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Fourier-based spectral method solution to finite strain crystal plasticity with free surfaces

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ABSTRACT

A plastically dilatational material model is proposed that enables to simulate the mechanical response of non-compact geometries (containing free surfaces) by means of established spectral methods without any particular adaptations, i.e. in combination with arbitrary constitutive laws describing the remainder of the simulated geometry and under mixed boundary conditions. The versatility of this material model and more accurate representation of empty space in comparison to an isotropic elastic model employing low stiffness is demonstrated for the cases of void growth under biaxial extension and grain-scale deformation behavior of an oligocrystalline dogbone-shaped aluminum sample under uniaxial tension.

Classically, the crystal plasticity finite element method (CPFEM) has been the vehicle of choice to simulate and understand the mechanical behavior of engineering components with structural dimensions approaching the grain size of the intrinsic microstructure. Examples of such oligocrystalline mechanics can be found in the fields of lead-free solder joints, thin wires, cardiovascular stents, and mesostructured materials such as foams or photonic crystals. The spatial resolutions achievable by CPFEM within reasonable computation times are limited by the substantial numerical effort inherent in the FEM strategy to solve the underlying partial differential equation system. Spectral methods have emerged as an efficient [1–3] substitute for CPFEM [4–7], but only recently were improved sufficiently to overcome their unfavorable convergence when large gradients in mechanical properties are present [8,9]. This enhanced capability allows the mechanics of porous structures to be solved using spectral methods by replacing the open space (or voids) with soft material [10] in the simulated periodic domain. Examples of such simulations have been demonstrated in recent works [11–14]. The methodology used in these works tightly links the behavior of the spectral solution *algorithm* to the specifics of the constitutive behavior of each material point, i.e., making a binary distinction between how to address void and filled points. Furthermore, any nucleation of additional voids not yet present in the initial geometry will require to propagate the information about such a change in local constitutive behavior to the spectral solution algorithm. Such a rigid approach is akin to element elimination in FEM simulations of crack propagation, where a particular constitutive response, i.e. loss of stiffness, is treated through *ad hoc* modification of the geometry instead of properly at the constitutive level, as achieved by, for instance, cohesive zone elements. Following this spirit of keeping any boundary value problem solver as general as possible, i.e., independent of the constitutive material behavior that is simulated, voids should only distinguish themselves through their constitutive model, which, classically, has been vanishingly small elastic stiffness. Here, to describe void regions, a plastically dilatational material is proposed that enables simulations of non-compact geometries such as open or closed-cell foams, or other geometries with free surfaces, by means of established spectral methods without any particular adaptations.

A plastic plate with a circular inclusion under biaxial extension and a dogbone-shaped tensile sample of oligocrystalline aluminum serve to compare this dilatational material model to a low-stiffness isotropically elastic model of all void regions.

Constitutive model for void like regions. A finite strain framework incorporating two intermediate configurations is adopted, similar to the work of Tjahjanto et al. [15] and following Shanthraj et al. [16]. The total deformation gradient $\mathbf{F} = \mathbf{F}_e\mathbf{F}_i\mathbf{F}_p$ at each material point is multiplicatively decomposed into isochoric, and lattice preserving, plastic deformation $\mathbf{F}_p$, non-isochoric, but stress-free, dilatation $\mathbf{F}_i$, and elastic deformation $\mathbf{F}_e$, consecutively mapping the reference

