Published in final edited form as:

Eng Fract Mech. 2015 July 1; 142: 50–63. doi:10.1016/j.engfracmech.2015.05.039.

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

Liqiang Lin and Xiaowei Zeng*

Department of Mechanical Engineering, University of Texas, San Antonio, TX 78249, USA

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.

Keywords

interface zone model; high-speed impact; spall fracture; polycrystalline solid; intergranular fracture; transgranular fracture; multiscale

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

*Corresponding author. Tel: +1 210 458 7698, xiaowei.zeng@utsa.edu (X. Zeng).

Publisher's Disclaimer: This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final citable form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

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 [17].

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.

2. Constitutive modeling of the atomistic-based interfacial zone model

2.1 Local Cauchy-Born rule continuum method

To calculate the potential energy for a crystalline solid, the Cauchy-Born rule is employed in the proposed atomistic-based interfacial zone model. The so-called Cauchy-Born can describe the material behavior from atomistic information and is widely used as a standard method in continuum mechanics [21, 22]. It refers to the following procedure: let $\mathbf{x}$ denote the spatial position of a material point $\mathbf{X}$ at the time t , thus the local continuum deformation

gradient is given by $\mathbf{F} = \frac{\partial \mathbf{x}}{\partial \mathbf{X}}$. Since in a given element $e (e = 1, \dots, n_{elem})$, the deformation gradient, $\mathbf{F}_e$, is a homogeneous tensor, the relative deformed bond vector $\mathbf{r}_i$ in a unit cell results from the corresponding related undeformed atomic bond vector $\mathbf{R}_i$ can be defined as:

$$\mathbf{r}_i = \mathbf{F}_e \mathbf{R}_i, \quad i=1, 2, \dots, n_b. \quad (1)$$

where n_b is the total number of bonds in a unit cell.

Consequently, the elastic energy density in any given element can be calculated by computing the potential energy density of an arbitrary unit cell inside the element:

$$W_e(\mathbf{F}_e, \mathbf{R}_i) = \frac{1}{2\Omega_0^b} \sum_{i=1}^{n_b} \phi(r_i) = \frac{1}{2\Omega_0^b} \sum_{i=1}^{n_b} \phi(\mathbf{F}_e \mathbf{R}_i), e = 1, 2, \dots, n_{elem} \quad (2)$$

Where Ω_0^b denotes the volume of the unit cell in the referential configuration and b indicates bulk element, $\phi(r_i)$ is the atomistic potential, $r_i, i = 1, 2, \dots, n_b$ is the current bond length in a unit cell.

Based on the Cauchy-Born rule, the constitutive relations for the bulk medium can be established. For instance, the second Piola-Kirchhoff stress can be expressed in the following form:

$$\mathbf{S}(\mathbf{C}) = \frac{1}{2\Omega_0^b} \sum_{i=1}^{n_b} \phi'(r_i) \frac{\partial r_i}{\partial \mathbf{C}} = \frac{1}{2\Omega_0^b} \sum_{i=1}^{n_b} \frac{\partial \phi(\mathbf{F}_e \mathbf{R}_i)}{\partial r_i} \frac{\mathbf{R}_i \otimes \mathbf{R}_i}{r_i} \quad (3)$$

where $\mathbf{C} = \mathbf{F}^T \cdot \mathbf{F}$ is the right Cauchy-Green tensor.

2.2 Effective deformation gradient in the interfacial zone

Since we consider the interfacial zone as an actual physical zone, the Cauchy-Born rule can be applied in the interfacial zone area. Additionally, the thickness R of interfacial zone is chosen as $10^{-3}|s_0^\mp| \leq R \leq 10^{-1}|s_0^\mp|$, and $s_0^\mp$ are the length of the sides of the adjacent bulk elements. The lower limit aspect ratio is a restriction limit beyond which numerical ill-conditioning may happen in computations. The upper limit aspect ratio may limit how much refinement we can do as the mesh size approaches to atomistic scale, because R has to be greater than 4-5 lattice spacings in order to apply the Cauchy-Born rule to the effective displacement field in the cohesive zone. Based on Cauchy-Born rule, the relative deformed lattice bond vector in each interfacial zone can be calculated as follows:

$$\mathbf{r}_i^{inter} = \mathbf{F}_e^{inter} \mathbf{R}_i, \quad i = 1, 2, \dots, n_{inter}. \quad (4)$$

If we consider the interfacial zone as one quadrilateral element sandwiched by two triangle bulk elements(see Fig. 1), the interfacial zone deformation gradient, $\mathbf{F}_e^{inter}$, can be expressed by the four finite element nodal displacement[19, 20]:

$$\begin{bmatrix} F_{11}^{inter} \\ F_{12}^{inter} \\ F_{21}^{inter} \\ F_{22}^{inter} \end{bmatrix} = \frac{1}{ad - cd} \begin{bmatrix} d & 0 & -b & 0 \\ -c & 0 & a & 0 \\ 0 & d & 0 & -b \\ 0 & -c & 0 & a \end{bmatrix} \begin{bmatrix} x_{l+1}^+ - x_l^- \\ y_{l+1}^+ - y_l^- \\ x_l^+ - x_{l+1}^- \\ y_l^+ - y_{l+1}^- \end{bmatrix} \quad (5)$$

where $a = X_{l+1}^+ - X_l^-$, $b = Y_{l+1}^+ - Y_l^-$, $c = X_l^+ - X_{l+1}^-$, $d = Y_l^+ - Y_{l+1}^-$.

