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# Effect of loading direction on grain boundary failure under shock loading

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**Abstract**

We investigate the effect of grain boundary inclination with respect to the loading direction on void nucleation at a boundary, using plate impact experiments on polycrystalline copper. Examination of damaged specimens reveals that boundaries perpendicular to the loading direction are an order of magnitude more susceptible to failure than those parallel to the loading direction. We investigate the mechanisms and reasons behind this experimental observation through molecular dynamics (MD) simulations, as a function of loading direction, in a copper bicrystal. Two extremes of loading directions are considered, either parallel or perpendicular to the grain boundary plane, spanning the range that grain boundaries within a polycrystalline sample will ordinarily experience under uniaxial strain conditions. Using MD simulations, we demonstrate that, during shock compression, the ability of a boundary to undergo plastic deformation is altered measurably by changing the loading direction with respect to the boundary plane. This change in the plastic response of the GB affects the development of stress concentrations believed to be responsible for void nucleation. MD simulations show that boundaries perpendicular to the loading direction do not undergo as much plastic deformation, by dislocation emission, as those parallel to the loading direction. The lack of plastic deformation at the GB, in the perpendicular loading case, can decrease the stress required for void nucleation. The MD results are consistent with experimental observations, and support the contention that plastic response of a grain boundary under shock compression can be a contributing, or even dominating, factor in determining the stress for void nucleation.


*Keywords:* Copper; Grain boundary structure; Dynamic phenomena; Molecular dynamics; Loading direction

## 1. Introduction

Under dynamic loading conditions, microstructural features such as grain boundaries, inclusions, vacancies and heterogeneities can affect the response of a material to varying degrees [1–7]. During dynamic loading, material failure, characterized by void nucleation, growth and coalescence, can lead to fracture and is frequently termed "spall" [2,8]. To accurately predict the spall strength of a ductile material, it is most important to understand the first of these processes, void nucleation.

To understand and predict void nucleation, it is essential to recognize the stresses required for void nucleation and how the stress concentrations within the microstructure develop to overcome this void nucleation stress. One of the most important factors in comprehending this process, is to understand the competition between processes that either dissipate or accumulate stress at various microstructural features. Dissipative processes delay, retard or prevent void nucleation, while cumulative processes promote

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or enhance the formation of voids. One such example of a dissipative process is plastic work, such as Shockley partial and perfect dislocation emission from grain boundaries, and a similar example of a cumulative process involves dislocation pile-ups at grain boundaries, which create high stress sites. The microstructure further complicates an in-depth understanding of these dissipative and cumulative events. It is well known that there are inherent stresses associated with various microstructural features [2]. However, the total stress at a given microstructural feature is a sum of this inherent stress and the external stress from mechanical loading. For specific loading conditions, if this total tensile stress is greater than the critical stress required for void nucleation, a material will nucleate a void at the specific microstructural feature. Nevertheless, the competition between the dissipative and cumulative processes in the local region of a microstructural feature determines whether or not this critical stress for void nucleation can be reached in a material.

In fact, it has been previously shown that a dissipative process like plastic deformation in ductile metals is closely coupled to void nucleation, imbuing this process with importance in the contexts of both deformation and material failure [9–11]. In addition to the microstructure, it is believed that the sense of dynamic loading with respect to the microstructural features can also be pivotal under the right conditions. For example, the inclination of grain boundaries with respect to the loading direction may play an important role in promoting or retarding plastic deformation and void nucleation. Consequently, in this work we focus on studying this orientation effect for void nucleation at grain boundaries.

The behavior of grain boundaries (GB) under dynamic mechanical loads is of particular interest as it has been observed that, especially in high-purity materials, grain boundaries are important void nucleation sites. The majority of the previous work has focused on studying the effect of grain boundary structure on void nucleation. Recent observations of spall failure in high-purity Cu metal demonstrate that not only do voids nucleate preferentially at grain boundaries [12], but certain boundaries are more susceptible than others to void nucleation [13]. These observations are also supported by the work of Wayne et al. [14] on dynamically loaded copper, where it is observed that grain boundaries with a certain range of misorientations are preferred locations for intergranular damage.

These observations regarding damage nucleation at high strain rates apply equally to damage at lower strain rates. Work by Mikhailovskij et al. [15], on body-centered cubic tungsten shows that, under uniaxial stress conditions, special boundaries such as $\Sigma1$, $\Sigma3$ and $\Sigma9$ require higher stresses for void nucleation in comparison with other types of coincident site lattice (CSL) and non-CSL boundaries. Experiments by Lim [16] on low-cycle fatigue of polycrystalline face-centered cubic (fcc) nickel samples show that low-order CSL boundaries such as $\Sigma3$ and $\Sigma5$ do not crack during the deformation process. Evrard et al. [17] and McMurtrey et al. [18] make similar observations through both experiment and simulation, showing that special boundaries are more resistant to void nucleation in pre-irradiated austentic stainless steels. These results collectively suggest that all grain boundaries are not equal in terms of their propensity for nucleating voids and that they can be an influential factor controlling material failure.

In previous MD simulation work, we have tried to understand and predict failure at grain boundaries by using average and local properties associated with specific GBs [19,20]. To help frame the relationship between plasticity and failure [19], we considered a standard model for the fracture toughness of a material [9,10],

$$\gamma_f = 2\gamma_s - \gamma_{gb} + \gamma_p \tag{1}$$

where $\gamma_f, \gamma_s, \gamma_{gb}$ and $\gamma_p$ are the fracture energy, surface energy, grain boundary energy and plastic work energy associated with intergranular fracture. In a brittle material, where $\gamma_p = 0$, the growth of a intergranular crack simply requires separating a GB ($\gamma_{gb}$) into two new surfaces ($2\gamma_s$). The fracture energy ($\gamma_f$) calculated for these materials is then used as an important input in the Griffith criterion to calculate the stress at which a material would rupture [9]. However, the plastic energy term, $\gamma_p$, can be dominant in ductile materials [12–14,19]. We [19] have examined the importance of $\gamma_s$ and $\gamma_{gb}$, and related average properties, such as excess volume, to predict the failure strength of a grain boundary in a ductile metal. Those results suggest that the plastic work term, $\gamma_p$, is a better determinant of the failure strength of an interface in ductile bicrystals [19].

The plastic work during the early stages of void nucleation generally increases resistance to void nucleation by dissipating the stress that might otherwise nucleate a void. The total applied stress needed to nucleate a void therefore increases to meet the combined requirements for plastic, dissipative work and void nucleation. However, it is important to note that plasticity as a dissipation mechanism is only true during the early stages of void nucleation. An increase in the ability of a material to plastically deform can lead to plastic instabilities or localization of plastic work during later times. This deformation process, at later times, can actually promote void growth, as shown in mesoscale models for crack growth developed by, amonst others, Gurson, Tvergaard and Hutchinson [21–25]. These mesoscale models treat both void nucleation and growth together, whereas in this paper we are focusing solely on void nucleation.

To fully understand and predict void nucleation at a grain boundary, both the grain boundary structure and the boundary inclination with respect to the loading direction need to be taken into account. The majority of experiments performed under low strain rate, uniaxial stress loading conditions have already shown that the inclination of a boundary with respect to the loading direction can significantly affect void nucleation [7,18,26]. It is widely accepted that, in these cases, boundaries perpendicular to the loading direction are more susceptible to void