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configuration into the "lattice" configuration ($\mathbf{F}_p$), then into the "intermediate" configuration ($\mathbf{F}_i$), and finally into the deformed one ($\mathbf{F}_e$). Only the elastic lattice distortion gives rise to stress, which takes the form $\mathbf{S}_p = \mathbb{C} : \frac{1}{2}\mathbf{F}_i^T(\mathbf{F}_e^T\mathbf{F}_e - \mathbf{I})\mathbf{F}_i$ in the lattice configuration and $\mathbf{S}_i = \mathbf{F}_i\mathbf{S}_p\mathbf{F}_i^T/\det(\mathbf{F}_i)$ in the intermediate one, with $\mathbb{C}$ being the fourth-order elastic stiffness tensor (in the lattice configuration). The stress $\mathbf{S}_i$ drives the dilatational velocity gradient $\mathbf{L}_i(\mathbf{S}_i, \boldsymbol{\eta}) = \dot{\mathbf{F}}_i\mathbf{F}_i^{-1}$, while $\mathbf{S}_p$ drives the plastic velocity gradient $\mathbf{L}_p(\mathbf{S}_p, \boldsymbol{\eta}) = \dot{\mathbf{F}}_p\mathbf{F}_p^{-1}$ and the evolution $\dot{\boldsymbol{\eta}}$ of internal state variables. The total velocity gradient follows as $\mathbf{L} = \mathbf{L}_e + \mathbf{F}_e\mathbf{L}_i\mathbf{F}_e^{-1} + \mathbf{F}_e\mathbf{F}_i\mathbf{L}_p\mathbf{F}_i^{-1}\mathbf{F}_e^{-1}$.

To capture the mechanical response of a void, an isotropic plasticity model that combines an isochoric response due to the deviatoric stress with a dilatational response due to the hydrostatic pressure (mean stress) is formulated. The kinetics and internal state parameterization of the model are inspired by the phenomenological crystal plasticity model introduced by Peirce et al. [17] that postulates a power-law relation and an internal deformation resistance, termed g.

Thus, in an isotropic setting, the strain rate $\dot{\epsilon}_p$ connected to isochoric deformation is given as

$$\dot{\epsilon}_p = \dot{\epsilon}_0\left(\frac{\sqrt{3J_2}}{Mg}\right)^n = \dot{\epsilon}_0\left(\sqrt{\frac{3}{2}}\frac{\parallel \mathbf{S}'_p \parallel}{Mg}\right)^n, \quad (1)$$

with J_2 as the second invariant of $\mathbf{S}'_p$ (deviatoric second PIOLA–KIRCHHOFF stress), stress exponent n, Taylor factor M, and $\parallel\cdot\parallel$ the FROBENIUS norm. The associated plastic velocity gradient $\mathbf{L}_p$, acting in the lattice configuration, is then formulated as

$$\mathbf{L}_p = \dot{\epsilon}_p\frac{\mathbf{S}'_p}{\parallel \mathbf{S}'_p \parallel} = \dot{\epsilon}_0\left(\sqrt{\frac{3}{2}}\frac{1}{Mg}\right)^n \mathbf{S}'_p \parallel \mathbf{S}'_p \parallel^{n-1}. \quad (2)$$

To mimic the dilatational response of a void region, a similar constitutive law but for the dilatational expansion rate $\dot{\epsilon}_i$ and the dilatational velocity gradient $\mathbf{L}_i$ is formulated in the intermediate configuration

$$\mathbf{L}_i = \dot{\epsilon}_i\frac{\mathbf{I}}{\parallel \mathbf{I} \parallel} = \dot{\epsilon}_0\left(\frac{p}{Mg}\right)^n \mathbf{I} \quad (3)$$

where p is the hydrostatic pressure calculated from $\mathbf{S}_i$, and $\mathbf{I}$ is the 2nd order identity tensor. The evolution of deformation resistance follows

$$\dot{g} = M\dot{\epsilon}_p h_0\left|1 - \frac{g}{g_\infty}\right|^a \ \text{sign}\ \left(1 - \frac{g}{g_\infty}\right) \quad (4)$$

where a, $\dot{\epsilon}_0$, and h_0 are adjustable parameters.

Solution to mechanical boundary value problem. To solve the mechanical boundary value problem of static equilibrium, the finite strain spectral method outlined in [3,9] and implemented as part of the Düsseldorf Advanced Material Simulation Kit (DAMASK) is used. The constitutive law described above was integrated into the flexible material point model offered by DAMASK. Since the solution fields resulting from the spectral method are a superposition of a homogeneous and a fluctuating part, where the mean value of the latter vanishes over the domain, any boundary conditions can only prescribe the average (homogeneous) fields.

