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Nucleation and growth of damage in polycrystalline aluminum under dynamic tensile loading

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Plate-impact experiments were conducted to study the features and mechanisms of void nucleation and growth in the polycrystalline of pure aluminum under dynamic loading. Soft-recovered samples have been analyzed by metallographic microscopy, electron back scattering diffraction (EBSD), and synchrotron radiation x-ray tomography technology. It was found that most of the void nucleation in grains neared the boundaries of "weak-orientation" grains and grew toward the grain boundaries with fractured small grains around the boundaries. This was mainly caused by the accumulation and interaction of slip systems in the "weak-orientation" grains. In addition, the micro voids were nearly octahedron because the octahedral slip systems were formed by 8 slip planes in the polycrystalline of pure aluminum. The EBSD results are consistent with the three-dimensional structure observed by synchrotron radiation x-ray. [http://dx.doi.org/10.1063/1.4914919]

I. INTRODUCTION

Spallation of ductile metals from high strain-rate loading is a complex physical and mechanical process. The shock wave from the loading induces the void nucleation, growth, and coalescence, which is closely related to the microstructure of the material. The microstructure such as the grain spatial orientation, size, and boundary misorientations can strongly affect spall strength and damage evolution.[1–6] The fracture process can be induced to polycrystalline metals from the loading by a gas gun. During this process, different grains have different levels of slip and ductile deformation because of different spatial orientation of the grain and tensile stress. For example, in FCC metals, every grain includes 4 (111) slip planes, and every plane includes 3 [110] packed directions, namely slip directions. Therefore, there are 12 equivalent slip systems. Under tensile loading, the 12 systems do not start to slip at the same time. The slipping start time is related to the direction of tensile loading. Therefore, in a certain loading direction, the grains with a different orientation have a different slipping mode and deformation degree. The grain that is easy to deform is called a "weak orientation" grain. Otherwise, it is called a "hard orientation" grain. The "weak orientation" grain deforms quickly and significantly, which can affect the deformation of other grains and cause strain concentration. Y. Z. Guo et al.[4] investigated the tensile deformation behavior of a copper bicrystal with a perpendicular grain boundary and found that the strain level at the grain boundary was lower than that within the grain, and the concentration of both ductile deformation and strain tended to occur in the grains with "weak orientation." They stated that the large-angle grain boundary in the material affected the uniformity of deformation, which can induce a "double-necking" phenomenon.

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X. Chen et al.[5] studied the spall behavior of pure aluminum with a different microstructure and found that the spall strength of [100] single-crystal Al is higher than that of [111] single-crystal Al, and the orientation of grains strongly affect the mechanical response. Ziegler et al.[6] studied the effects of grain boundary on tantalum bicrystals and found that the grain boundary limited the localization of deformation. W. M. Roger et al.[7] quantitatively studied the effect of microstructure characteristics on the spall behavior of copper and stated that the spall strength of the single-crystal was higher than that of polycrystalline, and the resistance to damage of polycrystalline with tiny grains was lower than that of polycrystalline with coarse grains. P. Peralta et al.[8] analyzed the initial dynamic damage of polycrystalline copper and found that the transcrystalline fracture tended to appear in the thin copper sheet with an average grain size of 320 μm. They also found that the voids occurred near the grain boundary, not on the boundary, and the intergranular fracture was always observed in the material with the smaller grain size. These studies have shown that the grain boundary is not the weakest microstructure in materials, while the grain boundary modifies the uniformity of plastic deformation and induces the localization of strain in the grain with special orientation, which can reduce the strength of the materials. Although there were studies on the microstructure effects on polycrystalline damage, there were not any studies on the accurate description about the nucleation of the initial damage, or on the spatial structure of dynamic damage. A lot of studies focused on the simulation of dynamic molecular damage. Experiments are needed to evaluate and verify the simulation and to better understand the dynamic evolution of damage.

This paper reports experiments on the initial spall of polycrystalline aluminum to better understand the nucleation and growth mechanism. The relationship of grain orientation and the degree of damage, as well as the feature of slips and the shape of initial microvoids in grains, were observed using EBSD. The observations from EBSD were verified by synchrotron radiation x-ray.