Subsequently, the averaged first Piola-Kirchhoff stress tensor in each interfacial zone can be written as:

$$\mathbf{P}_{inter} = \frac{1}{2\Omega_0^b} \sum_{i=1}^{n_b} \frac{\partial \phi_{inter}}{\partial r_i} \frac{\mathbf{r}_i \otimes \mathbf{R}_i}{r_i} \quad (6)$$

Once we obtain the stress inside the interfacial zone, the interfacial cohesive tractions along the boundaries of adjacent bulk elements can be readily written as:

$$\mathbf{T}^{inter} = \mathbf{P}_{inter} \cdot \mathbf{N} \quad (7)$$

where $\mathbf{N}$ is the out normal of adjacent bulk FE elements.

In this model, the interfacial zone is assumed a relatively “soft” zone and the intermolecular interaction inside the interfacial zone is a type of the Van der Waals interaction between non-covalent bonds or quasi-covalent bonds. When the atomistic potential for a given bulk medium is available, the interfacial zone potential can be calculated by integrating the bulk potential over the bulk medium half space. For example, if the potential in the bulk element is considered as Lennard-Jones potential:

$$\phi_{bulk} = 4\epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right] \quad (8)$$

the coarse graining interfacial potential can be obtained by analytical integration[23]:

$$\phi_{inter}(r) = \int_{\text{half space}} \beta \phi_{bulk}(r - r') dV' = \pi \beta \epsilon r_0^3 \left[\frac{1}{45} \left(\frac{r_0}{r} \right)^9 - \frac{1}{3} \left(\frac{r_0}{r} \right)^3 \right] \quad (9)$$

where ϵ is the depth of the potential well; σ is the finite distance at which the inter-atom potential is zero; $r_0 = 2^{1/6}\sigma$ is the equilibrium bond distance in the bulk material; β is the atomic density in the solid. In the interfacial zone, the crystal lattice structure is modeled as hexagonal structure and the arrangement of atoms is regular in the undeformed state, but its lattice constants and atomistic potential are different from those of the bulk medium.

2.3 Finite element implementation

A displacement-based finite element formulation is developed from the weak form of virtual work. The Lagrangian finite deformation formulation is used to account for finite strain. If $\mathbf{x}$ denotes the current spatial position of a material point $\mathbf{X}$ at the time t , the displacement vector are defined as $\mathbf{u} = \mathbf{x} - \mathbf{X}$. During the deformation process, a Galerkin weak formulation including a contribution from the interfacial surfaces may be expressed as following[24]:

$$\int_{\Omega} \mathbf{P} : \delta \mathbf{F} d\Omega + \int_{\Omega} \mathbf{B} \delta \mathbf{u} d\Omega + \int_{\Omega} \rho \frac{\partial^2 \mathbf{u}}{\partial t^2} \cdot \delta \mathbf{u} d\Omega = \int_{S_{inter}} \mathbf{T}^{inter} \cdot \delta \mathbf{u} dS + \int_{S_{ext}} \bar{\mathbf{T}} \cdot \delta \mathbf{u} dS \quad (10)$$

where Ω , S_{inter} , S_{ext} are the volume, interfacial surface and external surface of solid body in the reference configuration, respectively. $\mathbf{B}$ is the body force; ρ is the material density in the

reference configuration; $\mathbf{T}^{inter}$ is the interfacial surface traction vector and $\bar{\mathbf{T}}$ is the external traction vector.

In addition, the explicit time integration scheme is based on the Newmark β -method with $\beta = 0$ and $\gamma = 0.5$ to obtain the nodal velocities and the nodal displacements[25].

