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Different Characteristics of Unstable Atoms in Monatomic Amorphous Ni and Al: Local Lattice Instability Analysis

***Masaomi Nishimura[1], Kisaragi Yashiro[2] and Yoshihiro Tomita[2]**

[1] Student of Graduate School of Science and Technology, Kobe University
Rokkodai 1-1, Nada, Kobe, 657-8501, JAPAN
nishimura@solid.mech.kobe-u.ac.jp

[2] Graduate School of Engineering, Kobe University
Rokkodai 1-1, Nada, Kobe, 657-8501, JAPAN
yashiro@mech.kobe-u.ac.jp
tomita@mech.kobe-u.ac.jp

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ABSTRACT

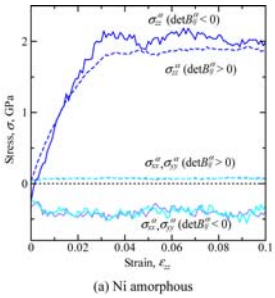
Short range orders (SROs) such as icosahedral clusters play important roles in the formability and deformability of amorphous metals. We are thus trying to reveal their role and deformation mechanism based on the "local lattice instability analysis[1-3]". That is, we discuss about the curvature of local energy surfaces, by the positiveness of atomic elastic stiffness coefficients, $B_{ij}{}^{\alpha}$. In the present study, the different characteristics of unstable atoms in monatomic amorphous metals of Ni and Al are discussed.

Both amorphous metals is made by usual melt-quench simulation, and then subjected to tension by means of molecular dynamics simulations. Figure 1 illustrates the changes in the average of atomic stresses, $\sigma_{ij}{}^{\alpha}$, acting on the unstable ($\det B_{ij}{}^{\alpha} < 0$) atoms and that on the stable ones ($\det B_{ij}{}^{\alpha} > 0$) under tension. Here, the system stress is controlled to zero at the initial equilibrium, $\varepsilon_{zz} = 0$, so that the average of $\sigma_{ij}{}^{\alpha}$ becomes zero if we do not distinguish the stable and unstable atoms. At the strain of $\varepsilon_{zz} = 0$, the average stress on unstable atoms is larger than that on stable ones, negative (compression) in Ni while positive (tension) in Al. In both cases, we can deduce that the local structure around unstable atoms largely deform than that around stable ones. As we have previously reported, this initial stress of unstable atoms in Ni amorphous works as "deformation buffer" against elongation; the stress of unstable atoms catches up with that on stable ones in the loading direction, and this point corresponds to the onset of blunting in the stress-strain curve[3]. On the other hand, the stress increase in Al is far smaller than that in Ni. The unstable atoms always show higher stress than stable ones in the loading direction, and they never cross each other.

Figure 2 shows pair distribution functions separately evaluated for stable and unstable atoms at the initial equilibrium. The end of abscissa is the cut-off distance, 0.479 nm for Ni and 0.556 nm for Al. The most remarkable difference between Ni and Al can be found in the position and magnitude of the first peak. In the Ni's case, the magnitude, or the probability of finding neighbor atoms, is almost same for stable and unstable atoms while the distance becomes slightly shorter for the unstable atoms. On the other hand,

the Al amorphous has almost same distance for the nearest neighbor atoms from both center of stable and unstable ones, while the probability decreases for the unstable atom center; that is, the unstable atoms find less atoms at the nearest neighbor distance than the stable ones.

In order to divide the atomic stress into the contribution from the nearest neighbor atoms and the outer surroundings, we have performed Voronoi polyhedra analysis and separated the atomic stress. Table 1 shows the stress contributions for stable and unstable centers at the initial state. Whichever the atom is stable or not, all the atoms feel compression from the nearest atoms, and tension from the outer surroundings. The unstable atoms always show smaller magnitude than the stable ones in the absolute value; however, it is noteworthy that the difference in the contribution from the nearest neighbors is very subtle in the Ni amorphous. This could be attributed to the slight difference in the 1st peak of Fig.2 (a). On the other hand, Al amorphous shows much larger difference in the stress contribution from the nearest neighbors, since the unstable atoms find fewer neighbors as shown in Fig.2 (b). The difference between stable and unstable atoms is about 0.3GPa in the outer surroundings, and it is almost same for both Ni and Al. Thus we can conclude that the different characters of unstable atoms in Ni and Al would be dominated by the nearest neighbor atoms.



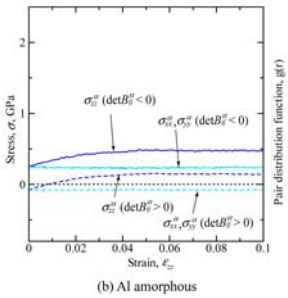
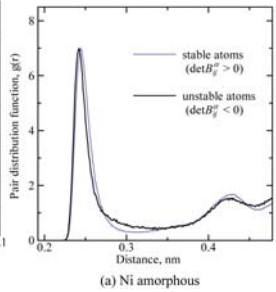


Fig.1 Change in normal stresses on stable and unstable atoms.



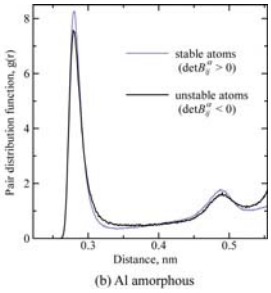


Fig.2 Pair distribution functions separately evaluated for stable and unstable atoms.

Table 1 Stresses contribution from the nearest neighbor and the outer surroundings.

	Ni amorphous		Al amorphous	
	$\det B_{ij}^{\alpha} > 0$	$\det B_{ij}^{\alpha} < 0$	$\det B_{ij}^{\alpha} > 0$	$\det B_{ij}^{\alpha} < 0$
Stress by nearest neighbor atoms	-12.039 GPa	-12.019 GPa	-9.663 GPa	-8.864 GPa
Stress by 2nd and further surrounding atoms	12.086 GPa	11.74 GPa	9.537 GPa	9.249 GPa

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