II. EXPERIMENTS METHOD

A group of plate-impact experiments were performed using a light gas gun for ultrapure polycrystalline samples (99.999% pure) with different impact velocities. The detailed parameters of samples and the experimental process can be found in Ref. 9. To understand the effect of microstructure of materials on the damage evolution and the mechanism of damage nucleation and growth, one sample was characterized by metallographic microscopy, EBSD, and synchrotron radiation x-ray. The sample and flyer was 6 mm and 3 mm thick, respectively, and the impact velocity of the flyer was 201 m/s. The sample was at the stage of incipient spallation which was visually observed on the free surface of the sample.[9] The recovered sample was cut symmetrically. The cross-section was polished using SiC papers with the particle sizes from big to small until the cross-section had few scratches. Then the sample was polished again using a diamond polishing spray on an automatic polishing machine until the surface looked like a mirror. Part of the sample with prepared cross-section was etched using the hydrofluoric acid with 10% concentration until grain boundaries were clear. The prepared sample was observed by metallurgical microscope to obtain the figure of cross-section (Figure 1). Another part of the sample with a prepared cross-section was handled using electropolishing with a solution of alcohol and perchloric acid (5 : 1 proportion) and cooled with LN_2. Then the prepared sample was observed by scanning electron microscopy with EBSD to obtain the EBSD figure of the cross-section (Figure 2).

III. ANALYSIS AND DISCUSSION

In Fig. 1, the vast large of voids nucleated and grew on the grain boundary. In fact, due to the limit of resolution of the optical microscope, mostly voids look like on the grain boundary. But the result of EBSD in Fig. 2 shows that a lot of voids are not just on the grain boundary and they always tend to locate at a grain with some orientation or three-grain intersections. Furthermore, some initial plastic deformation can be found near many grain boundaries, this also shows the void did not nucleate on the grain boundary. Previous studies stated that voids or cracks in the materials were easy to appear on grain boundaries and expand along them, and the grain boundaries were relatively

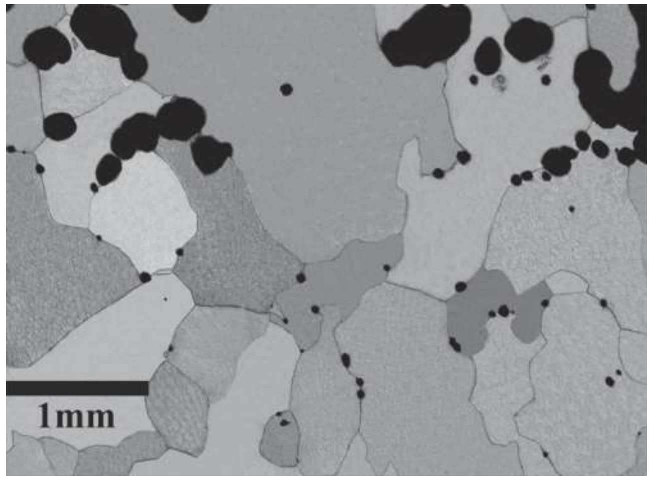

FIG. 1. Metallographic figure of the crosssection of part sample. It seems that the vast large of voids nucleated and grew on the grain boundary.

weak microstructures in the materials.[10–12] However, in this experiment, voids tend to appear in the grains with some special orientation or at the intersection of three grains, but we still need to do a lot of research for understanding voids is more likely to appear in what kind of grains, which will be continued in our following work. Robert E. Rudd et al.[13] obtained similar results using a simulation method and concluded that voids are easy to nucleate at the intersections of three grains, which is the weak location, and on some areas near the grain boundary with special misorientations. Based on the analysis of EBSD characteristic, L. Wayne et al.[14] provided the range of grain boundary misorientations where damage is easier to occur in polycrystalline copper. Because both of polycrystalline copper and aluminum are typical FCC ductile metals, Wayne's work can provide some important knowledge and guidance for our study on the nucleation of voids in ultrapure aluminum. These results are similar to that produced by experiments of damage nucleation in ultrapure aluminum. The area of the sample by EBSD shows clearly that voids occurred in the grains with special orientations (Orientation is listed in Table I)(see Fig. 2(a)), and there were a lot of broken crystals around the voids. For example, voids occurred on the intersection of grains 1, 2, and 7,

