International Journal of Plasticity 64 (2015) 1–25

Contents lists available at ScienceDirect

International Journal of Plasticity

journal homepage: www.elsevier.com/locate/ijplas

The stored energy of cold work, thermal annealing, and other thermodynamic issues in single crystal plasticity at small length scales

Lallit Anand [a,*], Morton E. Gurtin [b], B. Daya Reddy [c]

[a] Department of Mechanical Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139, USA
[b] Department of Mathematical Sciences, Carnegie Mellon University, Pittsburgh, PA 15213, USA
[c] Department of Mathematics and Applied Mathematics, University of Cape Town, 7701 Rondebosch, South Africa

ARTICLE INFO

Article history:
Received 7 June 2014
Received in final revised form 26 July 2014
Available online 6 August 2014

Keywords:
A. Dislocations
Thermomechanical processes
B. Crystal plasticity

ABSTRACT

This paper develops a thermodynamically consistent gradient theory of single-crystal plasticity using the principle of virtual power as a paradigm to develop appropriate balance laws for forces and energy. The resulting theory leads to a system of microscopic force balances, one balance for each slip system, and to an energy balance that accounts for power expended during plastic flow via microscopic forces acting in concert with slip-rates and slip-rate gradients. Central to the theory are an internal energy and entropy, plastic in nature, dependent on densities that account for the accumulation of glide dislocations as well as geometrically necessary dislocations – and that, consequently, represent quantities associated with cold work. Our theory allows us to discuss – within the framework of a gradient theory – the fraction of plastic stress-power that goes into heating, as well as the reduction of the dislocation density in a cold-worked material upon subsequent (or concurrent) thermal annealing.

1. Introduction

The plastic deformation of metals when conducted at temperatures less than $\approx 0.35\,\vartheta_m$, where ϑ_m is the melting temperature of the material in degrees Kelvin, is called *cold-working*.[1] In this temperature range the underlying mechanism of plastic deformation of metal single crystals is the glide of *dislocations*, which are crystalline line-defects, on certain crystallographic slip systems in the material. This process of plastic deformation is usually accompanied by a rapid multiplication (and eventual saturation) in the number of dislocations. However, the dislocations so produced are seldom homogeneously distributed in the material; instead they form a heterogeneous "cell-structure", with cell-walls made of clusters of dislocations and with cell-interiors which are relatively free of dislocations. The increased dislocation density and resulting dislocation cell-structure leads to an increased resistance to subsequent plastic flow. This increase in the resistance to plastic flow is called *strain-hardening*.

When a metal is cold-worked, most of the plastic work done is converted into heat, but a certain portion is stored in the material. In nominally pure metals, the dominant contribution to the stored energy is the energy associated with the evolving dislocation density and sub-structure of the material. The dislocations – being line defects in the crystalline

* Corresponding author.
E-mail address: anand@mit.edu (L. Anand).

[1] Plastic deformation in the temperature range ≈ 0.35 through $\approx 0.5\,\vartheta_m$ is called *warm-working*, while *hot-working* refers to the plastic deformation of metals into desired shapes at temperatures in the range of ≈ 0.5 through $\approx 0.9\,\vartheta_m$.

http://dx.doi.org/10.1016/j.ijplas.2014.07.009
0749-6419/

lattice – cause distortion of the lattice and thereby store a certain amount of elastic energy, which is called the *stored energy of cold-work*.

The microscale dislocation substructure in a ductile metal that has been cold-worked and unloaded, is generally unstable. Upon subsequent heating to a temperature in the range ≈ 0.35 through $\approx 0.5\,\vartheta_m$ it undergoes a restoration process called *recovery* or *annealing*, during which the dislocation configurations in the cell-walls annihilate, the cell-walls sharpen, and the stored energy is released.[2]

The extensive literature on the experimental and theoretical developments concerning the stored energy of cold work has been reviewed by Bever et al. (1973). The reported values of the ratio of the stored energy to that expended plastically ranges from near zero to approximately 15 percent (cf., e.g., Farren and Taylor, 1925; Taylor and Quinney, 1934; Taylor and Quinney, 1937). A discussion of the notion of stored energy of cold work and its ramifications, within a one-dimensional conventional (non-gradient) theoretical framework, is the focus of an important study of Rosakis et al. (2000). For a recent two-dimensional, discrete-dislocation-plasticity-based numerical study regarding the stored energy of cold work, see Benzerga et al. (2005).

