PAMM · Proc. Appl. Math. Mech. **10**, 351 – 352 (2010) / **DOI** 10.1002/pamm.201010168

Gradient Plasticity for Single Crystals

Stephan Wulfinghoff[1,*] and **Thomas Böhlke**[1,**]

[1] Institute of Engineering Mechanics (Chair for Continuum Mechanics), Karlsruhe Institute of Technology (KIT), PO Box 6980, 76128 Karlsruhe, Germany

The kinematic relationship between classical single crystal kinematics and geometrically necessary dislocations will be clarified by a demonstrative example. The starting point for the dynamics is the contribution of geometrically necessary dislocations to the free energy, which leads to a kinematic hardening law. A simple two-dimensional shear example will be discussed.

1 Introduction

Metals exhibit strong size effects, when the length scale associated with inhomogeneous plastic deformation is in the order of microns. This effect has been demonstrated in various experiments using micro-specimens. Typical examples are the compression of micro-pillars [9], indentation tests [5] or torsion of thin wires [3]. In all of these examples the strength of the material is underestimated by classical continuum plasticity theories, which possess no internal length scale.

2 Kinematics

A crucial observation is that all experiments suggest a strong correlation between the unexpected increase in strength and the spatial variation, i.e. inhomogeneity, of the plastic deformation of small specimens [3]. Hence, from a phenomenological point of view, it is reasonable to assume the material strength to depend on the gradient of some plastic strain variable and thereby introduce an internal length scale.
In 1953, Nye [7] showed that the gradients of the plastic slips γ_α of a single crystal (α is the index of the slip system) also have a physical meaning: they represent a subsection of the underlying dislocation structure, which is regularly called Geometrically Necessary Dislocations (GNDs).

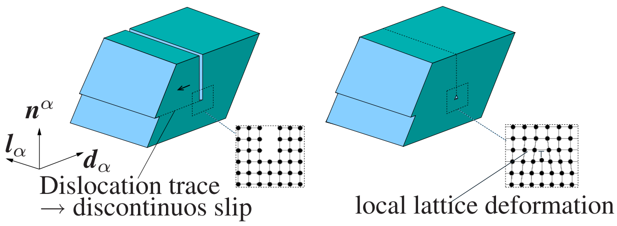

Fig. 1 Introduction of a discrete dislocation into a homogeneously deformed single crystal

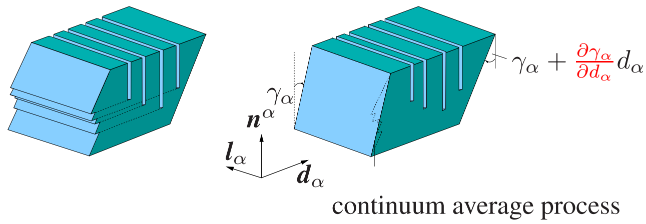

Fig. 2 Typical GND-example: several parallel edge dislocations of equal sign lead to a non-vanishing strain gradient

Fig. 1 shows the introduction of an edge dislocation into a perfect single crystal. The illustrated discontinuous slip as well as the local lattice deformation are not captured precisely by the classical continuum theory as they are averaged. Fig. 2 shows, as an example for a typical GND-configuration, the introduction of a set of parallel edge dislocations into a perfect single crystal and the average procedure of the continuum representation. Moreover, it can be seen from Fig. 2, that this dislocation configuration leads to a nonvanishing strain gradient, which the other way round was by many authors interpreted as dislocation density $\rho^\alpha_\vdash := -\partial\gamma_\alpha/\partial d_\alpha$ (e. g. Gurtin [4], Acharya [1] or Fleck [3]). Similar considerations lead to a strain gradient due to screw dislocations $\rho^\alpha_\odot := \partial\gamma_\alpha/\partial l_\alpha$. It can be shown, that these (signed) densities represent the complete GND-state (Nye's tensor) of the crystal.
GNDs constitute a limited geometric representation of the underlying dislocations structure. Energetically, however, they are much more representative, because their interaction energy can by far succeed the sum of the discrete self-energies, while the opposite is the case for dislocation arrangements, which are not captured by $\rho^\alpha_\vdash$ and $\rho^\alpha_\odot$ (statistically stored dislocations).

* Stephan Wulfinghoff, E-mail: wulfinghoff@itm.uni-karlsruhe.de, Phone: +00 49 721 608-8133, Fax: +00 49 721 608-4187
** Thomas Böhlke, E-mail: boehlke@itm.uni-karlsruhe.de