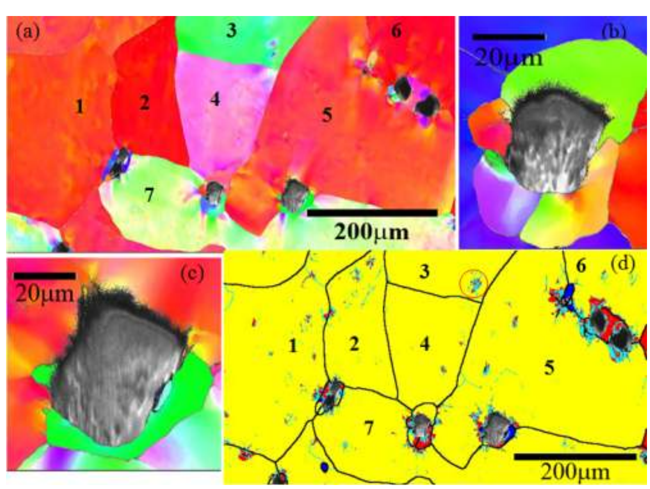

FIG. 2. EBSD figures of the cross-section of part sample (a) Distribution feature of grains with different orientation, grain boundaries and voids. (b) The void near the grain boundary among grain 4 and 7. (c) The void near the grain boundary between grain 5 and 7. (d) The distribution of grain boundaries and deformation. The deformation in the red "solid" circle was an early sign of void nucleation, which is about 10 microns.

TABLE I. Orientation of every grain.

Grain's number	1	2	3	4	5	6	7
Orientation	[001]	[136]	[104]	[456]	[106]	[016]	[346]

TABLE II. Misorientation angle of every grain boundary.

Grain boundary's number	Grains' number on both sizes of the grain boundary	Misorientation angle
1	1 and 2	21.50°
2	2 and 3	36.66°
3	2 and 4	46.05°
4	3 and 4	59.78°
5	3 and 5	19.35°
6	4 and 5	40.02°
7	1 and 7	40.47°
8	2 and 7	28.55°
9	4 and 7	45.39°
10	5 and 6	24.02°
11	5 and 7	40.95°

and the intersection of grains 4, 5, and 7, because these areas had relatively weak microstructures. However, in the area near grain boundaries between grains 5 and 7, a void was more inclined to nucleate in grain 5 (orientation is [106]), and the void would grow toward the grain 5 boundary. In the area near the boundary of grains 5 and 6, a void was more likely to nucleate in grain 6, and then would grow toward the grain boundary. Around these voids, there were a lot of broken small grains. With an increasing number of grains, some of them were squeezed into other grains. In addition, all voids in Fig. 2 were not round or oval, but similar to the diamond shape, as shown in Fig. 2(c). Figure 2(d) clearly shows the distribution of grain boundaries and voids. There were a lot of grain boundaries with very small curvatures around the void. The angles of these boundaries were within 2°, and the boundaries were small-angle grain boundaries, while in the original sample, the grain boundaries were big-angle grain boundaries (Misorientation is 45.39°and 40.95°, see Table II). Therefore, these grain boundaries should be newly formed by the broken matrixes around the voids. The plastic deformation near the grain boundary between grains 3 and 5 was an early sign of void nucleation, which was 10 microns(see the region in the solid circle). Y. Z. Guo et al.[4] observed similar results, i.e., a "double-necking" phenomenon in the bycrystal copper with a grain boundary perpendicular to the tensile direction, which also showed that plastic deformation occurred in the area near grain boundaries.

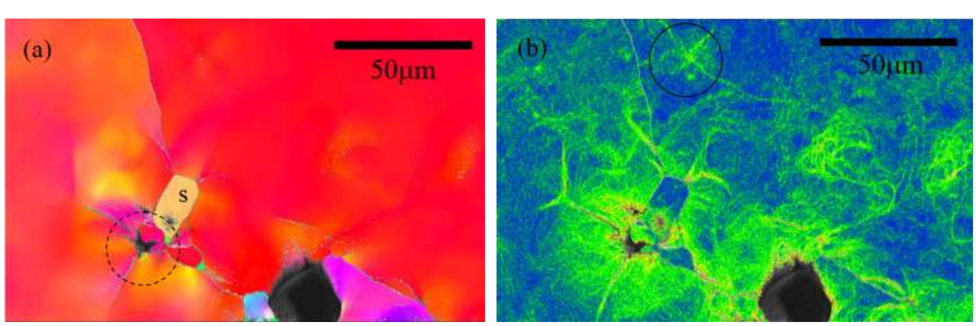

FIG. 3. The void and plastic deformation between grain 5 and 6 in Fig. 2. (a) Features of grains and voids. The grain with label "s" is an initial small grain in the ultrapure aluminum. There is a lot of serious damage around it. (b) Plastic deformation and slips.

