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Characterization of mechanical heterogeneity in amorphous solids

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The structural geometry and size distribution of the local atomic rearrangements induced by external stress in amorphous solids are investigated by molecular dynamics studies. We find that the size distribution exhibits a generic power-law behavior and their structural geometry shows fractal feature. This indicates that the local atomic rearrangements in amorphous solids are self-organized during deformation. A simple theoretical model based on the interaction of the heterogeneous elastic field sources is proposed which predicts the power-law scaling and characterizes the properties of the local atomic rearrangements in amorphous solids. © *2012 American Institute of Physics*. [http://dx.doi.org/10.1063/1.4739260]

I. INTRODUCTION

In amorphous materials, the characteristics of the local atomic rearrangements are crucial for the understanding of the deformation mechanism.[1–5] The shear transformation zone (STZ) model proposed by Argon provides a picture of the local atomic rearrangements and reveals that atomic rearrangements are confined in clusters of particles.[1] Based on Argon's work, Falk and Langer introduced mean-field equations of motion for the number density of STZs and their two-state translation.[6] All these efforts have been successful in explaining many phenomena, such as shear localization, strain hardening, and emergence of yield in amorphous solids.[7] On the other hand, some other studies investigated the property of the avalanches which are the accumulations of the local atomic rearrangements defined by stress drops or energy drops during deformation.[8,9] It is found that during deformation the amorphous solids undergo cascades of local atomic rearrangements, which induce quadrupolar energy fluctuation and organize into lines of slips spanning the length of simulation box. These studies indicate that local atomic rearrangements are not independent, but correlate to each other.[8,9]

It is known that the stress-induced local atomic rearrangements give rise to long range elastic fields, and act as stress sources similar to elliptic Eshelby inclusions.[10] Since every local atomic rearrangement can alter the stress field surroundings, all the local atomic rearrangements embedded in the elastic matrix may interact with each other and are subjected to a self generated dynamic noise.[11] This noise-like complexity makes it difficult to model the deformation behavior with the concern of the interaction between local atomic rearrangements.[12] The difficulty leads to some critical issues, for example, how these local atomic rearrangements distribute in space during plastic deformation, and in what manner these local atomic rearrangements cooperate with each other. All these issues are still less understood, but they are vital for understanding plastic deformation mechanism in amorphous materials.

In this work, we characterize the structural geometry feature and size distribution of the local atomic rearrangements with external shear stress by molecular dynamics (MD) simulation for two-dimensional (2D) and three-dimensional (3D) Lenard-Jones (LJ) binary mixtures and 3D CuZr metallic glass (MG) in shear deformation. A universal scaling of size distribution of local atomic rearrangements is found in the form of power-law distribution. The structural geometry of the local atomic rearrangement exhibits fractal feature, indicating that the local atomic rearrangements are self-organized during shear deformation. The simulation results show that this power-law distribution of local atomic rearrangements is generic, independent of the atomic potential or system size, reflecting the nature of structural heterogeneity in amorphous solids. A simple theoretical model based on the interaction of the elastic field sources is proposed, which predicts the power-law scaling behavior.

II. MODEL AND METHOD

In LJ binary mixture of particle A and B, all particles have the same mass, $m = 1$, and the composition $A_{65}B_{35}$ is selected because it is stable against crystallization especially in two dimension.[13] The interatomic potential is given by $U_{\alpha\beta}(r) = 4\varepsilon_{\alpha\beta}[(\sigma_{\alpha\beta}/r)^{12} - (\sigma_{\alpha\beta}/r)^{6}]$, where $\alpha, \beta \in \{A,B\}$, $\sigma_{AA} = 1.0$, $\varepsilon_{AA} = 1.0$, $\sigma_{AB} = 0.8$, $\varepsilon_{AB} = 1.5$, $\sigma_{BB} = 0.88$, $\varepsilon_{BB} = 0.5$. Following common practice, the potential is truncated and shifted at $r = 2.5\sigma_{\alpha\beta}$. Reduced units are used, with σ_{AA} being the unit of length, ε_{AA} the unit of energy, and $(m\sigma_{AA}^2/48\varepsilon_{AA})^{1/2}$ the unit of time.[14] Two structure models containing $N_1 = 100\,000$ and $N_2 = 500\,000$ atoms are generated for both 2D and 3D systems. The initial structure configurations are equilibrated at $T = 5.0$, then cooled down to target temperatures using NPT (constant number of atoms, pressure and temperature) ensemble with hydrostatic pressure fixed at 10.0 and cooling rate of 7×10^{-4}. For 2DLJ system, structure samples at $T = 0.1$ and $T = 0.2$ are obtained with box length of 282.7 and 283.6 for N_1 structure model, and 632.1 and 634.2 for N_2 structure model, respectively. For 3DLJ system, samples at $T = 0.4$ are fabricated (with box length of 40.6 for N_1 structure model and 69.5 for N_2

