# **Crystal Plasticity-Based Spalling Damage Model for Ductile Metals**

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## Abstract

Spalling is a typical tensile failure that results from the coupling evolution of microstructure and microdamage under high strain-rate loading. To understand the spalling damage behavior of polycrystalline materials at mesoscale, this paper develops a spalling model by integrating the crystal plasticity theory and the microvoid growth theory. The model is implemented in ABAQUS simulation via the VUMAT subroutine to simulate a planar impact process of copper, and the results are compared with experimental data. Due to the inhomogeneity of crystal plastic slip, the local stress fluctuates severely near the grain boundary. Therefore, without introducing the fluctuation in the threshold stress for microdamage evolution, this model can simulate the heterogeneous feature of microvoid nucleation, growth, and coalescence in materials. The results show that microvoids tend to nucleate at  $25^{\circ}$ – $50^{\circ}$  misorientation angle grain boundaries, which undergo a high probability of stress fluctuation.

Keywords Spalling · Crystal plasticity · Microvoid nucleation and growth · Grain boundary · Finite element method

# **1** Introduction

Spalling is a typical tensile failure that results from the nucleation, growth, and coalescence of microvoids or microcracks produced in materials under high strain-rate loading [1-3]. In the spalling process, the microstructural features of materials, e.g., the grain size, grain orientation, precipitates, inclusions, etc., evolve under impact loading and cause the evolution of microdamage. The coupling between the microstructural and microdamage evolution and the external impact loading poses fundamental challenges to spalling prediction.

Numerous efforts have been devoted to modeling the microstructural and microdamage evolution in the spalling process [4–9]. The dynamic crystal plasticity theory is one of the fundamental theories for describing plastic deformation [10–18], which is widely used in simulations of material impact dynamic process, microstructural evolution, and dynamic failure. For example, Chao Ling [19] used

a reduced micromorphic single crystal plasticity model to simulate void growth in ductile metals; Clayton [20, 21] simulated a spalling process with only grain boundary damage based on the weak connection model; Wilkerson and Ramesh [22, 23] developed the micro- and nano-scale void growth theory based on the dislocation density theory and the relativistic effect of dislocations. Although these studies help understand the dynamic deformation behavior and failure process of materials, a predicting model involving both intragranular and grain boundary microdamage evolution is still lacking.

To investigate the effect of grain boundaries on spalling, in this study, we first performed plate impact experiments of high-purity polycrystalline oxygen-free high-thermalconductivity (OFHC) copper samples on a one-stage lightgas gun; and then developed a new spalling damage model based on crystal plasticity and microvoid nucleation and growth theory. The model was implemented in the finite element simulation via the VUMAT subroutine of ABAQUS to investigate how damage nucleates and propagates in the target. The agreement between the simulation and experiments proves the validation of the new model. The simulation shows that resulting from high-stress fluctuations on grain boundaries with  $25^{\circ}$ - $50^{\circ}$  misorientation angle, microvoids are prone to nucleate on these boundaries in the initial damage evolution stage. With the increase in loading time,

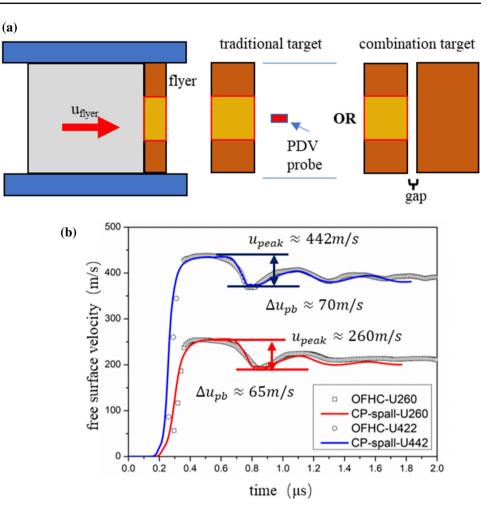


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**Fig. 1 a** Experimental setup, the traditional target for recording particle velocity curve by PDV probe, the combination target for freezing damage; **b** the particle velocity profiles of the free surface of the targets, where the discrete points are experimental data, and the curves are obtained from the finite element simulation



intragranular microvoids dominate damage evolution, followed by the coalescence of microvoids inducing final spalling.