From a fundamental theoretical standpoint, mechanical and thermal effects should be coupled within a consistent thermodynamical framework. Accordingly, the purpose of this paper is to formulate a *thermo-mechanically coupled gradient theory of single-crystal plasticity* at low homologous temperatures, $\vartheta \lessapprox 0.35\,\vartheta_m$. In this temperature range plastic flow of metals is only weakly dependent on the strain-rate; accordingly we limit our considerations to a *rate-independent theory*. Central to our continuum-mechanical theory are an internal energy and entropy, plastic in nature, dependent on dislocation densities that account for the accumulation of statistically-stored as well as geometrically-necessary dislocations – and that, consequently, represent quantities associated with cold work. Our theory allows us to meaningfully discuss – within the framework of a gradient crystal plasticity theory – the fraction of plastic stress-power that goes into heating, as well as the reduction of the dislocation density in a cold-worked material upon subsequent thermal annealing.

2. Basic equations

2.1. Kinematics

We begin with the requirement that the displacement gradient admit a decomposition

$$\nabla\mathbf{u} = \mathbf{H}^e + \mathbf{H}^p \qquad \left(u_{i,j} = H^e_{ij} + H^p_{ij}\right) \tag{2.1}$$

in which $\mathbf{H}^e$, the *elastic distortion*, represents stretch and rotation of the underlying microscopic structure, here a lattice, and $\mathbf{H}^p$, the *plastic distortion*, represents the local deformation of material due to the formation and motion of dislocations through that structure. We define *elastic* and *plastic strains* $\mathbf{E}^e$ and $\mathbf{E}^p$ as the symmetric parts of $\mathbf{H}^e$ and $\mathbf{H}^p$, so that the (total) strain $\mathbf{E}$ – which is the symmetric part,

$$\mathbf{E} = \frac{1}{2}\left(\nabla\mathbf{u} + (\nabla\mathbf{u})^\top\right), \tag{2.2}$$

of the displacement gradient $\nabla\mathbf{u}$ – is the sum

$$\mathbf{E} = \mathbf{E}^e + \mathbf{E}^p. \tag{2.3}$$

Single-crystal plasticity is based on the physical assumption that the motion of dislocations takes place on prescribed *slip systems* $\alpha = 1, 2, \ldots, N$. And the presumption that plastic flow take place through slip manifests itself in the requirement that the plastic distortion $\mathbf{H}^p$ be governed by *slips* γ^α on the individual slip systems via the relation

$$\mathbf{H}^p = \sum_\alpha \gamma^\alpha \mathbf{s}^\alpha \otimes \mathbf{m}^\alpha \qquad \left(H^p_{ij} = \sum_\alpha \gamma^\alpha s^\alpha_i m^\alpha_j\right), \tag{2.4}$$

where for each α the *slip direction* $\mathbf{s}^\alpha$ and the associated *slip-plane normal* $\mathbf{m}^\alpha$ are *constant* orthonormal lattice vectors; viz.

$$\mathbf{s}^\alpha \cdot \mathbf{m}^\alpha = 0, \qquad |\mathbf{s}^\alpha| = |\mathbf{m}^\alpha| = 1. \tag{2.5}$$

Here and in what follows: lower case Greek superscripts $\alpha, \beta, \ldots$ denote slip-system labels and as such range over the integers $1, 2, \ldots, N$; we do not use the summation convention for Greek superscripts; we use the shorthand

$$\sum_\alpha = \sum_{\alpha=1}^{N}.$$

A consequence of (2.1) and (2.4) is that

[2] Heavily cold-worked metals when heated to a sufficiently high temperature, $\vartheta \gtrapprox 0.5\,\vartheta_m$, may also undergo a restoration process called recrystallization. We do not consider recrystallization processes in this paper.