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Summary In this work, a single crystal strain gradient plasticity model is derived at finite strains. The gradient enhancement is base on a scalar strain measure of plastic slip of single crystals. It is implemented in finite element code Zset and then used to investigate void size effect on its growth and coalescence in single crystals. 3D unit cell finite element simulations are performed and the results are compared with those obtained with classical single crystal plasticity model.

CONTEXTS

In pressurised water reactors, irradiation leads to formation of various defects in their components. Especially in the core internals made of austenitic stainless steels, intragranular voids and bubbles can be created, which may induce macroscopic swelling at high irradiation levels. When the material is subjected to mechanical loading, the formed voids and bubbles can probably play a role in the process of ductile fracture, which is generally known as a result of void nucleation, growth and coalescence. At initial stage of fracture, voids are much smaller than the grain size so that one can consider the voids as embedded in an infinitely large single crystal matrix under homogeneous loading. In this work, effects of void size on its growth and coalescence in single crystals are investigated.

Size-dependent behaviours have been widely observed in metallic materials, such as size-dependent strength of micro-specimen, the Hall-Petch effect, etc. As classical continuum theories can not predict these behaviours, many authors are motivated to develop non-local models (see [1] and references therein). These enriched models suppose that the stress state of a material point depends on the state of a finite neighbourhood.

MODEL DESCRIPTION

A single crystal strain gradient plasticity model is proposed at finite strains. The strain gradient enhancement is based on a scalar strain measure of plastic slip (cf. [2]). One additional degree of freedom γ_χ is introduced. The set of degrees of freedom (DOF) and that of their Lagrangian gradients are therefore defined as

$$\text{DOF} = \{\underline{\boldsymbol{u}}\,, \gamma_\chi\} \;\text{ and }\; \text{GRAD} = \left\{ \underset{\sim}{\boldsymbol{F}} := \underset{\sim}{\mathbf{1}} + \frac{\partial \underline{\boldsymbol{u}}}{\partial \underline{\boldsymbol{X}}}, \underline{\boldsymbol{K}} := \frac{\partial \gamma_\chi}{\partial \underline{\boldsymbol{X}}} \right\}. \tag{1}$$

As a result, an additional balance equation and boundary condition are derived for the crystalline body V:

$$\operatorname{div} \underline{\boldsymbol{m}} - s = 0 \; \forall \underline{\boldsymbol{x}} \in V \tag{2}$$

and

$$m = \underline{\boldsymbol{m}} . \underline{\boldsymbol{n}}\,, \; \forall \underline{\boldsymbol{x}} \in \partial V, \tag{3}$$

where s and $\underline{\boldsymbol{m}}$ are the generalised stresses respectively work conjugate to the microdeformation γ_χ and the eulerian gradient of the microdeformation $\underline{\boldsymbol{k}} := \dfrac{\partial \gamma_\chi}{\partial \underline{\boldsymbol{x}}}$, m is the surface double force density and $\underline{\boldsymbol{n}}$ is the unit normal vector to the surface.

The deformation gradient $\underset{\sim}{\boldsymbol{F}}$ is multiplicatively decomposed into elastic and plastic parts $\underset{\sim}{\boldsymbol{F}} = \underset{\sim}{\boldsymbol{F}}^e . \underset{\sim}{\boldsymbol{F}}^p$. The elastic strain is defined as

$$\underset{\sim}{\boldsymbol{E}}^e := \frac{1}{2}(\underset{\sim}{\boldsymbol{F}}^{eT} . \underset{\sim}{\boldsymbol{F}}^e - \underset{\sim}{\mathbf{1}}), \tag{4}$$

and the plastic strain rate is

$$\dot{\underset{\sim}{\boldsymbol{F}}}^p \underset{\sim}{\boldsymbol{F}}^{p-1} := \sum_s \dot{\gamma}^s \underset{\sim}{\boldsymbol{N}}^s, \tag{5}$$

with plastic slip rate $\dot{\gamma}^s$ and the Schmid tensor $\underset{\sim}{\boldsymbol{N}}^s = \underline{\boldsymbol{l}}^{\,s} \otimes \underline{\boldsymbol{n}}^{\,s}$ for the slip system s, where $\underline{\boldsymbol{l}}^{\,s}$ is the slip direction vector and the normal to the slip plan $\underline{\boldsymbol{n}}^{\,s}$. Inspired from the form of the residual dissipation, the plastic slip rate $\dot{\gamma}^s$ is assumed to be

$$\dot{\gamma}^s = \left\langle \frac{|\tau^s| - (\tau_c^s - J_e s)}{K} \right\rangle^n \operatorname{sign}(\tau^s)\,. \tag{6}$$

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The microdeformation γ_χ is related to the total cumulative slip $\gamma_{\text{cum}} = \sum_s |\gamma^s|$ via the relative cumulative slip e

$$e(\underline{\boldsymbol{X}}, t) = \gamma_{cum} - \gamma_\chi. \tag{7}$$

e measures the departure of the microdeformation γ_χ from the total cumulative slip, which will be associated with a cost in free energy potential.