# 2 Plate Impact Experiment

The plate impact experiments of oxygen-free high-thermalconductivity (OFHC) copper were conducted on a one-stage light-gas gun, as shown in Fig. 1a. The study involved three experiments, denoted as OFHC-U260, OFHC-U442, and OFHC-U442F. OFHC-U260 and OFHC-U442 adopted the traditional target and recorded the free-surface velocity profiles by a photonic Doppler velocimeter (PDV), as shown in Fig. 1b. OFHC-U442F adopted the combination target to achieve damage freezing [24] (due to the back target, the free-surface curve could not be recorded, we used the same pressure-to-mass ratio to drive the flyer to obtain a speed similar to that of OFHC-U442), and the equation for tensile pulse width is:

$$\tau \approx \frac{d_{\rm gap}}{u_{\rm p}} \tag{1}$$

Table 1 The details of three shot experiments

	OFHC- U260	OFHC- U442	OFHC-U442F
The diameter of targets	30 mm		
The diameter of flyers	> 30 mm		
The thickness of targets	2.24 mm	2.20 mm	2.20 mm
The thickness of flyers	1.20 mm	1.24 mm	1.24 mm
Peak stress	4.66 GPa	8.29 GPa	_
Spall strength	1.13 GPa	1.22 GPa	-

where  $d_{\rm gap}$  is the gap between combination targets,  $u_{\rm p}$  is the free-surface particle velocity, and  $\tau$  is tensile pulse width. For OFHC-U442F,  $d_{\rm gap} = 40 \ \mu \text{m}$ ,  $u_{\rm p} \approx 442 \ \text{m/s}$ , so  $\tau \approx 90 \ \text{ns}$ . The details of the three experiments are shown in Table 1.

The electron backscatter diffraction (EBSD) microscope images clearly show that the sample has a grain size of about  $300 \ \mu m$  (Fig. 2a).

The peak stress  $\sigma_{\text{peak}}$  can be approximately calculated as:

$$\sigma_{\text{peak}} \approx \frac{\rho_0}{2} \left( c_0 + \frac{1}{2} s u_{\text{peak}} \right) u_{\text{peak}} \tag{2}$$

where  $\rho_0$  is the initial density of OFHC,  $c_0$  is the sound velocity in the material at zero pressure, *s* is the linear Hugoniot slope coefficient, and  $u_{\text{peak}}$  is the peak velocity of free-surface particles. The spall strength is calculated from the pullback velocity with the sound velocity approximation:

$$\sigma_{\rm spall} \approx \frac{\rho_0}{2} c_0 \Delta u_{\rm pb} \tag{3}$$

where  $\Delta u_{pb}$  is the pullback velocity, which is the difference between peak and rebound velocities. According to the above formulae, the corresponding calculation results are shown in Table 1. After the impact test, the targets of OFHC-U442F were cut, ground, and polished for EBSD observation. As shown in Fig. 2b, the microvoids spread across the grain boundaries, near-grain boundaries and inside grains. Figure 2c is an optical microscope photo, which is used for damage statistics.

## **3 Theoretical Model**

In this section, a new theoretical model is developed, which integrates shock dynamics of solid, the rate-dependent crystal plasticity theory [25], and the nucleation and growth theory of microvoids [26].

## 3.1 Volumetric Stress

The update of the volumetric stress in the model is through the shock dynamics of solid. Based on the  $u_s - u_p$  equation of state of solid impact and the Rankine–Hugoniot relationship [27] (mass, momentum, and energy continuity conditions of