3 Dynamics

The deformation field of discrete dislocations can be interpreted to be averaged by the continuum plasticity theory, consequently the associated discrete local strain energy can be assumed to be underestimated. Hence, it is reasonable to add a "correction term" to the total free energy density $\psi = \psi_e(\boldsymbol{\varepsilon}_e) + \psi_d(\rho_{\vdash}^{\alpha}, \rho_{\odot}^{\alpha})$, which (with the arguments from above) only takes the energy of GNDs into account and was called defect energy by Gurtin [4] (for clearness the isotropic hardening potential is here set to zero). Similar free energy approaches were introduced by several authors (e. g. Menzel and Steinmann [6] or Reese and Svendsen [8]).
Using this ansatz, the evaluation of the principle of virtual displacements yields as field equations the classical linear momentum balance $\mathrm{div}(\boldsymbol{\sigma}) + \rho \boldsymbol{f} = \boldsymbol{0}$ (with the stress tensor $\boldsymbol{\sigma}$, the mass density ρ and the body force $\boldsymbol{f}$) and an expression for the dissipative force $\tau_\alpha^{\mathcal{D}} = \tau_\alpha - \tau_\alpha^B$, where $\tau_\alpha^{\mathcal{D}}$ is defined by the classical decoupled model of the total dissipation $\mathcal{D}_{tot} = \sum\limits_\alpha \mathcal{D}(\dot\gamma_\alpha) = \sum\limits_\alpha \tau_\alpha^{\mathcal{D}} \dot\gamma_\alpha$. Here, τ_α is the resolved shear stress of slip system α and

$$\tau_\alpha^B := -\,\mathrm{div}\left(-\frac{\partial \psi_d}{\partial \rho_{\vdash}^{\alpha}} \boldsymbol{d}_\alpha + \frac{\partial \psi_d}{\partial \rho_{\odot}^{\alpha}} \boldsymbol{l}_\alpha\right). \tag{1}$$

can be interpreted as a backstress resulting from the presence of GNDs.

4 Example: Two-Dimensional Shear Test

To achieve a complete set of differential equations, the dissipation $\mathcal{D}(\dot\gamma_\alpha)$, the strain energy $\psi_e(\boldsymbol{\varepsilon}_e)$ and the defect energy $\psi_d(\rho_{\vdash}^{\alpha}, \rho_{\odot}^{\alpha})$ must be constitutively modeled. For the numerical computation, a classical quadratic approach is chosen for $\psi_e(\boldsymbol{\varepsilon}_e)$, the dissipation $\mathcal{D}(\dot\gamma_\alpha)$ is modelled such that the dissipative force $\tau_\alpha^{\mathcal{D}}(\dot\gamma_\alpha)$ follows a classical power law and two decoupled approaches $\psi_d = c_n \sum_\alpha |\rho_{\vdash}^{\alpha} L|^n$ with $n = 2$, which was also analysed by Gurtin, and $n = 4$ (a more progressive approach) are compared to identify the physical meaning of the exponent n (c_n is another material property and L is a normalization parameter).
The analysed strip has two slip systems, the slip directions of which are $\pm 60°$ with respect to the horizontal. The displacement of the top is a prescribed function $u_0(t)$. The results (see Fig. 3) show, that the first ansatz ($n = 2$) leads to smooth strain

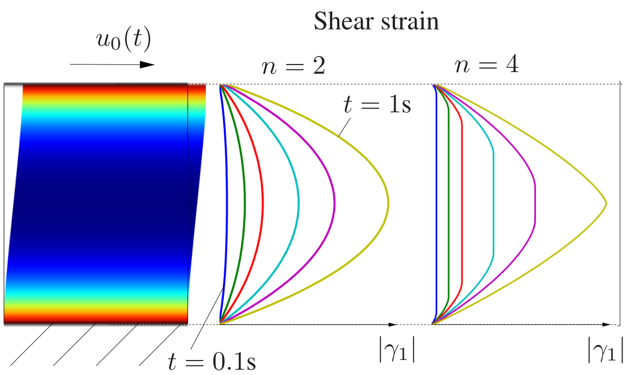

Fig. 3 Evolution of the absolute value of the plastic shear strain $|\gamma_1|$ for $n = 2$ and $n = 4$

curves, which can be explained by piled-up GNDs at the boundaries, which have a long-range influence from the boundary on the bulk behaviour due to the smooth quadratic approach.
In contrast, the progressive ansatz (with $n = 4$) generates a clearer distinction between bulk and boundaries and thereby leads to a clear hardening zone at the boundaries, which grows during the deformation process. This behaviour results from the dislocation pile-ups, which now constitute "harder" obstacles, i.e. show a weaker long-range but a stronger short-range influence.

References

[1] A. Acharya, J. Mech. Phys. Solids **49**, 761–784 (2001).

[2] P. Cermelli and M. E. Gurtin, Int. J. Solids Struct., **39**, 6281–6309 (2002).

[3] N. A. Fleck, G. M. Muller, M. F. Ashby and J. W. Hutchinson, Acta metall. mater. **42**, 475–487 (1993).

[4] M. E. Gurtin, L. Anand, and S. P. Lele, J. Mech. Phys. Solids **55**, 1853–1878 (2007).

[5] Q. Ma and D. R. Clarke, J. Mater. Res. **10**, 853–863 (1995).

[6] A. Menzel and P. Steinmann, J. Mech. Phys. Solids **48**, 1777–1796 (2001).

[7] J. F. Nye, Acta Metall. **1**, 153–162 (1953).

[8] S. Reese and B. Svendsen, Kluwer Series on Solids Mechanics and Its Application **108**, 141–150 (2003).

[9] M. D. Uchic, D. M. Dimiduk, J. N. Florando, W. D. Nix, Science **305**, 986 (2004).

