The Local Rearrangement of Tension Deformation in AlSi Amorphous Alloy: A Molecular Dynamics Study

Ye Li*, Hongyu Liang, Yinzhu She and Yulin Wang

Taiyuan Institute of Technology, Taiyuan 030008, P.R. China

Al$_{100-x}$Si$_x$ (x = 2, 4, 6, 8, 10) amorphous alloy models are constructed by using molecular dynamics (MD) simulations. In order to investigate the local rearrangement during the tension deformation, Honeycutt-Andersen (HA) method and Voronoi tessellation method are performed for the initial state. The HA method and the atomic local shear strain are used for the deformed states of the models. The structure of AlSi alloys is mainly amorphous structure. It is found that the Si element enhanced glass-forming ability. Moreover, the amorphous structure breaks and transforms into other tiny complex structure during the tension deformation. In addition, it is observed that the amorphous regions which preferentially undergo atomic rearrangement in the elastic stage and early plastic stage. [doi:10.2320/matertrans.MT-M2020351]

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1. Introduction

Amorphous metals have fairly attracted attention due to their high strength and hardness as a substitute for conventional crystalline metals. However, they usually suffer from a strong tendency towards shear localization and easily brittle failure, which restricts the application of these materials. Although the underlying deformation physics of these materials established less firmly as compared with crystalline metals, understanding of local rearrangement is particularly important in amorphous metals because local rearrangement plays a crucial role in forming to shear transformations zones (STZs). STZs occur to the atomic scale and are the elementary plastic events involving a few tens of atoms spanning within a few picoseconds. With the accumulation of STZs forming to shear band (SB), finally the failure of amorphous metals is induced by SB.

The MD simulations may be the most suitable tool to study plastic deformation in amorphous materials, because the lack of experimental device is able to identify plastic events in amorphous at the atomic scale. Thus far, MD simulation has been extensively applied to characterize the plastic deformation of pure amorphous metals and fixed composition amorphous alloys. Wang et al. studied amorphous structure of magnesium under compression with different strain rate; they revealed that the amorphous regions are dominant in the deformation and results of more homogenous deformation. In the case of magnesium, the crystalline zones are predominant in the deformation. However, they usually suffer from a strong tendency towards shear localization and easily brittle failure, which restricts the application of these materials. Although the underlying deformation physics of these materials are less firmly established as compared with crystalline metals, understanding of local rearrangement is particularly important in amorphous metals because local rearrangement plays a crucial role in forming to shear transformations zones (STZs). STZs occur to the atomic scale and are the elementary plastic events involving a few tens of atoms spanning within a few picoseconds. With the accumulation of STZs forming to shear band (SB), finally the failure of amorphous metals is induced by SB.

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2. Simulation Method

The MD simulations were performed for AlSi amorphous with a time step of 1 fs. The interatomic interactions were used by the modified embedded atom method (MEAM) potential proposed by B. Jelinek et al. All simulations were performed using the Large Scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) software. The AlSi amorphous models were made by “Atomsk”. We used the radial distribution function (RDF), the HA method and Voronoi tessellation method to investigate the initial structure of AlSi alloy. We performed the HA method to analyze local arrangement during the tension deformation. “OVITO” was used for visualizing and analyzing output date.

Al$_{100-x}$Si$_x$ amorphous alloy models on values of x of 2, 4, 6, 8 and 10 were prepared as follows. At first the modell was randomly packed with Al and Si atoms with specific composition into a small unit, which consisted of 4 x 4 x 4 FCC lattice constructions (256 atoms) and lattice constants set to 4 Å as seen in Fig. 1(a). The small unit was copied 5 times along X, Y, and Z to generate the final model consisting of 32000 atoms as seen in Fig. 1(b). The prepared model was numerically heated to 1800 K, which is much higher than the melt point of Al and Si. After a sufficient relaxation of 20 ps, it is cooled to 300 K at a rate of 10$^{13}$K/s in the isothermal and isobaric (NPT) ensemble. Periodic boundary conditions were applied to the three dimensional directions in order to eliminate surface effects as seen in Fig. 1(c). We investigated local rearrangement of the AlSi atomic models under uniaxial tension loading. The simulation cell was applied to a small
strain increment in each step at the speed of $10^2$ m/s along the x axis. The applied stress for the whole system was estimated using the atomic stress definition based on the virial theorem. Periodic boundary conditions (PBC) were used along the Y and Z axis, and free boundary condition was used along the X axis. The temperature was set at 300 K. Figure 1(d) was the snapshot of Al$_{96}$Si$_4$ at the tension strain of 50%.

