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On dislocation pileups and stress-gradient dependent plastic flow

Nasrin Taheri-Nassaj*, Hussein M. Zbib

School of Mechanical and Materials Engineering, Washington State University, United States

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ABSTRACT

In strain-gradient plasticity, the length scale controlling size effect has been attributed to so-called *geometrically necessary dislocations*. This size dependency in plasticity can also be attributed to dislocation pileups in source-obstacle configurations. This has led to the development of stress-gradient plasticity models in the presence of stress gradients. In this work, we re-examine this pileup problem by investigating the double pileup of dislocations emitted from two sources in an inhomogeneous state of stress using both discrete dislocation dynamics and a continuum method. We developed a generalized solution for dislocation distribution with higher-order stress gradients, based on a continuum method using the Hilbert transform. We qualitatively verified the analytical solution for the spatial distribution of dislocations using the discrete dislocation dynamic. Based on these results, we developed a dislocation-based *stress-gradient plasticity* model, leading to an explicit expression for flow stress. Findings show that this expression depends on obstacle spacing, as in the Hall–Petch effect, as well as higher-order stress gradients. Finally, we compared the model with recently developed models and experimental results in the literature to assess the utility of this method.

1. Introduction

Modeling the mechanical behavior of materials presents several challenges due to the complexity of the underlying microstructure. Depending on the objective, a material microstructure can be modeled explicitly or implicitly. Explicit modeling is an effective way to model the microstructure to study material behavior at the grain level, with each grain being a single crystal. By using averaging or homogenization methods, the overall polycrystalline properties of a material can be obtained. It is also possible to model microstructure implicitly by using internal state variables to represent the microstructure. Among the internal state variables, dislocations are the main carriers of plastic deformation, and contribute significantly to mechanical behavior such as strain hardening and ductility. The discrete dislocation dynamics (DDD) method is an explicit approach that considers the motion and interaction of individual dislocation segments to predict stress–strain response by direct simulation of dislocation assemblies. On the other hand, the continuum dislocation dynamics method is an implicit approach based on the concept of dislocation density. In this study, we formulated dislocation density-based models to represent the macroscopic material volume element encompassing mechanisms at the microscopic level. Dislocation

* Corresponding author. Tel.: +1 509 715 7279.
E-mail addresses: nasrin.taherinassaj@email.wsu.edu, nasrin.taheri.n@gmail.com (N. Taheri-Nassaj).

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density-based models can be used to bridge micro-level phenomena and macro-level continuum quantities such as stress and strain (e.g., Domkin, 2005).

Dislocation-based crystal plasticity models can be used to describe dislocation–obstacle interactions as well as dislocation–dislocation interactions to elucidate underlying dislocation mechanisms and microstructure. In such dislocation–obstacle configurations, dislocations pile up against impenetrable obstacles under applied stresses. For example, in polycrystalline materials, grain boundaries act as natural obstacles to dislocation motion. The classical problem of dislocation pileup goes back to investigations by Hall (1951), Petch (1953), Eshelby (1949) and Bilby and Eshelby (1968). Particularly, Hall (1951) and Petch (1953) investigated the pileup of dislocations against grain boundaries under a constant applied stress, leading to the well-known Hall–Petch relationship. This relationship describes the yield stress of a polycrystal as $\sigma_y = K/\sqrt{d} + \sigma_0$, where K is a material constant, d is the grain size, and σ_0 is the constant yield stress. The Hall–Petch relationship reveals the size-dependency of yield strength in polycrystals. It is based on the mechanism of pileup of dislocations against an obstacle (grain boundary) and the critical resolved shear stress required to cause the leading dislocation to penetrate the grain boundary under uniform applied stress.

Dislocation pileup problems have been analyzed explicitly using discrete approaches (see, e.g., Eshelby et al., 1951; Chou and Li, 1969; Lardner, 1969; Biby and Eshelby, 1968) or implicitly using continuum approaches (see, e.g., Leibfried, 1951; Le and Stumpf, 1996; Kochmann and Le, 2008; Chou and Louat, 1962; Head and Louat, 1955; Chakravarthy and Curtin, 2011, 2014; Hirth, 2006; Akarapu and Hirth, 2013). In the first approach, the balance of interaction forces among discrete dislocations in a pileup leads to a set of nonlinear algebraic equations for the equilibrium positions. The second approach uses a continuous distribution of infinitesimal dislocations on a slip-plane, as presented by Eshelby (1949) in the Peierls–Nabarro description (Nabarro, 1947; Peierls, 1940). The continuum model, along with the transform theory presented by Leibfried (1951), can readily describe the strain fields of pileups. Leibfried (1951) demonstrated that the equilibrium distribution in dislocation pileups could be described in terms of Hilbert Transforms and Tschebyscheff (Chebyshev) Polynomials.

