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Continuum modeling of dislocation interactions: Why discreteness matters?

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Abstract

Continuum frameworks of dislocation-based plasticity theories are gaining prominence in the research community. In these theories, the underlying discrete lattice defects are represented by an averaged continuous description of a signed dislocation density. The long-range stress fields are accurately characterized but the short-range interactions are modeled phenomenologically. In this paper, we demonstrate by a rigorous analysis that short-range interactions resulting from certain aspects of the underlying discreteness cannot be neglected. An idealized problem of dislocation pile-ups against a hard obstacle is used to illustrate this observation. It is also demonstrated that the modeling of short-range interactions by a local gradient of dislocation distribution has limitations. It is realized that even though the stress contribution for distant dislocations is relatively small, it is the accumulation of these stress contributions from numerous such dislocations which culminates in substantial contributions. It would be inaccurate to neglect these effects. Our benchmark problem can be used for calibration of current and future theories of plasticity that attempt to accurately model short-range interactions.

Keywords: Dislocation interaction; Short-range interaction; Modeling; Mesoscopic plasticity; Pile-up

1. Introduction

Most materials undergo permanent deformation beyond their elastic limit. In metals, this is mainly attributed to the motion of a large number of discrete defects, namely dislocations. Plastic deformation is being characterized across various length scales. Currently, much research is being pursued in making a fundamental connection between plasticity-related processes at an atomic scale and those at the engineering application scale. Once this is achieved, the development of a consistent, unified plasticity theory based on a multi-scale strategy seems at reach.

Discrete dislocation plasticity theories have been used extensively to study a variety of important problems in mechanics today [1–5]. In this framework, dislocations are modeled as line discontinuities in a linear elastic continuum. The extensive calculation of strains along the dislocation line poses a problem, since the effort becomes too large to be computable using linear elasticity theory. Moreover, dislocations are kept track of by a book-keeping scheme that increases in computational complexity with an increasing number of dislocations. The computational cost of performing these numerical computations at physically reasonable strain rates and spatial dimensions is so high that they are of limited practical use.

Continuum theories, on the other hand, are mathematically more tractable, with the advantage of being easily extendable to handle problems involving non-linear elasticity and anisotropy [6–8] without incurring a computational overhead as in discrete dislocation theories. The price that is paid for this efficiency is a loss in resolution, which is often acceptable in engineering applications. In a continuum setting, dislocation distributions are represented by an averaged continuous description through a signed dislocation density. Long-range stress fields are generally taken care of in a mechanistically rigorous sense [9,10]. However, the short-range interactions due to the spatially unresolved dislocation density distribution are modeled phenomenologically [9]. Groma et al. [10] emphasized the importance of correct characterization of the short-range interactions in a continuum setting and attempt to do so in a statistical mechanics framework. However, such an analysis has some limitations as we shall demonstrate in this paper. Specifically, we shall demonstrate that

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the use of nearest neighbor interactions to model short-range interactions locally may be inaccurate. Accurate physical characterization of the short-range interactions is a challenge and a detailed study is lacking in literature. This paper is an attempt in filling the gap. More specifically we shall strive to gain a better deterministic understanding of the importance of short-range interactions and their role in the overall dislocation evolution and resulting non-local effects. We shall demonstrate that the accumulation of these short-range interactions may eventually cause substantial long-range effects.

Apart from the statistical argument as used in [10], the need for short-range terms may also be evidenced in a purely deterministic framework. In this paper we shall limit ourselves to the study and analysis of pile-up groups. Pile-up groups play an important role in the understanding of the mechanical behavior of crystalline solids for both single crystals and polycrystals ([11–17], and many others). A simple pile-up is traditionally described as a set of identical parallel dislocations lying in the same slip plane which move in the same direction under the influence of an externally applied stress until the leading dislocation encounters a barrier. The remaining free dislocations "pile up" against this barrier and take up low-energy equilibrium positions. An infinite wall of dislocations on equidistant slip planes generates a constant long-range stress field (in fact zero stress for walls of edge dislocations) and since it is the short-range interactions that we are keen to study the problem is appropriate and ideal. An additional advantage is that the underlying mathematical problem of an infinite layer pile-up is simpler as the stress field of an infinite dislocation wall can be represented by a simple function. Hence, in this paper we shall restrict ourselves to dislocation walls of infinite length piling up against an obstacle in an infinite medium. The analysis of this assumption sheds light into the complexity of averaging out the dislocation distributions and elucidates that some information of the underlying discreteness simply cannot be ignored. We believe that this realization is a first step in gaining a full understanding of the effects of the underlying discreteness.