3. Polycrystalline microstructure modeling

To generate different randomly shaped grain structures in polycrystalline materials and to study the effect of polycrystalline grain morphology, Voronoi tessellation has been widely used[26-29]. Before the appearance of Voronoi tessellation method, the simplified grain shapes, such as hexagons for 2D case[30], or truncated octahedrons for 3D case[31, 32], were utilized to deal with polycrystalline microstructure. However, these regular structures cannot precisely predict local stress-strain fields inside the grains[33, 34]. Thus, Voronoi tessellation method has been emerging as a powerful tool to construct arbitrary polycrystalline microstructure. Initially, the Voronoi domain is considered as partitioning of a plane with a set of n random distinct points, or nuclei[35, 36]. For a 2D case, the Voronoi region of every nucleus is defined as:

$$V_i = V(X_i) = \{X : d(X_i, X) < d(X_j, X)\} \quad \text{for } i \neq j \quad (11)$$

where X_i represent the coordinates of kernel points i , $d(X_i, X)$ denotes the Euclidean distance between X_i and X , X belongs to Voronoi region V_i and is closer to nucleus i than other nuclei, as shown in Fig. 2. In addition, the slope of the line perpendicular to each closest point connection line, e.g. line $i-j$ as shown in Fig. 2, defines the polygonal boundary segment $\overline{ab}$.

The impact test samples are generated by centroidal Voronoi tessellation as shown in Fig. 3(a). Each Voronoi cell represents an individual grain cell and all edges of grain cells are considered as grain boundaries. It can be seen from Fig. 3(b) that triangular finite element is used to mesh all grain cells after the generation of grain cells. All interfaces among bulk elements are governed by the interfacial zone model.

4. Numerical simulations

4.1. Problem analyzed

Numerical simulations have been carried out for simulation of high speed impact induced spall fractures. For spall fracture, it is a very difficult problem that has been elusive to many existing numerical methods[37]. The exact problem statement is described in Fig. 4, in which the projectile is a rigid block with an impact velocity v_0 and the target is a plate with dimension ($L_x \times L_y = 0.4mm \times 0.2mm$) under free boundary condition.

To characterize the varying grain morphology, each grain can be assigned an individual set of material properties such as lattice orientation α (α^g is grain orientation angle and α^b is grain boundary orientation), see Fig. 5. For simplicity, the lattice structure is chosen as the hexagonal lattice in the simulations as shown in Fig. 5, and we use the Lennard-Jones potential for the hexagonal crystal structure.

To prevent penetration during the impact process, the so-called impenetrability condition is enforced during the computation, which means the contact forces are required to push out the penetrated nodes. The pushed-out contact force required to prevent penetration are given as following[14, 38]:

$$F_{s,j} = \frac{2M_{s,j}\delta_{s,j}}{\Delta t^2} \quad (12)$$

where $M_{s,j}$ is the mass of node j on the slave surface, $\delta_{s,j}$ is the penetration distances for all nodes j on the slave surface. Here, the surface on target plate is assumed as slave surface and the surface on rigid block is treated as master surface in the contact pairs.

4.2. Fracture growth in polycrystalline material

In this study, there are 128 grain cells in the target plate and the average grain size is around 25 μm [39-42]. Meanwhile, each grain is assigned a random lattice orientation α^g and the

lattice orientation in the grain boundary is set as $\alpha^b = \frac{1}{2}(\alpha_A^g + \alpha_B^g)$. The impact velocity is set as 100m/s and the time step is chosen as $\Delta t = 0.1 \times 10^{-10}\text{s}$ in time integration. For this case, the potential energy of the interfacial zone in grain boundaries is smaller than that in the grains, i.e. $\epsilon_{inter}^g = 3\epsilon_{inter}^b$, which means the grain boundaries is weaker than the grains [43].

When the rigid flyer impacts the target, a pulse of compression stress wave is generated at the contact surface. The simulation results are shown in Fig. 6 and the propagation and reflection of the stress wave from the top edge to the bottom free edge has been observed. The phenomenon of spall process under high-speed impact has been captured, as shown in Fig. 6.

The dynamic history of particles inside a material at micro-scale level cannot be recorded by the current experimental approach [4]. Thus, the free surface velocity history at the opposite side of contact surface is widely utilized to observe the spall behavior as an approach for indirect measurement. Within the acoustic approximation, the spall strength is defined as[44, 45]:

$$\sigma_{sp} = \frac{1}{2}\rho c V_{sp} \quad (13)$$

where ρ is the material density, c is the sound velocity in the material and $V_{sp} = V_o - V_m$. A compressive disturbance called a “spall signal” appears on the free surface velocity history as the tensile stress relaxes[4, 12]. It can be seen that the free surface velocity illustrates as dynamic behavior as shown in Fig. 7(a). Meanwhile, the reflected force on free bottom surface also appears as an oscillating force. With the spall crack initiation, the sign of reflected force changes from compression to tension as shown in Fig. 7(b). When $t > 0.3\mu\text{s}$, the amplitude of free surface velocity and reflected force decrease significantly, which implies the layer of bottom surface is completely separated from the target plane as shown in Fig. 6(e) and Fig. 6(f), then the velocity verge to approximately a constant value and the reflected force decrease to zero as shown in Fig. 7(a) and Fig. 7(b).