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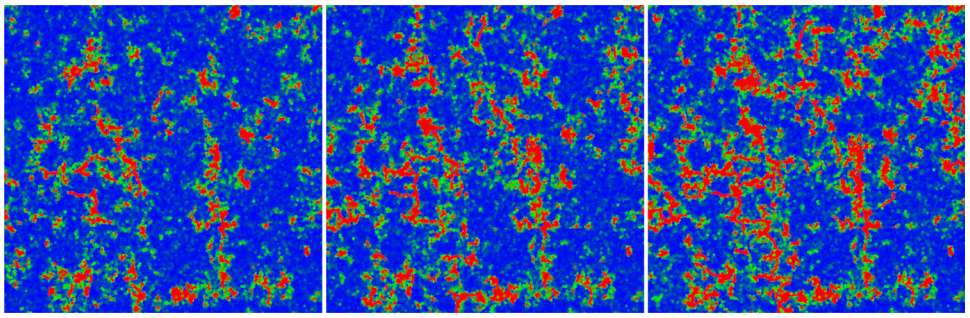

FIG. 1. Nonaffine displacement field in 2DLJ N_1 sample at the strain of 10% with the strain interval of 1% (a), 2% (b), and 3% (c), respectively. T = 0.2.

structure model). The glass transition temperature T_g is 0.33 and 0.58 for 2DLJ and 3DLJ systems, respectively.[13] In our simulations, simple shear deformation is applied to LJ binary mixtures along x axis with period boundary conditions in all directions. After each shearing with the strain interval of 0.1%, the system is relaxed for 2000 MD steps (with time step of 0.014 (Ref. 14)), which leads to the average strain rate of 3.6×10^{-5}. For $Cu_{50}Zr_{50}$ MG containing 40 000 atoms with a realistic interatomic potential,[15] compressive deformation is applied at T = 300 K. Detailed information about the sample preparation and deformation can be found in Ref. 16.

III. RESULT AND DISCUSSION

To investigate the plastic deformation behavior on atomic level, the nonaffine displacement of an atom relative to its nearest neighbors determined by Voronoi tessellation method under deformation $D^2(t, \Delta t)$ is calculated[6] by

$$D_i^2(t,\Delta t) = \frac{1}{N}\sum_j \left[\vec{r}_j(t) - \vec{r}_i(t) - \vec{\gamma}\left(\vec{r}_j(t+\Delta t) - \vec{r}_i(t+\Delta t)\right)\right]^2,$$

where i denotes the central atom, and j runs over the N nearest neighbors of central atom i, Δt is the time interval for plastic rearrangement, and $\vec{\gamma}$ is the maximum local elastic strain tensor.[6] Note that nonaffine displacement has been distinguished as a long-rang correlated continuous part and a localized fluctuating part, and a clear transformation from localized fluctuation to continuum at the length of about inter-particle distance has been shown.[17,18] Therefore, it is be reasonable that we use the nonaffine displacement within the inter-particle distance to characterize the local atomic rearrangement.