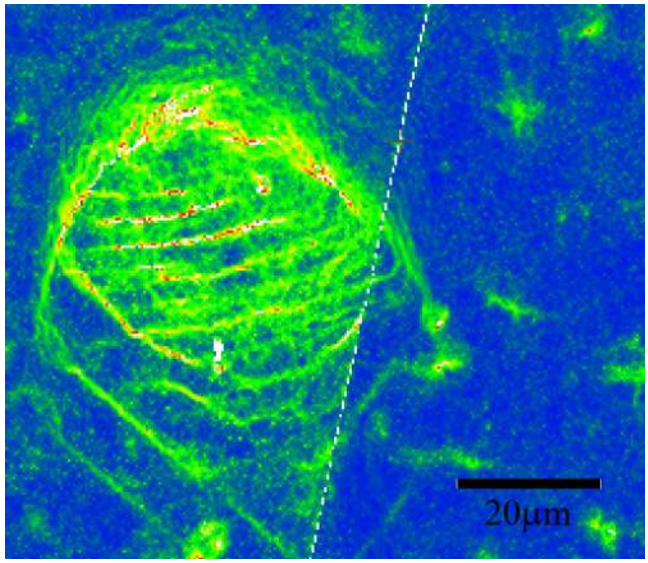

FIG. 4. Accumulated slips and the state of original damage near the grain boundary. The "dotted" line is a magnified grain boundary.

Figures 3(a) and 3(b) show the area between grains 5 and 6 in Fig. 2. There was a very small grain in Fig. 3(a) (see the grain with label "s"), which was not formed after shocking because its orientation was different from that of other grains around it, as shown from the plastic deformation characteristics in Fig. 3(b). After shocking, the grain boundary of the broken grains was small-angle, while the boundary around the grain was large-angle (>10°). There was a lot of microvoid nucleation near the small grain boundaries in grain 5 (in the dotted circle on Fig. 3(a)). Multiple slip lines from different directions appeared around the biggest void, and some of them would form sub-boundaries eventually. If the void continues to grow and connect with the adjacent ones, then the matrix around the grain 5 boundary will be divided into multiple broken grains. The plastic deformation in Fig. 3(b) clearly shows strain concentration in other locations near the grain 5 boundary (e.g., in the solid circle). With the crossing of multiple slips from different directions, the plastic concentration became violent, which caused the strain concentration, and the void nucleation was formed eventually.

Fig. 4 shows the initial nucleation state of a void, and a lot of slip lines gathered around the void. A large number of dislocations can be generated in materials under a compression wave, which migrate under the tensile stress generated by the intersection of a release wave, and the migration always begins to spread outward from the interior of a grain until it is blocked by the grain boundary. In this experiment, more than 90% of grain boundaries were large-angle, which had complicated structures and were made of interconnecting areas with a size of a few nanometers between disordered and ordered atoms areas. The large-angle boundaries can prevent the slip motion from spreading to adjacent grains. Therefore, multiple slips from different directions accumulated in the area near the grain boundaries because the wave migration was terminated by the grain boundaries. Because these slips overlapped each other, strain concentration occurred, which can form larger plastic deformation and voids nucleate. Under a higher tensile stress, with the accumulation of the dislocations around a grain boundary, slips can also cross the grain boundary and reach the adjacent grains, resulting in deformation of the grain boundary. Pure aluminum is one of face-centered cubic (FCC) metals. There are 4 {111} slip planes with different orientations in every grain. Every plane has 3 <110> packed directions, namely slip directions. Therefore, there are 12 equivalent sliding systems in each grain (Fig. 5). However, under a tensile stress, not all of the slip systems slip at the same time because they have different orientations. Part of the 12 slip systems have angles from the tensile stress direction close to 45°, which are called "soft-orientation" slip systems, while others are called "hard-orientation" slip systems. The "soft-orientation" slip systems are easy to slip under a small stress, while the "hard-orientation" slip systems need a large stress to slip. 4 {111} planes

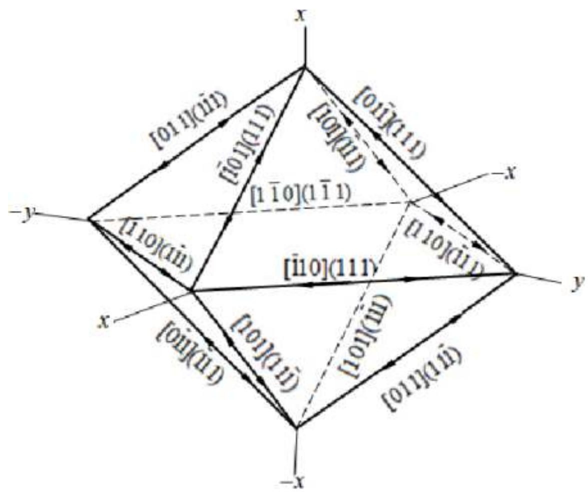

FIG. 5. Octahedron formed by 8 starting slips with different orientations at the same time.

