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Energy of periodic discrete dislocation networks

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Abstract

We present an approach to compute the stored energy associated with arbitrary discrete dislocation networks subjected to periodic boundary conditions. To circumvent the issue of conditional convergence while keeping the computational cost tractable, we develop a regularization procedure that involves two equivalent measures of the dislocation network energy. Taking advantage of the non-singular formulation, the energy is first evaluated by explicitly calculating the conditionally convergent sum of all interactions between dislocation segments. Regularization constants are then determined by volume integral of the smooth elastic stress fields produced for large values of the dislocation core radius. The approach is employed to investigate the stored energy of a series of idealized dislocation configurations and large-scale networks generated by discrete dislocation dynamics (DDD) simulations. It is found that (1) the stored energies predicted by DDD simulations are in good agreement with experimental measurements of about 5% of the work done, and (2) Taylor lattice configurations provide surprisingly good energetics models for complex DDD networks, thereby confirming the screening of long-range stresses in work-hardened dislocation structures.

Keywords: Dislocations, Energy, DDD

1. Introduction

Plastic deformation in metals is primarily caused by the motion of dislocations in response to the imposed mechanical loading. While this process is highly irreversible and results in dissipating most of the work done to the crystal into heat, a fraction of the energy remains stored within the crystal in the form of elastic and core energies of the dislocations. The stored energy is of particular interest since it depends both on the density of dislocations and on their arrangement. In addition, it provides the driving force for several phenomena that are important for the microstructure evolution, such as static and dynamic recovery, and recrystallization.

As such, the energy associated with dislocation structures has become a key ingredient in our understanding of plastic deformation, and a fundamental quan-