The paper is organized as follows: in Section 2, we construct a reference solution, by performing analyses based on discrete distributions of edge and screw dislocations. Section 3 comprises the analysis based on a semi-discrete/continuum distribution, where more specifically, discreteness is maintained within the individual edge or screw dislocation walls but the wall distribution is represented by a continuous function. In Section 4, the effect of representing the discrete wall of dislocations by a continuous description of infinitesimal dislocations is investigated. The intrinsic role of discreteness in upscaling short-range interactions is thereby revealed. Section 5 comprises a comparison with a model of statistical mechanics and discusses some limitations of this theory. The paper ends with some discussions and concluding remarks in Section 6.

2. Discrete analysis of pile-ups of infinite walls of dislocations

The representative problem chosen here has been a subject of research in several papers [18–22]. Stresses due to meso-

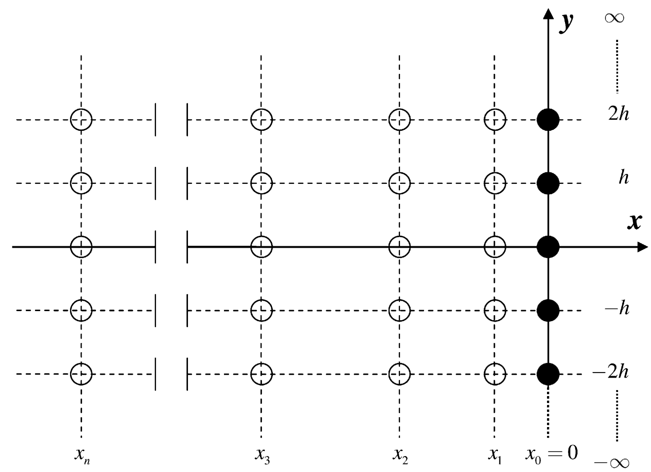

Fig. 1. Discrete dislocation representation of a pile-up in an infinite media. Slip plane separation is h . The circles represent either edge or screw dislocations. The solid circles represent the immobile wall at x = 0. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of the article.)

scopic variations are captured by continuum theories relevant at these scales and are therefore not our main interest. The idealized configuration chosen here eliminates the long-range stress variations and allows us to perform a rigorous analysis of the underlying short-range stress fields.

The problem is stated as follows: the infinite sequence of planes $y = 0, \pm h, \ldots, \pm nh$ are the active slip planes in a crystal, where h is the slip plane spacing and n is an integer index ranging from 0 to ∞. Dislocations on the slip plane are straight and are organized in vertical walls. The line direction of the dislocations is parallel to the z-axis. The Burgers vector for an edge dislocation is in the positive x direction and for a screw dislocation in the positive z direction. Here, x, y, z are orthogonal Cartesian coordinate axes. Fig. 1 is a schematic representation of such a configuration of infinite dislocation walls piling up against an obstacle at $x = 0$ in an infinite media under a constant externally applied shear stress σ. For our analysis we assume that the domain where a pile-up forms is in the range $[-a,0]$ with respect to the x-axis, where $a = 15\,\mathrm{h}$. The choice of $15\,h$ is arbitrary and does not influence any of our conclusions for $a \gg h$.

Our main interest is in the analysis of edge dislocation walls, for which the configuration described is perhaps reasonable since dislocations are generally available only on a limited number of parallel slip planes. Nevertheless we also pursue an analysis of screw dislocation walls as analytical results are available and differences can be pointed out.

2.1. Screw dislocations

The physical relevance of the motion of infinite walls of screw dislocations on equidistant slip planes piling up against an obstacle is limited. Nevertheless we perform an analysis primarily as a mathematical exercise and also as a scheme for checking our numerical procedure as an analytical result is readily available in the literature (cf. Section 3.1).