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Instability origin of subgrain formation in plastically deformed materials

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ABSTRACT

The review is focused on two methods of formulation and solution of the subgrain formation problem: an energetic approach and a model of incremental deformations. Both methods are based on a reduced single slip version of crystal plasticity. The mathematical analysis of the energetic approach is done for a single slip model only; in the incremental approach the deformation are assumed small, hence, multi slip can be treated as a sum of single slips. The energetic approach has been employed in analysis of the crystal plasticity model of shear and kink bands. The incremental higher strain gradient model provides an insight into an initial stage of the subgrain formation and the mechanism controlling the subgrain size.

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1. Introduction

Formation of misoriented structural elements, typically in a form of subgrains or misoriented dislocation cells (in the following text we use the short term "subgrains"), is a fundamental process of dislocation patterning accompanying plastic deformation [1]. Subgrains can be found in plastically deformed metals on very different scales, from sub-micron subgrains induced by severe plastic deformation to mm-size subgrains in metals deformed near the melting temperature. The importance of the phenomenon is recognized by considering the process of work hardening, which is clearly correlated with formation of subgrains.

Conventional explanations of formation of subgrains assume either a pre-existing structure of obstacles in the crystal [2] or use statistical arguments [3,4]. In the statistical approach misoriented dislocation structures are considered as a random accumulation process of excess dislocations in dislocation boundaries. Two types of boundaries are distinguished: ordinary boundaries are assumed to be caused by a statistical mutual trapping of dislocations and excess dislocations are accumulated by stochastic reasons only, whereas a different activation of slip systems is expected on both sides of planar dislocation boundaries termed geometrically necessary boundaries. As noted in [4], such imbalance in the activation of slip systems between different regions can arise from an intrinsic instability of the deformation process.

As shown in the present paper, the reason for the plastic deformation being non-homogeneous is a possible instability of homogeneous plastic flow driven by energy minimization. The long-range internal stresses which would be set up by deformation of a single volume element are reduced by deformation and rotation of neighboring volume elements [5,6]. According this alternative approach, dislocations are forced by the laws of non-linear continuum mechanics to arrange themselves into patterns of varying density. From this point of view, the intrinsically developed inhomogeneity of plastic deformation is

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the basic reason for subgrain formation. In addition to the macroscopic instabilities of plastic deformation in the form of necking or shear band formation, there is an instability in the form of internal buckling [7–9]. This instability is made possible by the inherent anisotropy of plastic deformation. Under certain circumstances, more energy is needed in the uniform plastic deformation than is required to initiate an internal mode of buckling. In such a case, the internal instability makes its appearance. It has been suggested to interpret the internal instability of homogeneous plastic flow in terms of the formation of subgrains in [10–13]. It has been shown that the internal buckling leads to the build up of lattice misorientations between neighboring volume elements. The periodic patterns of excess dislocations necessary to accommodate the lattice misorientations were interpreted as the beginning of subgrain formation.

The aim of this work is to review shortly the latter approach, focusing attention on two methods of formulation and solution of the subgrain formation problem: an energetic approach, Section 3, and a model of incremental deformations, Section 4. The methods are of a different origin and remain disjointed at present using even different scientific language; hopefully they will converge in the future. Both methods are based on a reduced single slip version of crystal plasticity. The detail mathematical analysis of the energetic approach is done for a single slip model only; in another energetic attempt [14] multi slip is treated as a succession of single slips. In the incremental approach the deformation are assumed small, hence, multi slip can be treated as a sum of single slips.

The energetic method employed in crystal plasticity has been inspired by the very successful mathematical theory of rate-independent processes [15]. The energetic approach in crystal plasticity leads to a problem of a minimization of an energy functional subjected to boundary conditions and dissipation inequality. The minimization may result in a spontaneous structural inhomogeneity (subgrains can be treated as a composition of lamellar deformation modes, Sections 3 and 4). The exact mathematical proof of the existence of lamellar structures was given by Conti and Theil [16] for a single slip rigid-plastic model with zero hardening (elastic deformation is reduced to lattice rotations and the hardening coefficient $h = 0$). Moreover, they predicted existence of a boundary layer which accommodates the lamellar structure to displacement boundary conditions. Their results indicate that the dominant effect, which causes formation of the lamellar structure, is the minimization of the dissipative energy (the rigidity excludes the elastic energy and $h = 0$ causes no change of the dislocation stored energy). The energetic approach has been employed in analysis of the crystal plasticity model of shear and kink bands [17] summarized in Section 3.