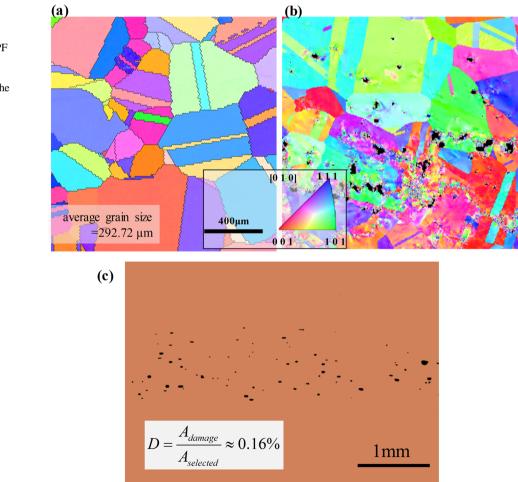


Fig. 2 a IPF map of initial oxygen-free high-thermal-conductivity (OFHC) copper sample; b IPF maps of samples of OFHC-U442F; c damage statistics of OFHC-U442F (the black spots are microvoids) impact), the relationship between volume change and volumetric stress under impact loading is:

$$\Delta \sigma^{\rm V} = -\Delta p = \frac{\rho_0^2 c_0^2 \Delta V}{\left(1 + s \rho_0 \Delta V\right)^2} \tag{4}$$

where  $u_s$  is the velocity of shock wave,  $u_p$  is the velocity of particle, p is pressure,  $\sigma^V$  is volumetric stress, which equals negative pressure,  $V=1/\rho$  is specific volume, and  $\rho$  is the current density of the material.

According to the Mie–Grüneisen equation of state, considering the contribution of plastic work to volumetric stress, Eq. (4) is modified as:

$$\Delta\sigma^{\mathrm{V}} = \frac{\rho_0^2 c_0^2 \Delta V}{\left(1 + s\rho_0 \Delta V\right)^2} - \frac{\gamma}{V} 0.9 W^p \tag{5}$$

where  $\gamma$  is the Grüneisen coefficient, and the second term on the right-hand side represents the contribution of the plastic work by assuming the work-heat conversion coefficient to be 0.9. The plastic work can be calculated from the following equation:

$$\mathrm{dW}^p = \boldsymbol{\sigma}' \,\mathrm{d}\boldsymbol{\varepsilon}' + \boldsymbol{\sigma}^{\mathrm{V}} \mathrm{d}f \tag{6}$$

where *f* is the porosity of the damage element. In Eq. (6), the plastic work consists of two parts: one is the contribution of the work of deviatoric stress  $\sigma'$  on the deviatoric strain e', the other is the contribution of volumetric stress  $\sigma^{V}$  on void expansion d *f*.

#### 3.2 Deviatoric Stress

The update of deviatoric stress in the model is made through the crystal plasticity theory [25]. The total deformation gradient tensor F can be decomposed as:

$$\boldsymbol{F} = \boldsymbol{F}^* \cdot \boldsymbol{F}^P \tag{7}$$

where superscript \* denotes lattice deformation, and superscript P denotes crystal slip. The deformation rate is given by:

$$\boldsymbol{D} = \operatorname{sym}\left[\dot{\boldsymbol{F}} \cdot (\boldsymbol{F})^{-1}\right] = \boldsymbol{D}^* + \boldsymbol{D}^P$$
(8)

where sym[] means the symmetric part of the tensor, and D can be divided into elastic part  $D^*$  and plastic part  $D^P$ . The elastic deformation rate can be further decomposed into spherical and deviatoric parts as:

$$\boldsymbol{D}^* = \boldsymbol{D}_m \boldsymbol{I} + \boldsymbol{D}' \tag{9}$$

where  $D_m$  is the value of spherical strain rate, I is the identical second-order tensor, and D' is the deviatoric part of elastic deformation rate tensor.

Since plastic deformation does not generate stress, the Cauchy stress is expressed as:

$$\nabla^*_{\boldsymbol{\sigma}} + \boldsymbol{\sigma} \left( \boldsymbol{I} : \boldsymbol{D}^* \right) = \mathbb{L} : \boldsymbol{D}^*$$
(10)

where  $\sigma^{\vee^*}$  is the Jaumann rate of Cauchy stress  $\sigma$ , and  $\mathbb{L}$  is the elastic modulus tensor, which has three independent crystallographic stiffnesses of materials,  $C_{11}$ ,  $C_{12}$ , and  $C_{44}$ .

