words, the value of $q_1$ obtained from the whole sample is contributed from all atoms including the supposedly fractal icosahedral and nonicosahedral clusters. Therefore, from the value of $q_1$, one cannot delineate the contributions from the atoms in the icosahedral clusters from the rest of the atoms. However, since the relations between $r_1$ and $q_1$ from the ICO and non-ICO samples are slightly nonlinear as compared with those of the whole sample [Fig. 2(c)], we noticed that the exponent $\zeta$ obtained from the scaling relation $v_{\xi} \sim q_1^{-\zeta}$ for the ICO and non-ICO clusters in Fig. 4(c) is larger. In other words, as the exponent $x$ is closer to 1 in $r_1 \sim q_1^{-x}$ for the ICO and non-ICO samples [see Fig. 2(c)], $\zeta \rightarrow d$. In the following, we shall further clarify the misconceptions in fractal packing in metallic glasses.

We showed that the atoms in the icosahedral clusters do form fractal-like packing [Fig. 4(b)] when separated from the rest of the atoms. This particular local atomic packing seen in many other Cu-Zr glasses [12–15] often leads to the conception that metallic glasses are made of these clusters which form interconnected percolating backbones [1,3,4,12–15]. A recent work, however, demonstrated that there are no percolating clusters in metallic glasses [18]. To understand this look-alike fractal packing in metallic glasses and how this "fractal-like" packing plays out in the dimensionality analysis, i.e., fractal dimensionality, we perform direct (fractal) dimensional sampling [1] using the mass scaling relation $M \sim r_0^d$ down to atomic scales, where $M$ is the total mass of Cu and Zr atoms within the sphere of the sampling radius $r_0$, which is taken at arbitrary positions in the sample with the increment of 0.4 Å. Once again, we perform this sampling in the three types of samples, the whole sample with all atoms included, ICO, and non-ICO sample.

Figure 5(a) shows the relation between $M$ and $r_0$ in the ICO sample. As seen from the inset in Fig. 5(a), the (fractal) dimension $d$ fitted is found to be a function of pressure $P$ and also sampling distance $r_0$. There is a crossover distance [see the inset in Fig. 5(a)] below which $d$ shows the fractional dimensionality ($<3$) and beyond $d$ becomes 3. The length scale associated with the crossover distance is about 12 Å at zero pressure and decreases to 8 Å at 80 GPa, which is the intermediate range at about the fourth- to fifth-nearest-neighbor distances, about the center-to-center distance between two or three clusters. The fractal dimension $d$ presented in the inset of Fig. 5(a) is obtained within this range of distance below the crossover distances which are also shown in the inset in Fig. 5(a) as function of applied pressure $P$. $d$ increases from 1.67 at zero pressure to 2.5 at and above 35 GPa within the crossover distance, or short- and medium ranges. Above the crossover distance, $d$ is always 3. The same is found for non-ICO samples, since ICO and non-ICO samples are complementary to each other. As a comparison, we plotted the mass scaling relation $M \sim r_0^d$ for the whole sample [Fig. 5(b)]. Here $d$ remains at 3 for all length scales and all pressures. The results confirm that, the local icosahedral cluster packing has fractal-like packing with $d < 3$ but only up to
FIG. 5. The mass scaling relation $M \sim r_d^s$ for (a) the samples containing the perfect icosahedral clusters at different pressures, where the inset shows the relation between the dimensionality $d$ and pressure and the crossover distance between the fractal and nonfractal regime versus pressure; and (b) the entire sample containing all atoms. (c) The scaling exponent $\zeta$ fitted in different pressure regions starting from zero pressure. (d) The scaling exponent $\zeta$ fitted piecewise in different pressure regimes toward the high pressure at 80 GPa.

the distance of the short- and medium range, beyond which the space packing does not look fractal anymore. In addition, as the pressure increases, or the system becomes more compacted, the atomic packing, including the icosahedra, becomes more dense and full-space filling with $d \to 3$. As we discussed above, the existence of the fractal-like packing in short- and medium range does not contribute solely to $q_1$ and, therefore, is irrelevant to fractal scaling in the amorphous packing using the relation $v_a \sim q_1^{-\zeta}$ involving $q_1$.

Lastly, we shall discuss the role played by the different atomic sizes in how they affect the fractal analysis in multicomponent amorphous alloys. One manifestation of the subtle size dispersity is in the variation of the exponent $\zeta$ with applied pressure. Figure 5(c) shows that in the binary metallic glass, $\zeta$ goes from 2.77 to 2.82 with the smaller value $\zeta (<3.0)$ occurring at the low-pressure regime (0–40 GPa) and approaching 3 at the high-pressure region (0–80 GPa). In Fig. 5(d), we plot the value of $\zeta$ fitted piecewise from different pressure intervals toward high pressure at 80 GPa. One can see that $\zeta$ increase monotonically from $\zeta = 2.880 \pm 0.030$, with the mean value fitted to the entire range of pressure from zero to 80 GPa, to $\zeta = 3.720 \pm 0.022$ in the range of pressure from 70 to 80 GPa. The higher the pressure, the larger $\zeta$. This observation is explained below.

Since the total volume of the sample is the summation of the volumes from each type of atoms with different nearest-neighbor-distances $r_1$’s, when these individual contributions are approximated by one single length scale, $r_1$ or $q_1$, errors may occur in the scaling analysis using $v_a \sim q_1^{-\zeta}$ as well as $v_a \sim r_1^d$. This can be understood in terms of the nonlinear responses to pressure of different atoms in the alloys [top panel in Fig. 2(c)]: Zr is a softer atom that can be compressed easily compared to the harder Cu atom. This size-dispersion effect becomes smaller with increasing pressure [19]. In other words, the sample looks more monoatomic at high pressure where the differences between the measured $r_1$’s (and $q_1$’s) from each type of atoms approach each other more closely, which makes the space filling look more compact. The sample with the more uniform atomic size distribution gives rise to larger $\zeta$ values as we see at higher pressure. This can also be seen in the variation of different scaling exponents in $x$ [Figs. 2(c), 3(b), and 4(c)] and $\zeta$ [Figs. 5(c) and 5(d)]. From this result, we could predict that in monoatomic metallic systems, crystal or glass, $x \to 1$, which leads to $\zeta \to d$ [20].
IV. CONCLUSIONS

Atomic structure in amorphous solids is still a mystery. Due to the absence of Bragg diffraction in this class of materials, the conventional experimental tools that have been used successfully for crystalline materials become powerless. Computer simulation, on the other hand, can fill some voids in providing detailed atomic information of atomic packing. However, this alternative approach needs to be coupled with rigorous and careful analysis in order to untangle the subtle structure information in amorphous solids.

As shown in this work, fractal-like packing does exist for various clusters including icosahedra but only in short- and medium range. The power-law scaling, therefore, does not extend to larger scales. The conception of non-space-filling by the local fractal cluster packing is simply the result of our selective viewing of certain subspace packing of the atoms classified as either icosahedral or some other types such as different alloy elements, or chemical and structural inhomogeneities. The (artificial) local fractal packing does not contribute uniquely to the first peak $q_1$ in the scattering function. Therefore, $q_1$ is not a faithful representation of space filling for atoms in amorphous solids. Consequently, in general one cannot use the scaling relation $v_0 \sim q_1^{-\zeta}$ for dimensional analysis. Our analysis from the extensive simulation shows that the atoms do not have fractal packing in the metallic glass, and neither the percolating substructure made of icosahedral clusters. The dimensionality of metallic glasses should remain at 3.

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