Several dislocation pileup analyses have been conducted for homogenous states of stress to formulate models for yield stress. Most notable is the double pileup problem resulting in the well-known Hall–Petch equation. However, especially on a small scale, the state of stress is generally non-uniform and can affect the assumed constitutive equation for flow strength. Thus, the pileup problem in an inhomogeneous stress state has garnered recent interest. Some studies have examined the pileup problem in the presence of stress gradients. Hirth (2006) proposed the stress-gradient dependent flow strength concept, using a continuum approach to analyze the pileup of dislocations emitted from two sources in the presence of a stress gradient. Hirth applied a continuum method by solving a singular integral equation with a kernel of Cauchy type on a finite interval. Other researchers extended this idea (Akarapu and Hirth, 2013; Chakravarthy and Curtin, 2011, 2014; Liu et al., 2013). For example, Chakravarthy and Curtin (2010, 2011, 2014). used a similar approach for a combined stress gradient for dislocations emitted from one source, with pileups at obstacles on either side of the source so that the dislocation density is zero at the center. These studies resulted in stress-gradient plasticity models that attribute the size effect to the dependence of flow stress on local stress gradients.

Studies show the size effect for plastic deformation at a small length scale in torsion experiments of wires with micrometer diameters (see, e.g., Fleck et al., 1994; Dunstan et al., 2009), uniaxial compression or tension experiments of nano and micropillars (see, e.g., Uchic et al., 2004), bending of thin beams and foils (see, e.g., Stölken and Evans, 1998; Evans and Hutchinson, 2009; Ehrler et al., 2008), etc. The classical theory of plasticity cannot describe size-dependent phenomena since it assumes that material strength is dependent only on local variables. To remedy this problem, several strain-gradient plasticity models have been developed (see, e.g., Zbib and Aifantis, 1988a,b,c, 1989, 1992; Fleck and Hutchinson, 1997). Strain-gradient theories are often based on so-called geometrically necessary dislocations which lead to the dependence of flow stress on strain gradients. One main drawback of these theories is that length scale, as a coefficient that multiplies strain gradient terms in constitutive equations, is phenomenological and must be determined experimentally. Moreover, experimental measurements indicate that length scale depends on stress states and loading conditions, suggesting that it is an evolving internal variable related to the underlying microstructure.

Stress-gradient plasticity models, however, arise from the classic analysis of dislocation pileups in source-obstacle configurations (Akarapu and Hirth, 2013; Chakravarthy and Curtin, 2011, 2014; Liu et al., 2013). They consider average obstacle spacing as a material length scale that controls material hardening. In this approach, flow strength relates to the force per unit length on the leading dislocation in the pileup. In terms of the crack problem, this force is based on the concept of a thermodynamic force derived from the rate of change of energy per unit crack length (Hirth and Lothe, 1982). To determine thermodynamic force at both ends of the crack or both tips of the pileup, both are treated equally by assuming symmetry. However, in terms of inhomogeneous stress, the pileup losses its symmetry (Liu and Gao, 1990), and thus the force based on that definition becomes ambiguous.

In this work, we identified closed-form analytical solutions for flow stress in the presence of inhomogeneous local stress as the main objective. We also generalized the traditional Hall–Petch relation to account for spatial stress gradients. The classical Hall–Petch relationship concerns yield stress vs. grain size in a homogenous state of stress. Our findings show that yield stress is not only dependent on grain size, i.e. obstacle spacing, but also on higher-order stress gradients. Many studies have generalized the traditional Hall–Petch relationship into two-dimensions (Zhu et al., 2014) or coupled it with a kinetic equation of dislocation evolution in polycrystals (see, e.g., El-Awady, 2015). In this study, we examined an idealized dislocation double pileup problem as a fundamental, simplified case. We derived an analytical solution to inform development of a generalized stress-gradient plasticity model. Although we could consider more complex pileups in anti-planes (see, e.g.,