4.3. Mesh convergence test

Generally speaking, the results of the interfacial zone method will be sensitive to its element size. To test mesh size dependence of interfacial zone model, the exact same condition was applied to the problem as in previous section with different mesh sizes. For comparison purpose, we defined the mesh ratio R_d in grain cell as:

$$R_d = \frac{\text{Average element size}}{\text{Average grain size}}$$

Three cases with different mesh ratio $R_d = 0.5, 0.33$ and 0.25 are employed, as shown in Fig. 8. From the study, we found out that the spallation is along the same path although the mesh size varies as shown in Fig. 9. That is, the current mesh can accurately capture the spall crack path.

On the other hand, the reflected forces r_b^i and velocities v_b^i on the free bottom surface are calculated in each case for further comparison. As shown in Fig. 10, the reflected force and free surface velocity become closer as mesh size decreases. The errors of free surface velocity and reflected force in different cases are defined as:

$$\begin{aligned} Err_v &= \int_0^t |v_b^i - v_b^{i-1}| dt, \quad i = 2, 3, 4 \dots \\ Err_f &= \int_0^t |r_b^i - r_b^{i-1}| dt, \quad i = 2, 3, 4 \dots \end{aligned}$$

From Table 1, it can be seen that errors from free surface velocity and reflected force both decrease as the element size decreases.

4.4. The effect of fracture morphology on spall strength

A given material can suffer transition from intergranular to transgranular fracture under different loading conditions[46]. The transition from intergranular to transgranular mode was observed by many researchers [47-49], which is determined by a variety of factors including loading conditions, microstructure of a material, interfacial properties etc. The fracture morphology, such as intergranular mode or transgranular mode, plays an important role on spall strength [45, 50].

In the atomistic-based interface zone model, the potential energy competition between grain and grain boundary will result in different fracture modes. Due to the hypothesis that the strength of grain boundaries are weaker than grains [43], we define the interfacial potential energy ratio between grain boundary and grain as $R_p = \epsilon_{inter}^b / \epsilon_{inter}^g$. Then we increase the potential energy ratio R_p from 30% to 100% gradually to observe the fracture mode transition. We found out that, when R_p reaches 75%, there is an intergranular to transgranular fracture mode transition. Before that the fracture are all intergranular. The Fig. 11 captured the process of fracture mode transition as $R_p = 75\%$. When R_p keeps increasing, the fracture mode changes from partially transgranular to completely transgranular as shown in Fig. 12.

The free surface velocity of the fracture process is illustrated in Fig. 13. From Fig. 13, it can be seen that the spall strength increases (*or V_{sp} increases*) during the intergranular to transgranular fracture mode transition. This result is qualitatively consistent with the experimental results observed by Brewer et al.[50].

We also calculated the J integral for different potential energy ratio. As described by Sorensen and Jacobsen [51], in Fig. 14, the locally evaluated J integral along the crack faces enclosing the interfacial zone is given as:

$$J_{loc} = \int_0^{\delta^*} T^{inter}(\delta) d\delta + J_{tip} \quad (14)$$

with assumption of $J_{tip} = J_o = 0$, where J_{tip} is the J integral evaluated around the crack tip and J_o is the fracture energy of the crack tip, δ^* is the opening of the interfacial zone.

The J integrals for different potential energy ratio R_p are shown in Fig.15. It can be seen that when J integral (J_{loc}) reaches approximately 45 (J/m²), there is an intergranular to transgranular fracture mode transition.

4.5. The effect of grain size on spall strength

The effects of the grain size on spall strength have not been well established in the literature. There are two conflicting conclusions about the grain size effect on spall strength in metals. Some researchers presented that spall strength decreases with increasing grain sizes[52], while other studies have observed that spall strength increases as grain size increasing[45, 53]. In this work, the atomic-based interfacial zone model is used to study the grain size effects on spall strength for three different grain sizes. As shown in Fig. 16, it is observed that the transgranular crack initiates for all three different grain sizes at potential energy ratio $R_p = 75\%$. By comparing the free surface velocity of intergranular and transgranular fracture modes for all three grain sizes, it can be seen from Fig. 17 and Fig. 18 that the spall strength σ_{sp} decreases as grain size decreases. Our results support the conclusion that spall strength is decreasing as grain size decreasing from experimental observations [45, 53].

In addition, as the grain size decreasing, the fraction of transgranular fracture versus intergranular fracture is decreasing as illustrated in Fig. 16. The reason for this trend (fraction of transgranular fracture versus intergranular fracture decreasing with decreasing grain size) might be that at small grain size, there exists more grain boundaries and these offer a low resistance path along grain boundaries for spalling. The fracture will prefer the grain boundaries to spall instead of grains. The similar phenomenon has been investigated from experiment [54].

4.6. The effect of lattice orientation on spall strength

It is known that the lattice orientation has effects on fracture toughness and fault energy[24, 55], which determines the fracture mechanism to some extent. On the other hand, 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]. In present work, three different lattice orientations of grains are studied to

investigate the variation of spall strength. The degrees of lattice orientation are 30° , 45° and 60° , as shown in Fig. 19.