The rate of plastic deformation gradient tensor  $F^P$  is related to the slipping rate  $\dot{\gamma}^{(\alpha)}$  of the slip system  $\alpha$ :

$$\dot{\boldsymbol{F}}^{P} \cdot \left(\boldsymbol{F}^{P}\right)^{-1} = \sum_{\alpha} \underline{\dot{\boldsymbol{\gamma}}}^{(\alpha)} \boldsymbol{s}^{(\alpha)} \boldsymbol{m}^{(\alpha)}$$
(11)

where the sum ranges over all activated slip systems,  $s^{(\alpha)}$  and  $m^{(\alpha)}$  are the unit vectors of the slip direction and the normal to the slip plane, respectively.

The corresponding resolved shear stress  $\tau^{(\alpha)}$  of the slip system  $\alpha$  is:

$$\tau^{(\alpha)} = \boldsymbol{m}^{(\alpha)} \cdot \frac{\rho_0}{\rho} \boldsymbol{\sigma} \cdot \boldsymbol{s}^{(\alpha)}$$
(12)

Based on the Schmid law, the slipping rate  $\underline{\dot{\gamma}}^{(\alpha)}$  of the slip system  $\alpha$  in a rate-dependent crystalline solid is determined by  $\tau^{(\alpha)}$  as:

$$\underline{\dot{\gamma}}^{(\alpha)} = \underline{\dot{a}}^{(\alpha)} \hat{f}^{(\alpha)} \left( \frac{\tau^{(\alpha)}}{g^{(\alpha)}} \right)$$
(13)

where  $\underline{\dot{a}}^{(\alpha)}$  and  $g^{(\alpha)}$  are the reference strain rate and the current strength of the slip system  $\alpha$ , respectively, and  $\hat{f}^{(\alpha)}$  is non-dimensional functions describing the dependence of strain rate on stress. In the current study, we follow the simple law proposed by Hutchinson [28] as:

$$\hat{f}(x) = x|x|^{N-1}$$
 (14)

The strain hardening is characterized through the incremental relation as:

$$g^{(\alpha)} = \sum_{\beta} h_{\alpha\beta} \underline{\dot{\gamma}}^{(\beta)} \tag{15}$$

where the sum ranges over all activated slip systems, and  $h_{\alpha\beta}$  is the slip hardening moduli of slip.  $h_{\alpha\alpha}$  (no sum) and  $h_{\alpha\beta}(\alpha \neq \beta)$  are self and latent hardening moduli, respectively. We use the expression of Bassani and Wu [29] for the hardening moduli to describe the three-stage hardening of

crystalline materials. Their expression depends on the shear strains  $\dot{\gamma}^{(\alpha)}$  of all slip systems as:

$$h_{\alpha\alpha} = \left\{ (h_0 - h_s) \operatorname{sech}^2 \left| \frac{(h_0 - h_s) \underline{\gamma}_0}{\tau_s - \tau_0} \right| + h_s \right\} \hat{G} \left( \gamma^{(\beta)}; \beta \neq \alpha \right)$$
  
no sum on  $\alpha$  (16)

$$h_{\beta\alpha} = qh_{\alpha\alpha} \quad (\beta \neq \alpha) \tag{17}$$

where  $h_0$  is the initial hardening modulus,  $h_s$  is the hardening modulus for easy slip stage,  $\tau_0$  is the yield stress,  $\tau_s$  is the break-through stress, and  $\hat{G}$  is the cross-slip-related function given by:

$$\hat{G}\left(\gamma^{(\beta)}; \beta \neq \alpha\right) = 1 + \sum_{\beta \neq \alpha} \tilde{f}_{\alpha\beta} \tanh\left(\frac{\gamma^{(\beta)}}{\gamma_0}\right)$$
(18)

where  $\underline{\gamma}_0$  is the amount of slip of the peak strength, and  $\overline{f}_{\alpha\beta}$  represents the interaction coefficient of the slips.