form an octahedron. When the tensile axis is in a [001] direction, the angle between the normal of any of the {111} slip planes and the tensile direction is 54.7° for all planes, and the angle between the slip direction ($[\bar{1}01]$, [101], [011] or $[0\bar{1}1]$) and tensile direction is 45°. Two <110> directions on the bottom of the octahedron are perpendicular to the tensile direction Therefore, 8 slip systems with same orientation in the octahedron start slipping simultaneously when the tension threshold causing slip is met. Slip systems in different octahedrons intersect when they slip, and multiple broken grains are produced. In Fig. 4, the orientations of these two grains were [166] and [012], respectively, which had angles with some of their slip systems. The "dotted" line in Fig. 4 is a magnified grain boundary. On the two-dimensional plane, slips come from 4 slip directions in "soft-orientation" grains can be seen (the green parallel in lines on Fig. 4). The 4 groups of slipping caused the area near the grain boundary to quasi-diamond-shape plastic deformation. When the tensile stress is large enough, the diamond area is cut into numerous small grains. Then, microvoids appear because of the decreasing of the material strength, which is the original state of void nucleation.

Therefore, the shape of the void is close to a diamond, as shown in Fig. 2. This phenomenon was also found in the three-dimensional characteristics. Fig. 6 shows the spatial shape and distribution of voids in the shocked ultrapure aluminum obtained by the 3D tomography of synchrotron radiation X-ray. The detailed process about the 3D tomography experiments and the reconstruction of 3D

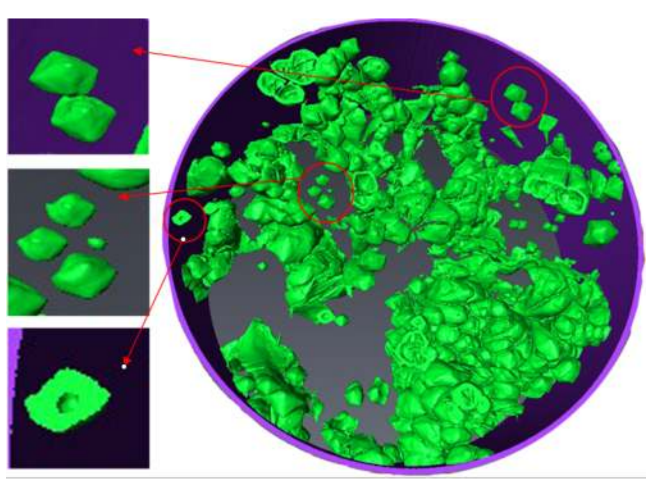

FIG. 6. 3D feature of voids was obtained by synchrotron radiation X-ray. There are a lot of octahedrons in this field.

images can be found in Ref. 15. In Fig. 6, the voids during the independent growth stage were octahedrons (see the areas in dotted circle), and their cross sections were diamond-shaped, which was consistent with the void shape observed by two-dimensional EBSD. But, the void shapes could be very complicated due to randomly disoriented grains in materials. For the octahedrons voids in this 3D characterization, they can be explained by the slip migration theory, but for the other shape, we still need other evidence to explain, especially, the voids at the intersection of three grains can not be explained by the slip migration theory.

IV. SUMMARY

In conclusion, the nucleation mechanism and features of the voids in an ultrapure aluminum polycrystalline after dynamic shock loading have been analyzed qualitatively. Combined with the characteristic methods of a metallographic microscope, EBSD, and synchrotron radiation X-ray, the formation and feature of damages in materials have been studied. The majority of the voids nucleated near the grain boundaries of "weak-orientation" grains and grew toward the grain boundaries. In the "weak-orientation" grains, all the slip systems started slipping almost simultaneously toward the grain boundaries and stopped slipping at the grain boundaries. The slip systems gathered near the boundaries and intersected with each other. This was the main reason why damage and broken grains were produced under dynamic loading. The voids at the initial stage were diamond shaped, observed by 2-D EBSD due to the motion of the octahedral slip systems in the ultrapure aluminum, which was confirmed by the observed 3-D void structure by 3D tomography of synchrotron radiation X-ray.

ACKNOWLEDGMENTS

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