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REVIEW ARTICLE

Modeling Dislocations at Different Scales

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Abstract. In this article, we give an introduction to the basic theory of dislocations and some dislocation models at different length scales. Dislocations are line defects in crystals. The continuum theory of dislocations works well at the length scale of several lattice constants away from the dislocations. In the region surrounding the dislocations (core region), the crystal lattice is heavily distorted, and atomistic models are used to describe the atomic arrangement and related properties. The Peierls-Nabarro models of dislocations incorporate the atomic features into the continuum theory, therefore provide an alternative way to understand the dislocation core properties. The numerical simulation of the collective motion and interactions of dislocations, known as dislocation dynamics, is becoming a more and more important tool for the investigation of the plastic behaviors of materials. Several simulation methods for dislocation dynamics are also reviewed in this article.

Key words: Dislocations; modeling; dislocation dynamics; Peierls-Nabarro model.

Contents

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1 Introduction

Dislocations are line defects in crystals. The dislocation theory had its origins in the early years of the last century [1–4], and has been an active research area ever since [5–7]. The dislocation theory is essential for the understanding of the plastic deformation (permanent deformation) properties of crystals. In this article, we shall briefly review the basic dislocation theory and some dislocation models at different length scales.

We first review the basic properties of dislocations. Fig. 1(a) shows the geometry of one type of dislocations: edge dislocations, in a simple cubic lattice, where the atomic arrangement is uniform in the direction perpendicular to the paper. An edge dislocation can be imagined as being formed by inserting an extra half plane of atoms into a perfect crystal, see Fig. 1(b). The boundary of the extra half plane, where the lattice is heavily distorted, is the edge dislocation. An edge dislocation can also be imagined as being formed by making a cut in a perfect crystal, and shifting the atoms on one side of the cut relative to those on the other side by one lattice spacing, in a direction in the cut plane and perpendicular to the cut boundary line, see Fig. 1(c). The boundary line of the cut is the edge dislocation. Note that the cut in the latter process is perpendicular to the extra half plane of atoms in the former one. Both processes give the same atomic arrangement for an edge dislocation. Fig. 2 shows the geometry of another type of dislocations: screw dislocations, in a simple cubic lattice. A screw dislocation can be imagined as being formed by shifting the atoms on one side of a half plane relative to the atoms on the other side by one lattice constant, in a direction parallel to the boundary of the half plane. The boundary of the half plane is the screw dislocation.

The motion of dislocations leads to plastic deformation in crystals. When single crystals are stressed, they undergo plastic deformation when the stress is high enough. However, the critical stress in a real material is several orders of magnitude lower than the theoretical stress to shear a perfect crystal [8]. Taylor [2], Orowan [3] and Polanyi [4] first pointed out that dislocations are responsible for this low critical stress. A simple demonstration is given in Fig. 3. In Fig. 3, a single crystal containing an edge dislocation is shown. The edge dislocation is perpendicular to the paper and the atomic arrangement is uniform in this direction. Away from the edge dislocation, the atomic arrangement is close to that in a perfect crystal; while near the dislocation, the lattice is heavily distorted. Under an applied shear stress, near the dislocation, the bond between atoms A and C forms and the bond between atoms B and C breaks, see Fig. 3(a) and (b). In this way, the edge dislocation moves a distance of one lattice spacing. This process repeats under the applied stress. When the dislocation moves to the crystal boundary, a step is produced there and the crystal undergoes a plastic (permanent) deformation, see Fig. 3(c). The shear stress required in this process is much lower than that to shift a perfect crystal.

Burgers vector [9] is used to characterize a dislocation. First, the direction of the dislocation needs to be defined, which is the direction of the unit tangent vector of the dislocation. Consider a closed loop enclosing an edge dislocation, see Fig. 4(a). The edge dislocation is perpendicular to the paper, and the extra half plane of atoms are