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# Computational modeling and simulation of spall fracture in polycrystalline solids by an atomistic-based interfacial zone model

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## ARTICLE INFO

## ABSTRACT

The focus of this work is to investigate spall fracture in polycrystalline materials under high-speed impact loading by using an atomistic-based interfacial zone model. We illustrate that for polycrystalline materials, increases in the potential energy ratio between grain boundaries and grains could cause a fracture transition from intergranular to transgranular mode. We also found out that the spall strength increases when there is a fracture transition from intergranular to transgranular. In addition, analysis of grain size, crystal lattice orientation and impact speed reveals that the spall strength increases as grain size or impact speed increases.

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## 1. Introduction

Mechanical spall is a shock wave induced dynamic fracture process, such as armor penetration and blast loads. The macroscopic spall damage is strongly depending on the mesoscale structures of material based on some experimental results [1–3]. On the mesoscale level, most ceramics and metals are characterized by crystal grains and grain boundaries, heterogeneous impurities, and material defects and so on. Various experiments have been conducted to observe the shock wave propagation and material failure in various solids at micro-scale level or meso-scale level [4–8]. However, it is still difficult for the experimental methods to precisely record the dynamical process of spall inside solids because of the short time scales. Due to the limitations of experiments, some researchers attempted to develop numerical models and simulation tools to study the basic features of spall fracture. The spall simulation of copper by planar shock loading has been investigated by molecular dynamics simulations [9,10]. Besides, a coarse-grained molecular dynamics with a Lennard–Jones potential is employed to simulate spall phenomena of a flyer specimen system by Krivtsov and Mescheryakov [11]. Ren et al. [12] used the reproducing kernel particle method (RKPM) to capture some features of the spall fracture including the role of inelastic wave pulses. To study the dynamic thermo-mechanical response of a tungsten heavy alloy, Clayton [13] applied a cohesive finite element method developed by Camacho and Ortiz [14] to simulate dynamic spall process in tungsten heavy alloys. Qian and Li [15] simulated the spall fracture in polycrystalline solids by a multiscale cohesive zone method, which is developed by Zeng and Li [19].

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**Nomenclature**

| | |
|---|---|
| $\boldsymbol{B}$ | body force |
| $c$ | sound velocity in the material |
| $\mathbf{C}$ | right Cauchy–Green tensor ($\mathbf{F}^{\mathbf{T}} \cdot \mathbf{F}$) |
| $d(X_i, X)$ | Euclidean distance between $X_i$ and $X$ |
| $F_{s,j}$ | pushed-out contact force |
| $\mathbf{F}$ | deformation gradient |
| $M_{s,j}$ | mass of node $j$ on the slave surface |
| $n_b$ | total number of bonds in a unit cell |
| $n_{elem}$ | total number of elements |
| $\mathbf{P}$ | first Piola–Kirchhoff stress tensor |
| $\boldsymbol{r}_i$ | deformed atomic bond vector |
| $R_d$ | mesh ratio |
| $R_p$ | interfacial potential energy ratio between grain boundary and grain |
| $\boldsymbol{R}_i$ | undeformed atomic bond vector |
| $s_0^{\mp}$ | side length of the adjacent bulk elements |
| $S_{ext}$ | external surface of the solid body in the reference configuration |
| $S_{inter}$ | interfacial surface of the solid body in the reference configuration |
| $\mathbf{S}(\mathbf{C})$ | second Piola–Kirchhoff stress tensor |
| $\mathbf{T}^{inter}$ | interfacial surface traction vector |
| $\overline{\mathbf{T}}$ | external traction vector |
| $\mathbf{u}$ | displacement vector |
| $V_i$ | Voronoi region |
| $W_e(\mathbf{F}_e, \boldsymbol{R}_i)$ | potential energy density of an arbitrary unit cell inside the element |
| $X_i$ | coordinates of kernel points |
| $\alpha^b$ | lattice orientation in the grain boundary |
| $\alpha^g$ | lattice orientation in the grain |
| $\delta_{s,j}$ | penetration distance for node $j$ on the slave surface |
| $\epsilon$ | depth of the potential well |
| $\rho$ | material density |
| $\sigma$ | finite distance at which the inter-atom potential is zero |
| $\sigma_{sp}$ | spall strength |
| $\varphi(\boldsymbol{r}_i)$ | atomistic potential |
| $\Omega_0^b$ | unit cell volume |

*Sub and superscripts*

| | |
|---|---|
| *elem* | a given element |
| *g* | polycrystalline grain |
| *inter* | interfacial zone |
| *s* | slave surface |

Although extensive research has been carried out to investigate the mechanisms of spall fracture, there still exist many elusive issues that need to be explored for spall fracture in polycrystalline solids. In fact, micro-structural characteristics such as grain shape, spatial arrangement of grains and local crystallographic orientation have influenced the material response to some extent [16–18]. For instance, the severe mechanical anisotropy within materials may be caused by the grain rotations [16], and the onset of shear band location and width depend on the grain distribution and volume fraction [17,18]. To better understand the spall mechanisms in polycrystalline materials, we conduct an extensive analysis of spall strength when there is an intergranular to transgranular fracture transition by applying an atomistic-based interfacial zone model (AIZM). This model was developed by Zeng and Li [19,20] and it links the atomistic crystal structure with the mesoscale material properties of the interfacial zone, which provides an effective approach to describe material inhomogeneities such as grain boundaries, biomaterial interfaces [20], slip lines and inclusions. The contribution of current work focuses on the fundamental studies of spall fracture. In present work, the distributions of stress contour and shock wave propagation during high-speed impact process in polycrystalline materials are obtained to better illustrate the spall process and fracture mechanism. The relations of polycrystalline fracture mode transition with interfacial potential energy and microstructure configuration are discussed. It is shown that potential energy will affect the fracture morphology, causing the transition from intergranular to transgranular. Additionally, the fracture mode, grain size, lattice orientation and impact speed will affect the spall strength in polycrystalline materials.