From Fig. 20(a), it can be seen that, at intergranular fracture mode, the free surface velocity V_{sp} (spall strength) will decrease when we change the lattice orientation from 30° , 45° , to 60° . However, under the transgranular mode, the spall strength almost keeps unchanged for three different lattice orientations, as illustrated in Fig. 20(b). The possible reason is that under transgranular fracture mode, it is more like a single-crystal structure, the effect of lattice orientation on the spall strength appears to be negligible. This result is in consistency with Dalton et al. [56] who reported that crystallographic orientation has no discernible effect on spall strength in single-crystal.

4.7. The effect of impact speed on spall strength

To investigate how impact velocity affects the spall strength, we test three different impact velocities (80m/s, 100m/s and 125m/s) to observe the variation of spall strength. It can be seen that the spall strength will increase with increasing impact speed under intergranular or transgranular mode, as shown in Fig. 21.

5. Discussion and conclusion

In this paper, we have applied a recently developed atomistic-based interfacial zone model to investigate the failure mechanism and spall fracture patterns under impact loadings in polycrystalline materials. In the model, atomistic structure information is used to extrapolate constitutive relations of both polycrystalline grains as well as grain boundaries. By using the AIZM, we have successfully described both grains and grain boundaries of a given polycrystalline material at the mesoscale, and studied the failure mechanisms that may happen during impact loading.

From the simulations, some important findings of present work can be summarized as: (1) when the potential energy of interfacial zone inside grains is greater than that along grain boundaries, i.e. $\epsilon_{inter}^g = 3\epsilon_{inter}^b$, the spallation will follow the grain boundaries (c.f. Fig. 6). The intergranular/transgranular fracture patterns are sensitive to potential energy ratio R_p and the potential energy competition between grain and grain boundary will result in different fracture modes (c.f. Fig. 12). From the simulations, we also observed that the spall strength increases as R_p increases during the intergranular to transgranular fracture mode transition (c.f. Fig. 13); (2) the grain size study indicated that as the grain size decreasing, the fraction of transgranular fracture versus intergranular fracture is also decreasing (c.f. Fig. 16), and the spall strength decreases as well (c.f. Fig. 17 and Fig. 18). Besides, at intergranular fracture mode, the lattice orientation will affect the spall strength to some extent (c.f. Fig. 20(a)). However, at transgranular fracture mode, the effect of crystal lattice orientation on the spall strength appear to be negligible (c.f. Fig. 20(b)); (3) from the impact speed study, we found out that the spall strength increases as impact speed increases for both intergranular and transgranular fracture modes (c.f. Fig. 21).

The simulation results are qualitatively consistent with the experimental measurements, and the atomistic-based interfacial zone model can depict the crystal lattice orientation which is

not achievable by traditional cohesive zone model. We have demonstrated the potential of the AIZM as a major modeling and simulation technique in both polycrystalline materials modeling as well as multiscale simulations in general. However, it should be pointed out that the proposed interfacial zone model is a continuum model and the current model may not be able to capture the complex atomistic physical mechanisms such as dislocation activity, cavity nucleation and growth along grain boundaries involved in the polycrystalline material damage process. In the model, the interfacial constitutive relations are derived from atomistic potential to describe the material interface interactions. We believe the atomistic enriched interface zone model may provide a useful numerical simulation tool to study the material failure process of polycrystalline materials at mesoscale.

Acknowledgements

This work is supported by a grant from National Institute of Health (Grant No. R21AR066925).

Nomenclature

B	body force
c	sound velocity in the material
C	right Cauchy-Green tensor($\mathbf{F}^T\mathbf{F}$)
$d(X_i, X)$	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
$\mathbf{r}_i$	deformed bond vector
R_d	mesh ratio
$\mathbf{R}_p$	interfacial potential energy ratio between grain boundary and grain
$\mathbf{R}_i$	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
$\bar{\mathbf{T}}$	external traction vector
$\mathbf{u}$	displacement vector

V_i	Voronoi region
$W_e(\mathbf{F}_e, \mathbf{R}_i)$	potential energy density of an arbitrary unit cell inside the element
X_i	coordinates of kernel points
α^b	lattice orientation in the grain boundary
α^g	lattice orientation in the grain
$\delta_{s,j}$	penetration distance for node j on the slave surface
ϵ	depth of the potential well
ρ	material density
σ	finite distance at which the inter-atom potential is zero
σ_{sp}	spall strength
$\phi(\mathbf{r}_i)$	atomistic potential
Ω_0^b	unit cell volume

Sub and superscripts

<i>elem</i>	a given element
<i>g</i>	polycrystalline grain
<i>inter</i>	interfacial zone
<i>s</i>	slave surface