Comparison between a dilatational and soft-elastic void. Using a plastically isotropic plate with a circular void at its center as an exemplary case, the response of the dilatational material model outlined above is contrasted to an alternative description of the void as a (relatively) soft and purely elastic inclusion. Table 1 lists the material parameters used to model the plastic plate as well as the elastic and the dilatational version of the void. The largest elastic stiffness constant C_{11} of the dilatational and elastic version of the void is scaled down, respectively, one and three orders of magnitude relative to the plate surrounding it, with C_{12} and C_{44} calculated such that elastic isotropy and vanishing Poisson ratio for the void is ensured in both versions. The flow stress of the dilatational version of the void is set to be two orders of magnitude lower than that of the plate material. The chosen values reflect a compromise between vanishing stress in void regions and the associated computational cost, as detailed in the supplementary material. A 512 × 512 × 1 regular grid is used to discretize the fully periodic geometry, resulting in about 2100 grid points within the void taking up an area fraction of 0.8%. The plate is subjected to biaxial tensile elongation along the x and y direction (see top row of Fig. 1), which is enforced by fixing eight of the components of the average deformation gradient rate and requiring the remaining complementary first PIOLA-KIRCHHOFF stress component P_{zz} to vanish, i.e.

Table 1
Material parameters; elastic constants C_{ij}, reference strain rate $\dot{\epsilon}_0$, stress exponent n, initial and saturation flowstress g_0 and g_∞, hardening parameters h_0 and a, and Taylor factor $M = 3$.

	Plate	Void		
		Elastic	Dilatational	
C_{11}	100	0.1	10	GPa
C_{12}	60	0	0	GPa
C_{44}	30	0.05	5	GPa
$\frac{2C_{44}}{C_{11}-C_{12}}$	1.5	1	1	
$\dot{\epsilon}_0$	10^{-3}		10^{-3}	s^{-1}
n	20		20	
g_0	30		0.3	MPa
g_∞	60		0.6	MPa
a	2		2	
h_0	80		1	MPa

$$\frac{\langle\dot{\mathbf{F}}\rangle}{10^{-3}\mathrm{s}^{-1}} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & * \end{bmatrix} \quad \text{and} \quad \frac{\langle\mathbf{P}\rangle}{\mathrm{Pa}} = \begin{bmatrix} * & * & * \\ * & * & * \\ * & * & 0 \end{bmatrix}, \quad (5)$$

where '*' indicates that stress (or deformation) needs to be iteratively adjusted since deformation (or stress) is prescribed. In the simulations, the conditions of Eq. (5) are maintained for 400 increments of 1 s each (such that the final $\langle F\rangle_{xx} = \langle F\rangle_{yy} = 1.4$).

The elastic and dilatational version of the void are contrasted in the left and right column of Fig. 1, showing the simulation results at the final simulation step in terms of deformed geometry, determinant of deformation gradients (i.e. relative change in volume), hydrostatic stress, and VON MISES stress. The two cases reveal markedly different results. For the same final planar geometry (second row), the dilatational void expands to about six times its original diameter, while the purely elastically modeled void only about doubles its diameter. As the volume of the plastic plate is preserved, its final thickness is about 10% smaller when containing the elastically modeled void. The volumetric expansion of the void is fully carried by $\det(\mathbf{F}_e)$ for the elastic version, whereas the values of $\det(\mathbf{F}_e)$ are minute compared to $\det(\mathbf{F}_i)$ in the dilatational void version (third and fourth row). Since only the hydrostatic *elastic* strain connected to $\det(\mathbf{F}_e)$, but not $\det(\mathbf{F}_i)$, is giving rise to a hydrostatic stress $\sigma_{hyd} = K\epsilon_{hyd}$, with $K = 0.43$GPa, the σ_{hyd} inside the elastic void is much larger than inside the dilatational void and even exceeds the hydrostatic stress experienced by the surrounding plastic plate (row five). To the contrary, the dilatational void does not exhibit any appreciable hydrostatic stress as well as deviatoric stress (last row) since it is *plastically* growing in volume at a flowstress much lower than the flowstress of the plastic plate.