Figure 1 shows the nonaffine displacement field of the 2DLJ N_1 sample at the strain of 10% with strain interval of 1%, 2%, and 3%, respectively. It can be clearly seen that as strain increases, the plastically deformed zones tend to trigger the new local atomic rearrangements in the surrounding areas. The "nearby triggering" effect results from the strong interaction of elastic fields generated by quadruple-like plastic events,[8] so that the distribution of these local atomic rearrangements is directly correlated with the subtle interaction of elastic fields. Therefore, characterizing the nature of the distribution of these atomic rearrangements becomes quite important for understanding the deformation mechanism in amorphous solids.

First, we assume that an atom experiences plastic deformation if its $D^2(t, \Delta t)$ value is in the top 5% (Δt is set as a strain increment of 0.1% in the analysis below). With this definition, one can justify whether an atom participates in local irreversible rearrangements or not. Since the local environments or the distribution of the free volume, chemical order, and local atomic symmetry are inhomogeneous in amorphous solids, the local atomic rearrangements will occur in different regions and with different sizes.[19,20] Therefore, the size of the local atomic rearrangements and its distribution should reflect the dynamic response of the local structures to the external stress. Figure 2 shows the size distribution of the local atomic rearrangements in the 2DLJ sample during deformation. It is interesting that the number of atomic rearrangements monotonically decreases with the size, which follows a power-law distribution. This indicates that there is no characteristic size for the local atomic rearrangements during deformation.[9,21] To check the choice of top percentage threshold on the size distribution of the local atomic rearrangements, we chose different top percentages of $D^2(t, \Delta t)$ such as 10%, 20%, and 30% for the local irreversible rearrangements and investigated the size distributions. As shown in Fig. 2, with the choice of different top percentages of $D^2(t, \Delta t)$, the power-law behavior still holds. This indicates that in a certain range, the choice of top percentage of D^2 will not influence the result. For convenience, we will choose top 10% of D^2 value in the analysis below.

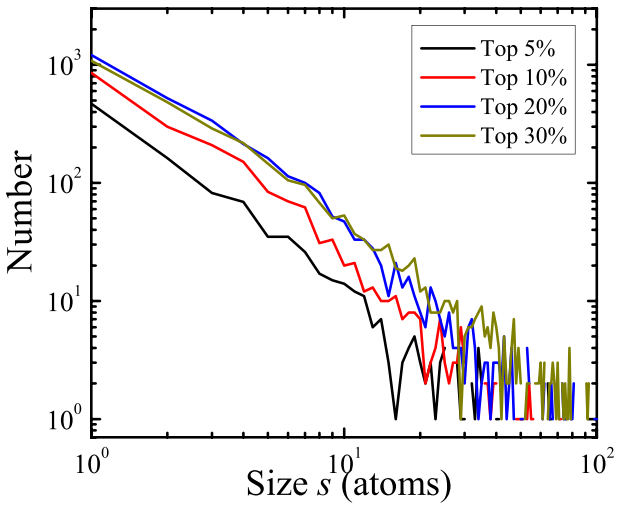

FIG. 2. The size distribution of local atomic rearrangements in a 2DLJ sample with different choices of top percentage of D^2 values at strain 10%.