It is assumed that the free energy potential ψ takes the following quadratic form:

$$\rho\psi = \frac{1}{2}\frac{\rho}{\rho_i}\underset{\sim}{\boldsymbol{E}}^e : \underset{\approx}{\boldsymbol{\Lambda}} : \underset{\sim}{\boldsymbol{E}}^e + \frac{1}{2}H_\chi e^2 + \frac{1}{2}A\underline{\boldsymbol{k}}.\underline{\boldsymbol{k}}\,. \tag{8}$$

As a results, one has

$$\underline{\boldsymbol{m}} = A\underline{\boldsymbol{k}} \quad \text{and} \quad s = H_\chi e = H_\chi(\gamma_{cum} - \gamma_\chi). \tag{9}$$

Considering the balance equation, it follows

$$s = \operatorname{div}\underline{\boldsymbol{m}} = A\operatorname{div}\operatorname{grad}\gamma_\chi = A\Delta_x\gamma_\chi, \tag{10}$$

which introduces the gradient effect in eq. (6).

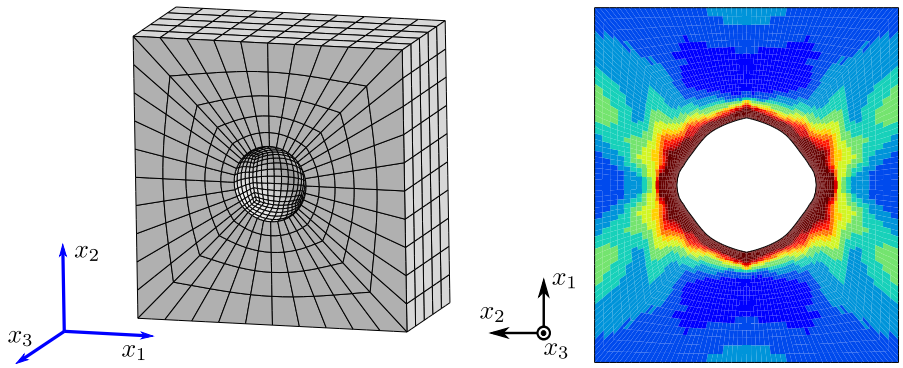
The free energy potential can also assume to be

$$\rho\psi = \frac{1}{2}\frac{\rho}{\rho_i}\underset{\sim}{\boldsymbol{E}}^e : \underset{\approx}{\boldsymbol{\Lambda}} : \underset{\sim}{\boldsymbol{E}}^e + \frac{1}{2}H_\chi e^2 + \frac{1}{2}\frac{\rho}{\rho_0}A\underline{\boldsymbol{K}}.\underline{\boldsymbol{K}}\,, \tag{11}$$

which leads to a linear relation in the reference configuration:

$$\underline{\boldsymbol{M}} = A\underline{\boldsymbol{K}} \quad \text{and} \quad s = A\operatorname{div}\left(\frac{\rho}{\rho_0}\underset{\sim}{\boldsymbol{B}}.\operatorname{grad}\gamma_\chi\right). \tag{12}$$

SIZE-DEPENDENT VOID GROWTH



(a) (b)

Figure 1: (a) 3D finite element mesh of voided unit cell. Only half of the mesh is shown. (b) Field of total cumulative slip, obtained by the local single crystal plasticity model, in the middle x_1-x_2 cross section of the unit cell for the [100]-[010]-[001] orientation at stress triaxiality $T = 3$.

The proposed model is used to investigate the size-dependent void growth by 3D finite element unit cell simulations (see fig. 1a). Void growth in single crystal matrix under triaxial loadings are simulated with different internal length scales. The evolution of void volume fraction, the overall stress-strain response, and the local plastic strain fields are compared to those obtained by classic single crystal plasticity. See fig. 1b for an example of unit cell simulation with local single crystal plasticity. The comparison of results can also be performed with those of dislocation dynamics and molecular dynamics simulations in the literature, e.g., [3].

References

[1] Aslan, O., Cordero, N. M., Gaubert, A., Forest, S.: Micromorphic approach to single crystal plasticity and damage. Int. J. of Eng. Sci., 49:1311-1325, 2011.

[2] Wulfinghoff S., Böhlke T.: Equivalent plastic strain gradient enhancement of single crystal plasticity: theory and numerics. Proc. of the Royal Society A, 468:2682-2703, 2012.

[3] Hussein, M., Borg, U., Niordson, C., Deshpande, V.: Plasticity size effects in voided crystals. J. of Mech. and Phy. of Solids, 56:114-131, 2008.