### 3.3 Void Nucleation and Growth Law

The critical volumetric stress  $\sigma_{nu}^{V}$  determines the spalling damage nucleation. When the volumetric stress of the element is greater than  $\sigma_{nu}^{V}$ , microvoid nucleates.  $\sigma_{nu}^{V}$  is assumed to be equal everywhere in the simulation. No initial pressure fluctuations are set, and no interface is set as a weak point.

Once the microvoid nucleates, the growth of the microvoid in the element will be considered. For an element with radius b containing a microvoid with radius a, the porosity of the element is given by:

$$f = \frac{a^3}{b^3} \tag{19}$$

According to the analysis of Czarnota et al. [30], the evolution of the microvoid radius *a* is governed by the following differential equation:

$$\sigma^{\rm V} - \sigma_{\rm gr}^{\rm V} = \rho \left\{ a\ddot{a} \left( 1 - f^{1/3} \right) + \frac{3}{2} \dot{a}^2 \left( 1 - \frac{4}{3} f^{1/3} + \frac{1}{3} f^{4/3} \right) \right\}$$
(20)

where  $\sigma_{gr}^{V}$  is the threshold stress for microvoid growth, which equals to the smaller one of  $\sigma_{nu}^{V}$  and the growth stress in the Gurson model  $\sigma_{G}^{V}$ :

$$\sigma_{\rm gr}^{\rm V} = \min\left(\sigma_{\rm nu}^{\rm V}, \sigma_G^{\rm V}\right) \tag{21}$$

The growth pressure in the Gurson model is:

$$\sigma_{\rm G}^{\rm V} = \frac{2k^{\rm poly}}{3q_2} \ln\left(\frac{1}{q_1 f}\right) \left\{ \varepsilon_0^{\rm poly} + \varepsilon^{\rm pre} + \frac{2}{3q_2} \ln\left[\frac{(q_1 f)^{-f/(1-f)}}{(1-f)}\right] \right\}^n$$

$$\times \left\{ \dot{\varepsilon}_0^{\text{poly}} + \frac{2}{3q_2} \ln\left(\frac{1}{q_1 f}\right) \frac{\dot{f}}{(1-f)^2} \right\}^m \tag{22}$$

where the constant coefficients  $q_1 = q_2 = 1$ ,  $\varepsilon^{\text{pre}}$  is cumulative plastic equivalent strain, *m* and *n* are the strain-rate sensitivity exponent and strain hardening exponent, respectively,  $\dot{\varepsilon}_0^{\text{poly}}$  and  $\dot{\varepsilon}_0^{\text{poly}}$  are the reference strain rate and the reference strain, respectively, and  $k^{\text{poly}}$  is a scaling factor for the flow stress level.

# 3.4 Reduction in Stiffness and Strength Caused by Temperature Increase and Damage Evolution

The stiffness of the material is reduced due to temperature rise and damage evolution. The initial equivalent shear modulus is [31]:

$$G_0 = \frac{C_{11} - C_{12} + 3C_{44}}{5} \tag{23}$$

The initial bulk modulus  $K_0$  is calculated by derivation of Eq. (4):

$$K_0 = -V \frac{d\Delta p}{d\Delta V} = V \frac{\rho_0^2 c_0^2 (1 - s\rho_0 \Delta V)}{(1 + s\rho_0 \Delta V)^3}$$
(24)

The temperature increment can be calculated as [27]:

$$\Delta T = \frac{\Delta E + p\Delta V}{c_v} - T\frac{\gamma}{V}\Delta V \tag{25}$$

where  $c_v$  is the specific heat. Temperature rise  $\Delta T$  can be obtained from the simultaneous Eqs. (5), (6), and (25).

The element stiffness is reduced with microdamages and temperature [32] as:

$$C_{ij} = C_{ij0}(1-f) \left( 1 - \frac{6K_0 + 12G_0}{9K_0 + 8G_0} f \right) \frac{T_r - T}{T_r}$$

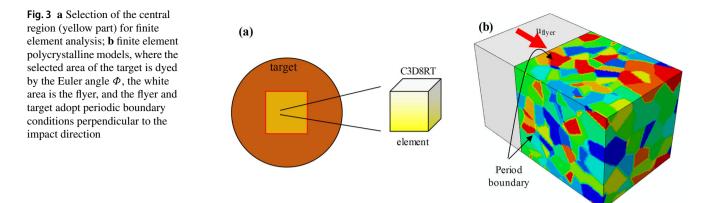
$$K = K_0 \frac{4G_0(1-f)}{3K_0 f + 4G_0} \frac{T_r - T}{T_r}$$
(26)

where  $T_r$  is the reference temperature equal to the melting temperature minus the loading temperature.