The other method presented in Section 4 is based on mechanics of incremental deformations proposed by Biot [9]. The theory provides rigorous and completely general equations governing the dynamics and stability of solids and fluids under initial stress in the context of small perturbations. It is applicable to anisotropic, viscoelastic, or plastic media. In Section 4 Biot's approach is employed in an analysis of a strain gradient rigid-plastic model of crystalline solids [13]. It provides an insight into an initiation of the subgrain formation and into the mechanism controlling the subgrain size. In order to introduce a physically relevant scale to our problem we assume, following earlier works of Dillon and Kratochvíl [18], that the energy in the system depends also on the gradient of the plastic variables. The gradient terms represent non-local effects caused by short-range interactions among dislocations. It is not clear, however, which function of the gradient should be used. We refer to Kratochvíl and Sedláček [19], and to Groma and Bakó [20] for attempts to derive it from statistics of discrete dislocations which reveal the complexity of the problem. Constitutive relations of gradient continua are advocated e.g. by Gurtin [21], Mainik and Mielke [22], or Conti and Ortiz [14] and also investigated in [23] mostly in relation to the so-called size effect. Mathematical theory of rate-independent isothermal evolution with gradients of plastic variables is developed in [24]. An interesting recent contribution by Gurtin and Anand [25] discusses the flow rules for rate-independent gradient plasticity proposed by Fleck and Hutchinson. As a key result, they showed that the flow rule of Fleck and Hutchinson [26] is incompatible with thermodynamics unless its nonlocal term is skipped. A physically sound gradient plasticity theory within the framework of small deformations is developed in [27]. A survey of non-local models in plasticity appeared in Bažant and Jirásek [28]. Numerical approaches are surveyed in [29,30].

2. Crystal plasticity

The energetic and incremental methods are based on the crystal plasticity framework introduced in classical papers, e.g. [31,32] and recalled e.g. in [21]. In the present paper the rigid-plastic, rate independent approximation to crystal plasticity is considered; this framework seems to be sufficient to catch the essence of the subgrain formation problem.

Each material point of a crystal can be identified by its position in a reference configuration. The point which was at position $\boldsymbol{X}$ in the reference configuration is in the current configuration in time t in the position $\boldsymbol{x}(\boldsymbol{X},t)$. The difference $\boldsymbol{u} = \boldsymbol{x} - \boldsymbol{X}$ is the displacement of the material point $\boldsymbol{X}$. The deformation of the material is described by the transformation $\boldsymbol{F}$ of an infinitesimal material fiber from the reference to the current configuration,

$$\mathrm{d}\boldsymbol{x} = \boldsymbol{F}\mathrm{d}\boldsymbol{X}. \tag{1}$$

Assuming that $\boldsymbol{x}(\boldsymbol{X},t)$ is a continuous and differentiable vector field, this transformation can be introduced as the deformation gradient $\boldsymbol{F} = \partial\boldsymbol{x}/\partial\boldsymbol{X} = \boldsymbol{I} + \partial\boldsymbol{u}/\partial\boldsymbol{X}$, where $\boldsymbol{I}$ is the second order identity tensor. In the rigid-plastic approximation the crystal lattice can (rigidly) rotate but it is not (elastically) strained. The plastic deformation of a crystal can be decomposed in two steps. First, the material flows through the crystal lattice by shearing along the active slip systems to reach an intermediate configuration. This step is described by the plastic deformation gradient $\boldsymbol{F}^{\mathrm{p}}$, $\det\boldsymbol{F}^{\mathrm{p}} = 1$. Second, the plastic deformation $\boldsymbol{F}^{\mathrm{p}}$ is

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