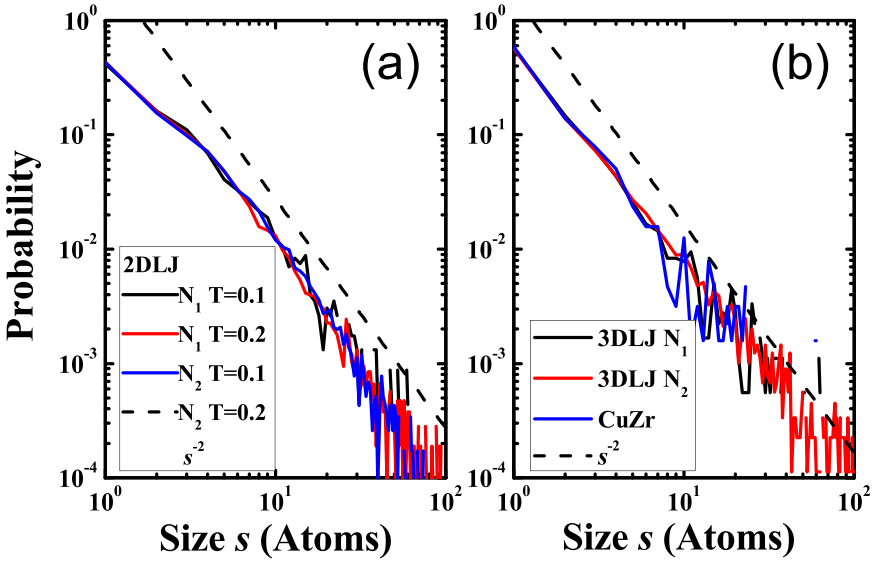

FIG. 3. Probability distribution of the local atomic rearrangements in 2D (a) and 3D (b) systems. The dashed lines are the power-law distribution with exponent of −2 predicted by the theoretical model.

Note that significant non-affinity can be present in purely elastic response due to the inhomogeneous relaxation in disordered structures, and it is important to explicitly distinguish the plastic rearrangements from elastic relaxation.[22] This issue is far beyond the topic of this work. To some extent, however, one may still use the nonaffine displacement to characterize the local atomic rearrangements.[6,7,16,26] In our study, the data were collected in plastic flow region where the local plastic rearrangements are dominant. Therefore, using nonaffine displacement to define the sites of plastic deformation should be a reasonable approximation.

Next we investigate the effect of system size and temperature on the power-law distribution of the local atomic rearrangements for 2DLJ and 3DLJ systems and $Cu_{50}Zr_{50}$ MG. As shown in Fig. 3, the size probability distribution of the local atomic rearrangements collapses together very well in the form of power-law distribution in both dimensionalities

$$P(s) \sim s^{-\nu}, \tag{1}$$

where P and s represent the probability and size of local atomic rearrangements, respectively. This finding indicates that the power-law behavior of size distribution of the local atomic rearrangements is generic, independent of the system size, temperature, and even the interatomic interaction in MGs, which is reminiscent of self-organized phenomena.

To examine the feature of these self-organized local atomic rearrangements, we analyzed their structure geometry feature by using box-counting method which is one of the most common methods for the fractal analysis[23]: in 2D (3D) case, for grids of squares (cubics) with edge length Δx, the number of squares (cubics) $N(\Delta x)$ containing at least one of atoms participating the local atomic rearrangements is determined. The "box-counting" dimension D_f is determined by $N(\Delta x) \sim \Delta x^{-D_f}$. Figure 4 shows the relationship between $N(\Delta x)$ and Δx in 2DLJ samples. By fitting the smaller Δx part of the curves, it is found that D_f is about 0.92, which indicates fractal geometry of the irreversible rearrangement regions. For top 20% and 30% of D^2, $D_f \sim 1.09$ and 1.20 in 2D case, respectively. In 3D case, it is found that $D_f \sim 1.09$, 1.25, and 1.47 for top 10%, 20%, and 30% of D^2, respectively. All these findings indicate the fractal geometry feature of the local atomic rearrangements. Therefore, the fractal geometry feature confirms that local atomic rearrangements are self-organized during plastic deformation.

In order to get deep insight into the self-organized behavior of the size distribution of local atomic rearrangements, we applied a simple theoretical model proposed by Holtsmark for the distribution of the gravitational forces created by the random distribution of stars.[23] In this model, it is found that the distribution of the gravitational forces follows a power-law behavior due to the heterogeneity of the distribution of stars.[23] In our case, local atomic rearrangements give rise to long-range elastic fields,[8–10] and the elastic fields trigger new local atomic rearrangements. Therefore, the distribution of the elastic stress should correspond to the distribution of local atomic rearrangements. As mentioned above, the location of local atomic rearrangements depends strongly