References

- [1]. Asay, JR.; Chhabildas, LC. High-Pressure Shock Compression of Solids VI. Springer; 2003. Paradigms and challenges in shock wave research; p. 57-119.
- [2]. Mescheryakov, YI. High-Pressure Shock Compression of Solids VI. Springer; 2003. Meso-macro energy exchange in shock deformed and fractured solids; p. 169-213.
- [3]. Vogler T, Clayton J. Heterogeneous deformation and spall of an extruded tungsten alloy: plate impact experiments and crystal plasticity modeling. J MechPhys Solids. 2008; 56:297–335.
- [4]. Kanel G. Spall fracture: methodological aspects, mechanisms and governing factors. International journal of fracture. 2010; 163:173–91.
- [5]. Larson D, Coppola J, Hasselman D, Bradt R. Fracture Toughness and Spalling Behavior of High- α -Al₂O₃ Refractories. Journal of the American Ceramic Society. 1974; 57:417–21.
- [6]. Chen X, Asay J, Dwivedi S, Field D. Spall behavior of aluminum with varying microstructures. Journal of Applied Physics. 2006; 99:023528.
- [7]. Rabczuk T, Eibl J. Modelling dynamic failure of concrete with meshfree methods. International Journal of Impact Engineering. 2006; 32:1878–97.
- [8]. Børvik T, Hopperstad O, Berstad T, Langseth M. A computational model of viscoplasticity and ductile damage for impact and penetration. European Journal of Mechanics-A/Solids. 2001; 20:685–712.
- [9]. Dremov V, Petrovtsev A, Sapozhnikov P, Smirnova M, Preston DL, Zocher MA. Molecular dynamics simulations of the initial stages of spall in nanocrystalline copper. Physical Review B. 2006; 74:144110.

- [10]. Luo S-N, An Q, Germann TC, Han L-B. Shock-induced spall in solid and liquid Cu at extreme strain rates. *Journal of Applied Physics*. 2009; 106:013502.
- [11]. Krivtsov A, Mescheryakov YI. Molecular dynamics investigation of spall fractures. *International Workshop on Nondestructive Testing and Computer Simulations in Science and Engineering: International Society for Optics and Photonics*. 1999:205–12.
- [12]. Ren B, Li S, Qian J, Zeng X. Meshfree simulations of spall fracture. *Computer Methods in Applied Mechanics and Engineering*. 2011; 200:797–811.
- [13]. Clayton J. Modeling dynamic plasticity and spall fracture in high density polycrystalline alloys. *Int J Solids Struct*. 2005; 42:4613–40.
- [14]. Camacho G, Ortiz M. Computational modelling of impact damage in brittle materials. *International Journal of solids and structures*. 1996; 33:2899–938.
- [15]. Qian J, Li S. Application of multiscale cohesive zone model to simulate fracture in polycrystalline solids. *Journal of Engineering Materials and Technology*. 2011; 133:011010.
- [16]. Schoenfeld SE. Dynamic behaviour of polycrystalline tantalum. *International Journal of Plasticity*. 1998; 14:871–90.
- [17]. Zhou M, Needleman A, Clifton R. Finite element simulations of shear localization in plate impact. *J MechPhys Solids*. 1994; 42:423–58.
- [18]. Zhou M. The growth of shear bands in composite microstructures. *International Journal of Plasticity*. 1998; 14:733–54.
- [19]. Zeng X, Li S. A multiscale cohesive zone model and simulations of fractures. *Computer methods in applied mechanics and engineering*. 2010; 199:547–56.
- [20]. Zeng X, Li S. Application of a multiscale cohesive zone method to model composite materials. *International Journal for Multiscale Computational Engineering*. 2012; 10
- [21]. Steinmann P, Elizondo A, Sunyk R. Studies of validity of the Cauchy–Born rule by direct comparison of continuum and atomistic modelling. *Modelling and Simulation in Materials Science and Engineering*. 2007; 15:S271.
- [22]. Ericksen J. On the Cauchy—Born Rule. *Mathematics and mechanics of solids*. 2008; 13:199–220.
- [23]. Israelachvili, JN. Intermolecular and surface forces. revised third. Academic press; 2011.
- [24]. Li S, Zeng X, Ren B, Qian J, Zhang J, Jha AK. An atomistic-based interphase zone model for crystalline solids. *Computer Methods in Applied Mechanics and Engineering*. 2012; 229:87–109.
- [25]. Hughes T, Belytschko T. A precis of developments in computational methods for transient analysis. *Journal of Applied Mechanics*. 1983; 50:1033–41.
- [26]. Bolander JE Jr, Saito S. Fracture analyses using spring networks with random geometry. *Engineering Fracture Mechanics*. 1998; 61:569–91.
- [27]. Espinosa HD, Zavattieri PD. A grain level model for the study of failure initiation and evolution in polycrystalline brittle materials. Part II: Numerical examples. *Mechanics of Materials*. 2003; 35:365–94.
- [28]. Ghosh S, Liu Y. Voronoi cell finite element model based on micropolar theory of thermoelasticity for heterogeneous materials. *International Journal for Numerical Methods in Engineering*. 1995; 38:1361–98.
- [29]. Liu Y, Kageyama Y, Murakami S. Creep fracture modeling by use of continuum damage variable based on Voronoi simulation of grain boundary cavity. *International Journal of Mechanical Sciences*. 1998; 40:147–58.
- [30]. Jivkov A, Stevens N, Marrow T. A two-dimensional mesoscale model for intergranular stress corrosion crack propagation. *Acta Materialia*. 2006; 54:3493–501.
- [31]. Evers L, Parks D, Brekelmans W, Geers M. Crystal plasticity model with enhanced hardening by geometrically necessary dislocation accumulation. *J MechPhys Solids*. 2002; 50:2403–24.
- [32]. Jivkov A, Stevens N, Marrow T. A three-dimensional computational model for intergranular cracking. *Computational materials science*. 2006; 38:442–53.
- [33]. Ghosh S, Nowak Z, Lee K. Tessellation-based computational methods for the characterization and analysis of heterogeneous microstructures. *Composites science and technology*. 1997; 57:1187–210.

