Minimal gradient-enhancement of classical crystal plasticity: finite-element treatment and size effects

Stanisław Stupkiewicz[1], **Henryk Petryk**[1]

[1]*Insitute of Fundamental Technological Reaserch (IPPT), Polish Academy of Sciences, Pawinskiego 5B, 02-106 Warsaw, Poland*
e-mail: ssupkie@ippt.pan.pl

Abstract

A novel 'minimal' framework for gradient-enhanced crystal plasticity has been developed with the aim to describe the effect of slip-rate gradients in a possibly simple manner. The basic assumptions adopted are consistent with phenomenological laws that are well-established in materials science. The model is formulated in the framework of classical continua, and the enhancement amounts to extending only the hardening law. Direct finite-element implementation of the model is not straightforward, and the present finite-element treatment relies on introducing non-local slip rates that provide a global continuous approximation of the local ones. The model has been applied to three-dimensional simulations of spherical indentation of a Cu single crystal, and the predicted indentation size effect shows a good agreement with that observed experimentally, even though there is no adjustable length-scale parameter.

Keywords: gradient plasticity, geometrically necessary dislocations, size effects, indentation, finite element method

1. Introduction

Several strain-gradient theories of crystal plasticity have been recently proposed to describe the size effects that accompany plastic slip at small length scales. Recently, we have proposed a minimal gradient-enhancement of the classical theory of plasticity of single crystals [1, 2] with the aim to describe the most essential size effects in a possibly simple manner. The essence of the proposed modification is in extending only the evolution equations for critical resolved shear stresses by a single non-conventional term involving slip-rate gradients [3].

The model has been formulated in the framework of classical continua, and as such it does not involve any additional balance equations. As shown in [4], an analytical solution describing the boundary layer in a constrained half-space can be found directly with no additional treatment. At the same time, direct finite element implementation of the model is not straightforward, and the present implementation relies on introducing non-local slip rates that provide a global continuous approximation of the corresponding local slip rates. The model has been applied to three-dimensional simlations of fcc single crystals. It has been found [4] that the experimentally observed indentation size effect in a Cu single crystal is captured correctly even though there is no adjustable length-scale parameter. The analytical solution mentioned above has also been used to show that the finite-element solution converges to the analytical one as the mesh is refined.

2. Classical crystal plasticity model

The classical theory of crystal plasticity at finite strain is based on the multiplicative decomposition of the deformation gradient $\mathbf{F}$, where the plastic part of deformation is assumed to result from plastic slip on individual slip systems,

$$\mathbf{F} = \mathbf{F}^{*}\mathbf{F}^{\mathrm{p}}, \qquad \mathbf{L}^{\mathrm{p}} = \dot{\mathbf{F}}^{\mathrm{p}}\mathbf{F}^{\mathrm{p}^{\mathrm{T}}} = \sum_{\alpha} \dot{\gamma}_{\alpha}\, \mathbf{s}_{\alpha} \otimes \mathbf{m}_{\alpha}, \tag{1}$$

where $\mathbf{s}_\alpha$ and $\mathbf{m}_\alpha$ are fixed orthogonal unit vectors that specify the slip direction and slip-plane normal, respectively. The yield criterion is formulated for each slip system in terms of the respective resolved shear stress $\tau_\alpha = \mathbf{M} \cdot (\mathbf{s}_\alpha \otimes \mathbf{m}_\alpha)$, where $\mathbf{M}$ is the Mandel stress tensor, and in terms of the critical resolved shear stress τ_α^{c}, namely

$$\tau_\alpha \le \tau_\alpha^{\mathrm{c}}, \qquad \dot{\gamma}_\alpha \ge 0, \qquad \dot{\gamma}_\alpha \tau_\alpha = 0. \tag{2}$$

Evolution of the critical resolved shear stress is governed by the anisotropic hardening law,

$$\dot{\tau}_\alpha^{\mathrm{c}} = \theta \sum_{\beta} q_{\alpha\beta} \dot{\gamma}_\beta, \tag{3}$$

where $q_{\alpha\beta}$ are dimensionless parameters describing self and latent hardening, θ is the instantaneous isotropic hardening modulus,

$$\theta = \theta_\tau(\tau), \qquad \dot{\tau} = \theta\dot{\gamma}, \qquad \dot{\gamma} = \sum_{\alpha} \dot{\gamma}_\alpha, \tag{4}$$

and $\theta_\tau(\tau)$ is a constitutive function.

3. Minimal gradient enhancement of the hardening law

In the proposed minimal gradient-enhancement, the slip-rate gradients are assumed to affect only the flow stress τ, i.e. the isotropic part of the critical resolved shear stress, so that the corresponding hardening rule $(4)_2$ becomes

$$\dot{\tau} = \theta(\dot{\gamma} + \ell\dot{\chi}), \tag{5}$$

and thus the anisotropic hardening law (3) is generalized to

$$\dot{\tau}_\alpha^{\mathrm{c}} = \theta\Big(\sum_{\beta} q_{\alpha\beta}\dot{\gamma}_\beta + \ell\dot{\chi}\Big). \tag{6}$$

Here, ℓ is the characteristic length that has been derived in the following simple explicit form,

$$\ell = \frac{a^2\mu^2 b}{2\tau\theta}, \tag{7}$$

and $\dot{\chi}$ is the effective plastic slip-rate gradient which is a function of slip-rate gradients $\nabla\dot{\gamma}_\alpha$, see [3] for details. Notably, the length-scale parameter ℓ of the form (7) possesses a direct physical interpretation that is frequently missing is other gradient-plasticity models, see [3]. The enhanced hardening law (5)-(6) has been derived by referring to the concept of the split of

the total dislocation density ρ into the densities of statistically-stored and geometrically-necessary dislocations and by exploiting the classical Taylor formula ($\tau = a\mu b\sqrt{\rho}$) in a rate form. Importantly, a, μ and b are known parameters, hence the above gradient-enhancement does not require any additional parameters with respect to the usual hardening law.