When the element contains damage, the equivalent strength and the effective cutting stress of the slip system are reduced as:

$$\widehat{g}^{(\alpha)} = g^{(\alpha)} \cdot (1-f), \quad \widehat{\tau}^{(\alpha)} = \tau^{(\alpha)} / (1-f)$$
(27)

The purpose of this model is to discuss the influence of inhomogeneity of plastic slip on the evolution of spalling damage. This model contains some approximate assumptions, for example, the variation of slip strength with temperature is not considered, and the quasi-static bearing capacity



of material with voids is calculated by the Gurson model. When the impact velocity is not high (the temperature rise is not high) and the details of the edge of each void are not considered, this model can give reliable averaged calculation results.

# **4 Finite Element Simulation**

Commercial finite element software ABAQUS/Explicit is utilized to simulate the planar impact test of OFHC. The target plate is  $2 \text{ mm} \times 2 \text{ mm} \times \text{thickness of the sample (Fig. 3a)}$ , with periodic boundaries perpendicular to the impact direction. The finite element polycrystalline model is generated by Voronoi polyhedrons of 300 random seeds, and three Euler angles determine the crystallographic orientation. The Euler angles are also randomly generated in the model. Figure 3b shows the polycrystalline models established for calculation. The C3D8RT element (an 8-node thermally coupled brick, trilinear displacement and temperature, reduced integration) is used in the simulation. A VUMAT subroutine is written to implement the above constitutive model in Sect. 3 in the FEM simulation. The corresponding parameters are shown in Table 2. The finite element simulation of OFHC-U260 and OFHC-U442 are carried out, which are denoted as CP-spall-U260 and CP-spall-U442, respectively.

In the simulation, to reduce the computational complexity, an equivalent polycrystalline plastic model is employed for the flyer material. The deviatoric viscoplastic flow follows the form of Czarnota et al. [27] A power-law equation is adopted to characterize the flow stress  $\sigma_y^{\text{poly}}$ , taking both strain hardening and strain-rate sensitivity into account:

$$\sigma_{y}^{\text{poly}} = k^{\text{poly}} \left( \dot{\varepsilon}_{0}^{\text{poly}} + \dot{\varepsilon}_{\text{eq}}^{\text{poly}} \right)^{m} \left( \varepsilon_{0}^{\text{poly}} + \varepsilon_{\text{eq}}^{\text{poly}} \right)^{n}$$
(28)

In Eq. (28), the corresponding symbols have the same meaning as Eq. (22).

# **5** Results and Discussions

## 5.1 Model Validation

To validate the constitutive model, we compare the simulation results of CP-spall-U442 with the experimental results of OFHC-U442F, and find that the experimentally measured damage in Fig. 6b (the red spot) falls near the simulated damage evolution curve (the tensile region appears at ~ 800 ns in CP-spall-U442, so the damage state of OFHC-U442F is the state of ~ 890 ns), which proves the validity of the constitutive model.

#### 5.2 Stress Wave Propagation and Damage Evolution

Figure 4 shows the stress wave propagation and the induced damage evolution in the simulated sample. In the shock compression stage, the wave head of the elastic precursor wave (the blue-green interface) is relatively flat, but the subsequent plastic wave head (the red-yellow interface) has noticeable stress fluctuations (Fig.  $4a_1b_1$ ). The shock waves are reflected on the free surfaces to form rarefaction waves, which transmit into the material and generate tensile stress inside the material. Since the plastic deformation of the crystal is not uniform, the tensile pressure fluctuates on grain boundaries (Fig.  $4a_2b_2$ ). When the tensile pressure is greater than the critical value  $\sigma_{nu}^{V}$ , microvoids nucleate on the grain boundaries (Fig. 4a<sub>3</sub>b<sub>3</sub>). With time going by, more microvoids nucleate on or near the grain boundaries (Fig. 4a<sub>4</sub>b<sub>4</sub>). However, many intragranular microvoids appear and disperse in the spall region (Fig. 4a<sub>5</sub>b<sub>5</sub>). In the later stage of damage evolution, the microvoids grow and coalesce, and the sample basically loses the load-bearing capacity (Fig.  $4a_6b_6$ ).