3. Results and Discussions

The RDF profiles of AlSi alloys are shown in Fig. 2. One can see the broad splitting second peak, which indicates the amorphous structure of AlSi alloy system. As the proportion of Si element increase, the heights of the first peak slightly decrease and the locations slightly move in the direction of the horizontal axis.

A further study into the structure distribution of AlSi alloy was conducted by HA pair analysis. The HA structural pairs utilize a sequence of four integers to classify the 3D atomic configuration between the centered and the surrounding atoms. According to the literature, amorphous and glassy structures are represented by the HA index 1551, 1541 and 1431. The bcc structure has the type 1441 and 1661, the fcc structure has the type 1421, and hcp has the type 1421 and 1422. Figure 3 shows the HA index distribution of AlSi amorphous system, which less than 3 percent of all the total number of HA pairs were added together as other pairs. There are 5 mainly kinds of HA pairs, which are 1551, 1541, 1431, 1441 and 1661 pairs in AlSi system. The fractions of amorphous structure (1551, 1541 and 1431) are over 40% in AlSi system. The fraction of 1551 pair is almost twice as much as 1541 and 1431 pair, respectively. The fractions of bcc structure are less than 30%. The 1441 and 1661 pair is about 14% and 12% respectively. However, the 1441 and 1661 pairs are also included in the defective icosahedra as well as in the Frank-Kasper polyhedra.

To further distinguish bcc structure, the defective icosahedra and the Frank-Kasper polyhedra in the 1441 and 1661 pairs, the Voronoi polyhedra method was used to classify the structure in the AlSi alloys. The method is constructed from all edges formed by the intersections of the planes halfway between the central atom and all of its first neighbor atoms. The Voronoi index $(n_3, n_4, n_5, n_6)$ represents different polyhedral structure. For example, the Voronoi indexes of the perfect icosahedra, BCC, and FCC/HCP are $(0,0,12,0)$, $(0,6,0,8)$ and $(0,12,0,0)$, respectively. However, these structures are distorted in the amorphous system. Figure 4 shows the Voronoi indexes of the AlSi alloy (less than 2% ignored). According to previous studies, these Voronoi indexes can be divided into two categories. The Voronoi indexes of deformed icosahedra include $(0,3,6,3)$, $(0,4,4,3)$, $(0,3,6,2)$, $(0,2,8,2)$ and $(0,2,8,1)$; The $(0,3,6,4)$ index represents deformed fcc structure. The remaining three Voronoi indexes are $(0,5,3,3)$, $(0,4,5,3)$ and $(0,5,3,4)$, these structures are very similar and no specified...
The results show that there are no Voronoi indexes for bcc structure, indicating no bcc structure in AlSi alloy. Meanwhile, the number of neighbor atoms has less than 13 in all these Voronoi indexes, indicating that there is as well no Frank-Kasper polyhedron in the AlSi alloy. It could be concluded that the structure of AlSi system was amorphous structure which includes a variety of deformed icosahedra. With the proportion of Si element increases, the fraction of most deformed icosahedra increases too. Combining the result of Fig. 3, it could be concluded that the Si element enhances glass-forming ability of AlSi system, the most likely reason is that Si doping prevents crystal formation leading to amorphous structure in the quenching process.

The calculated tension stress and applied strain relation are shown in Fig. 5 for different models. The stress increases linearly from the beginning to about 10%. Then the curves deviate from its initial linearity until to the critical strength at around 30%. Afterwards, the AlSi system shows a sustained decrease in strength. With the increasing the fraction of Si, the critical strength moved to the lower left, indicating the increasing of Si element slightly decreased strength and increased ductility of AlSi alloy.

Figure 6 shows the change in the number of different kinds of HA pairs under tension deformation of AlSi models. We pick the 5 most abundant HA pairs (The 1551, 1541, 1431, 1441 and 1661 pairs) and add the remaining HA pairs together (the other pairs) as shown in Fig. 6(a)–(e). It is clear that the fraction of 1551, 1541, 1441 and 1661 pairs decreased during the tensile process, indicating almost all kinds of the amorphous structure destroyed. Meanwhile the number of the other pairs shows large increasing, indicating that these amorphous structures transform into tiny and complex structures (There are more than 30 different types).
of these HA bond pairs, and all of them account for less than 2%.) during the tension deformation. It is worth noting that the 1431 pairs slightly increased in the strain region 0–15% while the 1551, 1541, 1441 and 1661 pairs decreased, it could be concluded that a small fraction of the other four pairs transform into the 1431 pairs. This means that the 1431 pair exhibits more stability than the other four pairs during deformation. Because the 1431 pairs would be related to the more defective amorphous structures than the other four pairs. The result can be observed in all of the AlSi alloy models. And the result is different from the previous studies,\textsuperscript{25–28} they found amorphous structure transform into crystalline structure in amorphous pure metal and alloy during deformation.