- [34]. Musienko A, Cailletaud G. Simulation of inter-and transgranular crack propagation in polycrystalline aggregates due to stress corrosion cracking. *Acta Materialia*. 2009; 57:3840–55.
- [35]. Du Q, Faber V, Gunzburger M. Centroidal Voronoi Tessellations: Applications and Algorithms. *SIAM Review*. 1999; 41:637–76.
- [36]. Lin L, Wang X, Zeng X. Geometrical Modeling of Cell Division and Cell Remodeling Based on Voronoi Tessellation Method. *CMES: Computer Modeling in Engineering & Sciences*. 2014; 98:203–20.
- [37]. Antoun, T.; Curran, DR.; Razorenov, SV.; Seaman, L.; Kanel, GI.; Utkin, AV. Spall fracture. Springer; 2003.
- [38]. Li S, Qian D, Kam Liu W, Belytschko T. A meshfree contact-detection algorithm. *Computer Methods in Applied Mechanics and Engineering*. 2001; 190:3271–92.
- [39]. Kraft R, Molinari J. A statistical investigation of the effects of grain boundary properties on transgranular fracture. *Acta Materialia*. 2008; 56:4739–49.
- [40]. Razorenov S, Garkushin G, Ignatova O. Resistance to dynamic deformation and fracture of tantalum with different grain and defect structures. *Physics of the Solid State*. 2012; 54:790–7.
- [41]. Tsuji N, Ito Y, Saito Y, Minamino Y. Strength and ductility of ultrafine grained aluminum and iron produced by ARB and annealing. *Scripta Materialia*. 2002; 47:893–9.
- [42]. Park S, Martin J, Guo J, Johnson JL, German RM. Grain growth behavior of tungsten heavy alloys based on the master sintering curve concept. *Metallurgical and Materials Transactions A*. 2006; 37:3337–46.
- [43]. Buban J, Matsunaga K, Chen J, Shibata N, Ching W, Yamamoto T, et al. Grain boundary strengthening in alumina by rare earth impurities. *Science*. 2006; 311:212–5. [PubMed: 16410521]
- [44]. Novikov S, Divnov I, Ivanov A. The study of fracture of steel, aluminium and copper under explosive loading. *Fizika metallov i Metallovedeniye*. 1966; 21:608–15.
- [45]. Dalton D, Brewer J, Bernstein A, Grigsby W, Milathianaki D, Jackson E, et al. Laser-induced spallation of aluminum and Al alloys at strain rates above 2×10^6 s⁻¹. *Journal of Applied Physics*. 2008; 104:013526.
- [46]. Gilath I, Eliezer S, Gazit Y. Fracture modes in alumina at hypervelocity impact conditions. *Journal of materials science*. 1991; 26:2023–5.
- [47]. Deshpande N, Gokhale A, Denzer D, Liu J. Relationship between fracture toughness, fracture path, and microstructure of 7050 aluminum alloy: Part I. Quantitative characterization. *Metallurgical and Materials Transactions A*. 1998; 29:1191–201.
- [48]. Wade RK, Petrovic JJ. Fracture modes in MoSi₂. *Journal of the American Ceramic Society*. 1992; 75:1682–4.
- [49]. Wang Q, Cáceres C. The fracture mode in Al–Si–Mg casting alloys. *Materials Science and Engineering: A*. 1998; 241:72–82.
- [50]. Brewer JL, Dalton DA, Jackson ED, Bernstein AC, Grigsby W, Taleff EM, et al. Influence of microstructure on the spall failure of aluminum materials. *Metallurgical and Materials Transactions A*. 2007; 38:2666–73.
- [51]. Sørensen BF, Jacobsen TK. Determination of cohesive laws by the J integral approach. *Engineering fracture mechanics*. 2003; 70:1841–58.
- [52]. Buchar J, Elices M, Cortez R. The influence of grain size on the spall fracture of copper. *Le Journal de Physique IV*. 1991; 1:C3-623–C3-30.
- [53]. Minich RW, Cazamias JU, Kumar M, Schwartz AJ. Effect of microstructural length scales on spall behavior of copper. *Metallurgical and Materials Transactions A*. 2004; 35:2663–73.
- [54]. Pedrazas NA, Worthington DL, Dalton DA, Sherek PA, Steuck SP, Quevedo HJ, et al. Effects of microstructure and composition on spall fracture in aluminum. *Materials Science and Engineering: A*. 2012; 536:117–23.
- [55]. Gumbsch P, Riedle J, Hartmaier A, Fischmeister HF. Controlling factors for the brittle-to-ductile transition in tungsten single crystals. *Science*. 1998; 282:1293–5. [PubMed: 9812888]