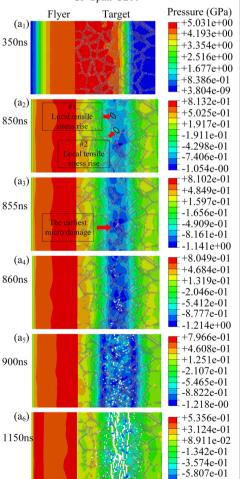
### 5.3 Grain Boundaries and Initial Nucleation Sites

We define an element as a grain boundary element (GBE) when the eight nodes of the element are not all in the same Voronoi polyhedron, as a near-grain-boundary element

#### Table 2 Parameters in the simulation

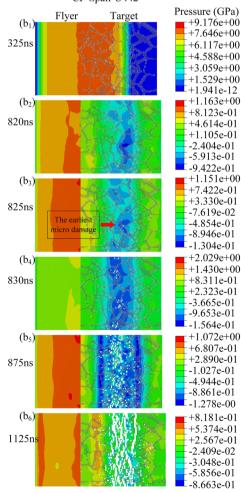
Name	Symbol	Numerical value	Remark
Density	$ ho_0$	8.93 g/cm <sup>3</sup>	From [31]
Elastic parameters	$C_{11}, C_{12}, C_{44}$	176, 118, 61 GPa	
Sound velocity	$c_0$	3.9 km/s	From [27]
Linear Hugoniot slope coefficient	S	1.49	
Grüneisen parameter	$\gamma_0$	2.0	
Specific heat	$c_{v}$	$384.9e^{-6} \text{ kJ/(g} \cdot ^{\circ}\text{C})$	
Crystal plasticity coefficient	$N, \dot{a}_0, h_0, h_{ m s}, \tau_0, \tau_{ m s}, f_{lphaeta}, q_{lphaeta}$	2.0, 0.05 s <sup>-1</sup> , 1.5 GPa, 0.5 GPa, 0.1 GPa, 0.3 GPa, 0.03, 0.01	Determination of parameters by curve fitting (Fig. 1b)
The critical nucleation volumetric stress	$\sigma_{ m nu}^{ m V}$	1.11 GPa	
Critical damage	$f_{c}$	0.024	
Equivalent polycrystalline coefficient	$k^{\text{poly}}, \dot{\varepsilon}_0^{\text{poly}}, m, \varepsilon_0^{\text{poly}}, n$	0.3 GPa·s <sup>m</sup> , 100 s <sup>-1</sup> , 0.48, 0.02, 0.4	Determination of the parameters by tensile simulation of the crystal plasticity model
The size of elements	$b_0$	25 μm	

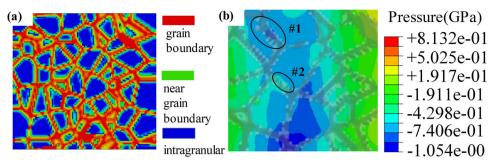
**Fig. 4** Pressure and damage evolution in target plates, where the shadow parts on the targets are the grain boundaries, and the white points are the damage (deleted unit) CP-Spall-U260



-8.040e-01







**Fig.5 a** A slice diagram of the polycrystalline target, where the red regions represent the grain boundary elements (GBE), the green regions represent the near-grain-boundary elements (NGBE), and the blue

regions represent the intragranular elements (IGE); **b** inhomogeneous distribution of pressure near-grain boundaries before microdamage nucleation (CP-spall-U442 820 ns)