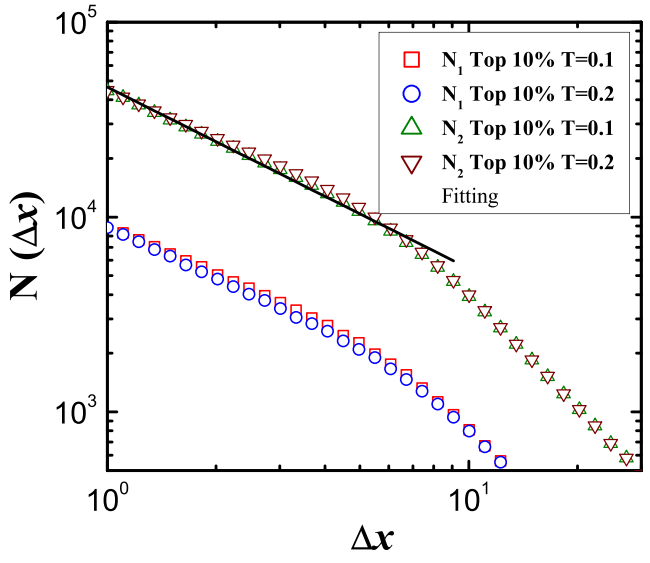

FIG. 4. Box-counting method for the relationship between N(Δx) and Δx, indicating the fractal geometry feature of the local atomic rearrangements.

on the complex local structures, so that it is natural to assume that local atomic rearrangements are randomly distributed in amorphous solids, and the probability of finding a local atomic rearrangement in the distance between r and $r+dr$ can be expressed as

$$P(r)dr \sim \rho r^{d-1}dr, \tag{2}$$

where d denotes the spatial dimensionality and ρ presents the average density of the local atomic rearrangements. Only the atomic rearrangements within a cutoff distance from the considered point are taken into account, because the elastic field generated by the atomic rearrangements far away from the point can be neglected.

On the other hand, the elastic field generated by one single atomic rearrangement decays with distance as $G(r) \sim r^{-\mu}$, and the decaying exponent μ is equal to 2 (3) in 2D (3D) system.[24] Here G is the elastic shear stress. Assuming that the atomic rearrangements that are further away do not contribute significantly compared to the closer ones, we may get the distribution $P(G)dG$ of the local shear stress G and $P(G)dG = P(r)dr$, which yields

$$P(G)dG \sim \frac{1}{\mu}G^{-\nu}dG, \qquad \nu = 1 + \frac{D}{\mu}. \tag{3}$$

In the case of a small strain interval, the local stress should correspond to the local atomic rearrangements, so that the sizes of local rearrangements are approximately proportional to the intensity of local stress, which leads to the form of Eq. (1) for the probability distribution of the local atomic rearrangements. Finally, $\nu = 2$ is obtained for the probability distribution of the local atomic rearrangements in both 2D and 3D cases.

As shown in Fig. 3, the dashed lines demonstrate that the power-law behavior predicted by this theoretical model is in good agreement with the simulation results, especially for 3D case. This is consistent well with the distribution of local stress in sheared 2DLJ amorphous solid.[25] It has been shown that strain field is heterogeneous.[26,27] According to our theoretical model, the self-organized stress-induced local atomic rearrangements result from the heterogeneous stress fields. If the plastic deformation is completely homogeneous, the elastic force will be zero in an infinite sample, due to the exact cancellation of the forces among all pairs of deformed points symmetric to each other. This theoretical model indicates that the nature of the elastic fields generated by local atomic rearrangements in plastic deformation finally leads to the self-organized behavior of these local atomic rearrangements.

We note that the heterogeneity-induced self-organized phenomenon is different from the evolution of the shear bands in deformed amorphous solids.[28,29] This is because the self-organized local atomic rearrangements emerge in short-time interval and are the processes of the creation and annihilation of STZs, which is closely related to the initial stage of plastic deformation. A relative long-time interval for deformation may break down the self-organization of the local atomic rearrangements. Strain rate is another ingredient that affects the self-organized behavior of local atomic rearrangements. High strain rate may also disrupt the self-organization, because the correlation between local atomic rearrangements will disappear as strain rate goes to $\dot{\gamma} \to \infty$.[11] We also did detailed analysis for various strain rates. Figure 5 shows that the probability distribution is gradually deviating from the power-law behavior as strain rate is getting higher in LJ system. However, for a realistic strain rate, the phenomenon of self-organization will sustain. We also note that instead of Voronoi tessellation, the first minimum of pair distribution function was also used as the clear length-scale cutoff to determine the nearest neighbors, which does not affect the above results.