- [56]. Dalton D, Worthington D, Sherek P, Pedrazas N, Quevedo H, Bernstein A, et al. Microstructure dependence of dynamic fracture and yielding in aluminum and an aluminum alloy at strain rates of $2 \times 10^6 \text{ s}^{-1}$ and faster. *Journal of Applied Physics*. 2011; 110:103509.

Highlights

- Modeling grain boundaries by interfacial zone model
- High-speed impact induced spall fracture in polycrystalline materials
- Investigation of intergranular/transgranular fracture transition under impact loading
- Investigating how grain size, crystal lattice orientation, and impact speed affect spall strength

Fig. 1.
Deformation gradient in interfacial zone

Fig. 2.
A schematic of Voronoi grain generation

Fig. 3. Polycrystalline grain cell and mesh generation: (a) grain cells and (b) finite element meshes over grain cells

Fig. 4.
The problem statement of the impact test

Fig. 5.
Lattice orientation in grains and interfacial zones

Fig. 6. Snapshots of stress distribution(σ_{22}) for an intergranular failure process: (a) $t=0.06\mu\text{s}$; (b) $t=0.12\mu\text{s}$; (c) $t=0.164\mu\text{s}$; (d) $t=0.208\mu\text{s}$; (e) $t=0.3\mu\text{s}$; (f) $t=0.4\mu\text{s}$.

Fig. 7.

(a) The velocity and (b) the reflected force on the bottom surface as a function of time

Fig. 8.

Different mesh ratio over grain cells: (a) Case 1 with $R_d=0.5$; (b) Case 2 with $R_d=0.33$; (c) Case 3 with $R_d=0.25$

Fig. 9.

The intergranular failure for different mesh ratio: (a) Case 1; (b) Case 2; (c) Case 3

Fig. 10.

(a) Free surface velocity and (b) Force profile at the free bottom surface for different meshes

Fig. 11. Snapshots of stress distribution(σ_{22}) for partially transgranular failure process with potential energy ratio $R_p=75\%$: (a) $t=0.048\mu s$; (b) $t=0.156\mu s$; (c) $t=0.204\mu s$; (d) $t=0.268\mu s$; (e) $t=0.34\mu s$; (f) $t=0.4\mu s$

Fig. 12.

The snapshot of transgranular failure intense with the increase of potential energy ratio R_p in a polycrystalline solid: (a) $R_p=75\%$; (b) $R_p=85\%$; (c) $R_p=100\%$

Fig. 13.

Free surface velocity as a function of time at different fracture mode: (a) Completely intergranular to partially transgranular; (b) Partially transgranular to completely transgranular

Fig. 14.
Integration paths locally around the interfacial surface for the J integral

Fig. 15.
 J integral curves for different potential energy ratio R_p

Fig. 16.

The snapshot of transgranular crack initiation for different grain sizes: (a) **grain No. = 128**;
(b) **grain No. = 200**; (c) **grain No. = 288**

Fig. 17.

The free surface velocity for different grain sizes at intergranular fracture mode:(a) $R_p=35\%$, (b) $R_p=50\%$

Fig. 18. The free surface velocities for different grain sizes at transgranular fracture mode:(a) $R_p=75\%$, (b) $R_p=85\%$

Fig. 19.
Lattice orientation: (a) 30; (b) 45; (c) 60°

Fig. 20.

Free surface velocity for different lattice orientations: (a) Intergranular fracture($R_p=35\%$);
 (b) Transgranular fracture($R_p=85\%$)

Fig. 21.

The free surface velocity for different impact speed: (a) Intergranular fracture ($R_p=35\%$);
(b) Transgranular fracture ($R_p=85\%$)

Table 1

Comparison of different meshes (Velocity & Force)

R_d	Bulk Element No.	Velocity Error	Force Error
0.50	2520	-----	-----
0.33	5101	4.78E-08	2.72E-10
0.25	8646	2.48E-08	1.40E-10