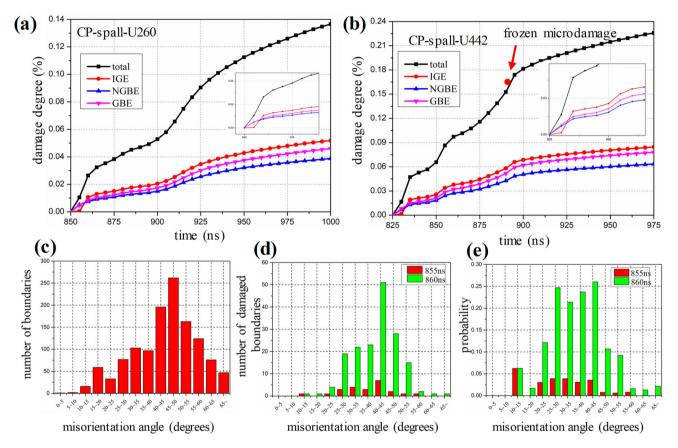


Fig. 6 a and b Damage evolution in different types of elements (the red point in (b) is damage statistics results of OFHC\_U442F); c statistics of misorientation angles of grain boundaries in the spalling damage zone

(shot CP-spall-U260); **d** and **e** statistics and the probability of misorientation angles of grain boundaries with damage at 855 ns and 860 ns (shot CP-spall-U260)

(NGBE) whenever there is a grain boundary element around it, and the others as intragranular elements (IGE) (Fig. 5a). In the simulations, the "random" nucleation of microdamage is due to the inhomogeneity of the stress distribution caused by crystal slippage, as shown (Fig. 5b), the volumetric stress of #1 grain boundary is greater than the average value near the spall area, so it is more prone to nucleation damage, while #2 grain boundary, on the contrary, prevents damage nucleation. The microvoids in different types of elements are counted and analyzed. Figure 6a and b shows the evolution of damage in these elements with time. The damage degree D is equal to the number of deleted elements  $N_{deleted}$  multiplied by the critical damage degree  $f_c$  and divided by the number of total elements  $N_{total}$ :

$$D = \frac{N_{\text{deleted}} f_{\text{c}}}{N_{\text{total}}}$$
(29)

As shown in the insets in Fig. 6a and b, the initial damage evolution is dominated by damage in grain boundary elements and near-grain-boundary elements. After that, the damage evolution in grain boundary elements and near-grainboundary elements slow down. Meanwhile, the damage in intragranular elements notably increases, manifested by relatively isolated and dispersed microvoids in grains, as shown in Fig. 4a<sub>5</sub> and b<sub>5</sub>. Then, the coalescence of microvoids dominates the damage evolution until an interconnected network of microvoids forms, as shown in Fig. 4a<sub>6</sub> and b<sub>6</sub>.

To understand the impact of grain boundary type on initial nucleation of microvoid, we analyze the misorientation angle distribution in the spalling damage zone. Figure 6c–e plots the distributions of the number of grain boundaries with different misorientation angles in the intact sample, the number of damaged grain boundaries with different misorientation angles, and the corresponding probability of the damaged grain boundary, respectively. It can be seen that the grain boundary with  $25^{\circ}$ – $50^{\circ}$  is more prone to damage, which is consistent with the relevant experimental observations [9]. Hence, it can be inferred that the grain boundaries with misorientation angles of  $25^{\circ}$ – $50^{\circ}$  are more susceptible to damage even without a weak interface, which may result from the heterogeneous stress distribution in the spalling region.

## 6 Summary

In this paper, a new spalling model, which combines the crystal plasticity and dynamic microvoid growth models, has been developed and implemented via the VUMAT subroutine in ABAQUS. The numerical results are compared with those of plate impact experiments of OFHC. The agreement between the simulation and experiments proves the validation of the new model. The simulation shows that microvoids are prone to nucleate on grain boundaries or near-grain boundaries at first, while with the increase in loading time, intragranular microvoids dominate damage evolution. In addition, grain boundaries with 25°–50° misorientation angle are more susceptible to damage due to higher stress.

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### Declarations

**Conflict of interest** The authors declared that they have no conflicts of interest in this work. And we declare that we do not have any commercial or associative interest representing a conflict of interest in connection with the work submitted.

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