So far, we have characterized the structural geometry feature and size distribution of local atomic rearrangements induced by shear deformation. It has been suggested that the structures of MGs consist of densely packed solid-like atomic clusters and loosely packed liquid-like regions.[14,20,26,30] Such a nanoscale structural heterogeneity leads to the local environments, the distribution of free volumes, chemical order, or local atomic symmetry quite different from one region to another in amorphous solids, so that local atomic rearrangements will occur in different regions and with different sizes.[19,20] It has been suggested that either

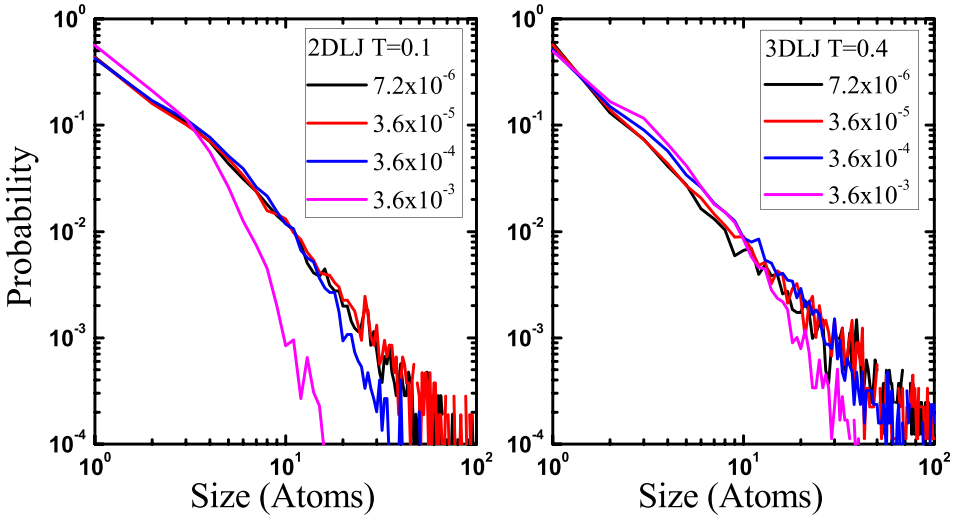

FIG. 5. Strain rate dependence of the probability distribution of the local atomic rearrangements in 2D (left panel) and 3D (right panel) systems.

temperature or applied shear stress can induce the glassy structure destabilization which prefers to be initiated in the loosely packed liquid-like regions,[31] so that the characteristics of the local atomic rearrangements reflect the dynamical response of the heterogeneous structures to the external stress.[32,33] Therefore, our results also have implications for the understanding of the structural and mechanical heterogeneity in MGs.

IV. CONCLUSION

In summary, we have characterized the local atomic rearrangements in shear deformation in amorphous solids. The size distribution of these local atomic rearrangements exhibits power-law behavior, far from the Gaussian distribution, which means the local atomic rearrangements can not be considered as randomly independent variables. We also find that these local atomic rearrangements are self-organized in plastic deformation. A simple theoretical model is proposed and predicts the power-law scaling behavior, indicating that the long-range heterogeneous elastic field sources induce the power-law size distribution of the local atomic rearrangements. The findings may shed light on the understanding of nature of the structural and mechanical heterogeneity in MGs.