In our observation from the data in Fig. 6, the ratio of broken of 1551, 1541, 1441 and 1661 pairs are different during the tension process. According to the result of the above study, these HA pairs are the deformed icosahedra. Since the maximum stress peak can be observed at around 30%, the number of the deformed icosahedra which breaks in tension is counted during the strain from 0% to 30%. The number of the broken deformed icosahedra decreased by 50,582 in Fig. 6(a), 49,914 in Fig. 6(b), and 47,763 in Fig. 6(c) 46,384 in Fig. 6(d) and 46,333 in Fig. 6(e). The change of decreased number becomes flat. It could be concluding that the number of amorphous structure which damage occurs in AlSi system has influence on the mechanical properties of the system. Combination with Fig. 5, we also could be concluding that the number of amorphous structure damaged decrease resulting in reducing strength and increasing ductility during the tension deformation.

To further reveal local rearrangement in AlSi amorphous alloy, we probed the atomic deformation process by using the atomic local shear strain $\eta_i^{\text{Mises}}$.\textsuperscript{29} The local strains were calculated by the atomic-level strain tensors based on two configurations of the system for identifying local irreversible shear transformations in amorphous solids. The deformation snapshots for Al$_{90}$Si$_{10}$ are illustrated with Fig. 7 at different strain.

Figure 7(a) shows all of atoms with $\eta_i^{\text{Mises}}$ is zero when the deformation starts. Figure 7(a) also shows the reference configuration, according to the von Mises strain calculation method, the Fig. 7(b)–(f) are calculated by comparing the reference and different strain configuration. Figure 7(b) shows all of atoms with $\eta_i^{\text{Mises}}$ greater than 10% at the tension strain of 10%, at which the sample mainly deformed elastically, as shown in Fig. 5. According to the previous result, the number of amorphous structure continuous decreases during tension strain from 0% to 10%. The colored areas are the regions with large deformation. We could be concluded that the structures in these colored areas are the amorphous structures. And amorphous structures in these areas gathered form the STZs. That is, the deformation region tends to occur in the amorphous region. Figure 7(c) shows all of atoms with state of atoms $\eta_i^{\text{Mises}}$ greater than 10% at the tension strain of 20%. The conclusion drawn in Fig. 7(c) is similar to that in Fig. 7(b). The deformation region occurs in amorphous structures during the elastic deformation and in the early stage of plastic deformation. Comparing the distribution of STZs in Fig. 7(b) and Fig. 7(c), these STZs show a certain complementarity. The result may be come from the amorphous in the STZs which broken and transformed into the tiny structure, these tiny structures reconstructed and formed new amorphous in the nearby regions.

Figure 7(d) shows strain on 30% which the sample deformed in plastic and near critical stress as shown in Fig. 5. There are fewer atoms in the STZ comparing the Fig. 7(b) and (c). This means that the number of easily deformable amorphous structures is becoming less and less. As the amorphous structure decrease, the number and size of STZs decrease too. Figure 7(e) shows the shear strain of atoms at the tension strain of 40% which is the final stage of
plastic deformation. There are the smallest numbers of atoms in STZ. Compared with Fig. 7(b), (c) and (d), the amorphous structures involved in deformation is least which means most atoms have formed structures that are quite resistant to deformation. That is, the STZ is almost no longer formed in AlSi system, finally the fracture occurs between these resistant structures as shown in Fig. 7(f). Similar conclusions can be drawn in other samples. It should be pointed out that the fracture regions are different from these samples, because the distribution of amorphous structures of the initial configuration largely determines the location of the fracture area. In addition, the influence of Si is not very obvious.

4. Conclusion

We compared the internal structures of Al$_{100}$-xSix alloys and the tension deformation of these structures. By using HA, Voronoi tessellation method and $\eta$Mises computational method, we obtain a detailed insight into the local arrangement in the Al$_{100}$-xSix system during the tension deformation, and transform relation between these internal structures. In detail we find the following results.

1. AISi amorphous samples of different component ratio were prepared by using MD simulations. We obtained the AlSi amorphous system mainly consisting of deformed icosahedra, and Si element enhances glass-forming ability because Si doping prevents crystallization of the AlSi system during quenching process.

2. The stress and strain relation showed that the increasing of Si element leads to slightly decrease of strength and increase of ductility of AlSi alloy. The amorphous structures transform into other tiny and complex structures during the tension deformation.

3. The simulation showed that the deformation region tends to occur in the amorphous region in the elastic and plastic deformation stages. The distribution of amorphous structures shows a certain complementarity and these amorphous structures gathered form the STZs during the tension deformation. As the amorphous structure continues to decrease, eventually the fracture occurs.

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