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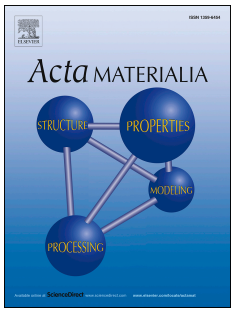

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Intragranular void formation in shock-spalled tantalum: Mechanisms and governing factors

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Abstract

Intragranular void formation in polycrystalline tantalum is investigated with plate impact experiments and molecular dynamics simulations, as regards its mechanisms and governing factors: grain boundary (GB) misorientation, grain orientation, grain size and shock pressure. Free-surface velocity history measurements are performed to obtain spall strength. Electron backscatter diffraction characterizations are used to obtain spatial distribution of voids, GB misorientation, and grain orientation associated with twins and intragranular voids. Intragranular voids are smaller in size but larger in number than intergranular voids, and nucleate in the GB vicinities. Smaller grains are favorable for the formation of intergranular and intragranular voids. At higher shock pressure, intragranular voids increase in fraction and tend to distribute at grain centers. Deformation twinning depends on grain orientation and prefers to form at high-angle GBs. However, intragranular voids have negligible dependence on grain orientation and favor medium-angle GBs, and the preference is enhanced slightly with increasing impact velocity and decreasing grain size. The simulations show GB-induced multiple-slip, slip-slip intersections and strain localizations act as the prerequisites to intragranular void formation.

Keywords: Polycrystalline tantalum, grain size, intragranular voids, void nucleation mechanism, grain boundary, slip-slip intersection.

1. Introduction

Understanding material behavior under elevated stresses and strain rates is essential to predicting and modeling damage initiation and evolution in engineering materials as well as terrestrial and extraterrestrial impact events [1–3]. Under impact loading, spall damage is the predominant mode of failure in metallic materials and is strongly influenced by microstructure [3–6]. For polycrystalline materials, grain boundaries (GBs) and triple junctions act as void nucleation sites (*intergranular voids*) and play a key role in damage process [2, 3, 7, 8]. The governing factors such as GB type [2, 3, 7, 9] and grain size [10–12] have been extensively investigated with experiments and molecular dynamics (MD) simulations [13–15]. Void nucleation within a grain interior (*intragranular voids*) is normally considered less likely or unlikely in polycrystalline materials, and this subject has been underexplored.

Intragranular damage (void nucleation and growth) as a dominant fracture mode was observed in polycrystalline tantalum, and the damage extent increases with increasing grain size [16]. However, the underlying mechanisms and governing factors are not fully understood for intragranular voids. Spall damage nucleation sites in polycrystalline tantalum were also examined under different shock loading conditions; damage can be induced at GBs after planer impact at low velocities [17], while voids tend to nucleate at twin-twin intersections and twin-GB intersections under sweeping detonation-wave loading [18]. Therefore, void formation in polycrystalline tantalum depends on loading and microstructure.

Intragranular damage is usually observed in monocrystals or bicrystals, and nucleates at highly deformed sites [19], dislocation cell boundaries [20] and twin GBs [21, 22] formed before spallation, due to the lack of GBs. Intragranular damage depends on shock-induced plasticity, which is in turn dependent on crystalline orientation and shock pressure, as shown for [100]/[110] bicrystal Cu [23]. In bicrystal Cu, dislocation cell size decreases with increasing shock pressure, and twinning occurs as the dominant substructure only in the [100] grain after shock loading at 10 GPa [23]. The [100] grain with finer dislocation cells is less resistant to damage than the [110], [111] grain with coarser dislocation cells in spalled bycrystal Cu [20]. Similarly, MD simulations of single crystal Ta [22] showed that twinning is dominant for the [100] and [110] orientations, and dislocation slip for the [111] orientation, and the spall

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