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[1]A. S. Argon, Acta Metall. **27**, 47 (1979).
[2]J. S. Harmon, M. D. Demetriou, W. L. Johnson, and K. Samwer, Phys. Rev. Lett. **99**, 135502 (2007).
[3]F. Delogu, Phys. Rev. Lett. **100**, 255901 (2008).
[4]D. Rodney and C. Schuh, Phys. Rev. Lett. **102**, 235503 (2008).
[5]S. G. Mayr, Phys. Rev. Lett. **97**, 195501 (2006).
[6]M. L. Falk and J. S. Langer, Phys. Rev. E **57**, 7192 (1998).
[7]C. A. Schuh, T. C. Hufnagel, and U. Ramamurty, Acta Mater. **55**, 4067 (2007).
[8]C. E. Maloney and A. Lemaître, Phys. Rev. Lett. **93**, 016001 (2004); C. E. Maloney and A. Lemaître, Phys. Rev. E **74**, 016118 (2006).
[9]E. Lerner and I. Procaccia, Phys. Rev. E **79**, 066109 (2009).
[10]J. D. Eshelby, Proc. R. Soc. London, Ser. A **241**, 376 (1957).
[11]A. Lemaître and C. Caroli, Phys. Rev. Lett. **103**, 065501 (2009).
[12]M. L. Manning, J. S. Langer, and J. M. Carlson, Phys. Rev. E **76**, 056106 (2007).
[13]R. Brüning, D. A. St-Onge, S. Patterson, and W. Kob, J. Phys.: Condens. Matter **21**, 035117 (2009).
[14]W. Kob and H. C. Andersen, Phys. Rev. Lett. **73**, 1376 (1994).
[15]M. I. Mendelev, D. K. Rehbein, R. T. Ott, M. J. Kramer, and D. J. Sordelet, J. Appl. Phys. **102**, 093518 (2007).
[16]H. L. Peng, M. Z. Li, and W. H. Wang, Phys. Rev. Lett. **106**, 135503 (2011).
[17]C. Goldenberg, A. Tanguy, and J.-L. Barrat, Europhys. Lett. **80**, 16003 (2007).
[18]M. Tsamados, A. Tanguy, C. Goldenberg, and J.-L. Barrat, Phys. Rev. B **80**, 026112 (2009).
[19]T. Egami, S. J. Poon, Z. Zhang, and V. Keppens, Phys. Rev. B **76**, 024203 (2007).
[20]Y. Q. Cheng, A. J. Cao, H. W. Sheng, and E. Ma, Acta Mater. **56**, 5263 (2008).
[21]N. P. Bailey, J. Schiøtz, A. Lemaître, and K. W. Jacobsen, Phys. Rev. Lett. **98**, 095501 (2007).
[22]C. E. Maloney, Phys. Rev. Lett. **97**, 035503 (2006).
[23]D. Sornette, Critical Phenomena in Natural Sciences: Chaos, Fractals, Selforganization and Disorder: Concepts and Tools, 2nd ed. (Springer, 2003).
[24]G. Picard, A. Ajdari, F. Lequeux, and L. Bocquet, Eur. Phys. J. E **15**, 371 (2004).
[25]M. Tsamados, A. Tanguy, F. Leonforte, and J. L. Barrat, Eur. Phys. J. E **26**, 283 (2008).
[26]Y. Shi and M. L. Falk, Phys. Rev. Lett. **95**, 095502 (2005).
[27]C. E. Maloney and M. O. Robbins, Phys. Rev. Lett. **102**, 225502 (2009).
[28]S. X. Song and T. G. Nieh, Intermetallics **17**, 762 (2009).
[29]B. A. Sun, H. B. Yu, W. Jiao, H. Y. Bai, D. Q. Zhao, and W. H. Wang, Phys. Rev. Lett. **105**, 035501 (2010).
[30]M. Li, C. Z. Wang, S. G. Hao, M. J. Kramer, and K. M. Ho, Phys. Rev. B **80**, 184201 (2009).
[31]P. Guan, M. W. Chen, and T. Egami, Phys. Rev. Lett. **104**, 205701 (2010).
[32]H. Wagner, D. Bedorf, S. Kuchemann, M. Schwabe, B. Zhang, W. Arnold, and K. Samwer, Nature Mater. **10**, 439 (2011).
[33]J. C. Ye, J. Lu, C. T. Liu, Q. Wang, and Y. Yang, Nature Mater. **9**, 619 (2011).