4. Finite-element treatment

In the finite-element implementation, the need to compute the slip-rate gradients constitutes the main difference with respect to the implementation of the usual non-gradient crystal plasticity models. The model is formulated in the framework of classical continua so that it involves no additional balance equations, and in that respect it differs from the other gradient crystal plasticity models. The present finite-element treatment relies on introducing non-local slip rates $\dot{\bar{\gamma}}_\alpha$ that provide a global continuous approximation of the local slip rates $\dot{\gamma}_\alpha$, through the following averaging equation

$$\dot{\bar{\gamma}}_\alpha - l_h^2 \nabla^2 \dot{\bar{\gamma}}_\alpha = \dot{\gamma}_\alpha, \tag{8}$$

where ∇^2 denotes the Laplace operator, and l_h is a numerical parameter of the dimension of length which is independent of the physical length scale ℓ and has been assumed proportional to the element size.

Further aspects of the present finite-element implementation involve: (i) a rate-independent regularization of the yield criterion (2) such that the well-known problems related to indeterminacy in selection of active slip systems are avoided; (ii) monolithic solution scheme in which the problem is solved simultaneously with respect to displacements and non-local slip rates; (iii) exact linearization by employing the automatic differentiation (AD) technique; (iv) automatic code generation using the *AceGen/AceFEM* system.

5. Sample results

An analytical solution to the problem of shearing of a constrained half-space has been used to validate the computational treatment based on the averaging equation (8) and the computer implementation itself. Subsequently, the model has been applied to simulate spherical indentation of Cu single crystal. Figure 1 shows the detail of the deformed mesh and the distribution of the norm of dislocation density tensor $\mathbf{G}$ [5], i.e. the finite-strain counterpart of the Nye's tensor. Figure 2 illustrates the predicted size effect which shows a very good agreement with experimental data [6] in spite of the absence of any adjustable length-scale parameter in the proposed framework.

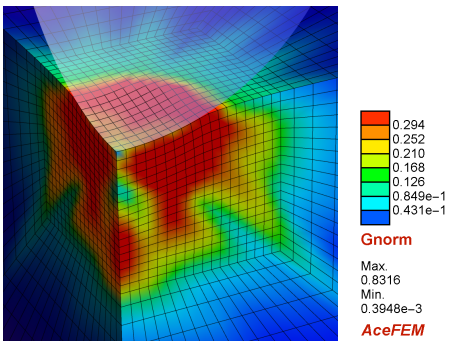

Figure 1: Spherical indentation of (001)-oriented Cu single crystal: norm of the dislocation density tensor $\mathbf{G}$ shown in the deformed configuration (indenter radius $R = 2\,\mu$m).

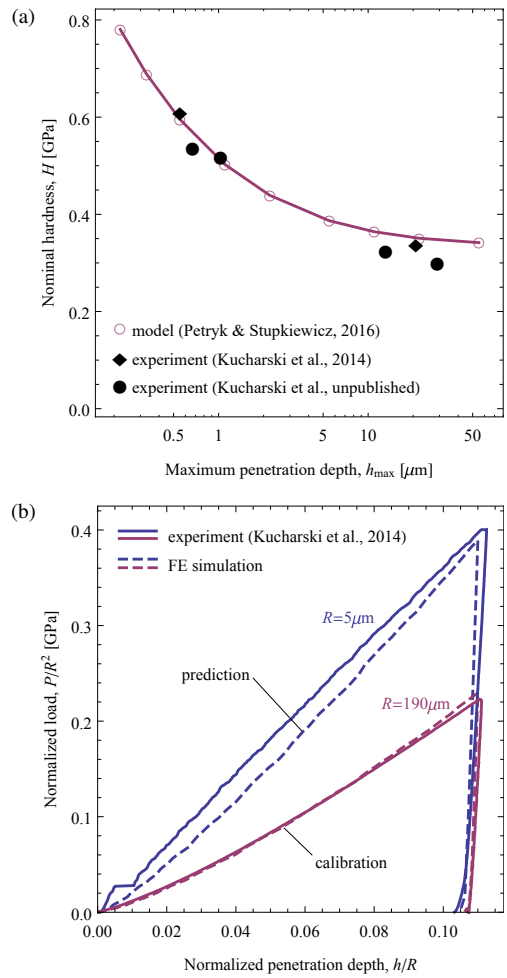

Figure 2: Indentation size effect: (a) dependence of hardness on the maximum penetration depth at fixed ratio $h_{\max}/R = 0.11$; (b) normalized size-dependent load–penetration curves.

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