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Atomistic simulations of lattice defects in tungsten

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ABSTRACT

The mechanical behavior of materials is ultimately determined by events occurring at the atomic scale. The onset of plastic yield corresponds to triggering of dislocation motion. Subsequent hardening is mainly controlled by interaction of gliding dislocations with other lattice defects such as forest dislocations, grain boundaries, interfaces and surfaces. Finally, material failure is influenced by processes at the tip of a crack propagating in a crystal lattice. In this work we review atomistic simulations of lattice defects in tungsten. We show that these studies are able to provide not only a detailed understanding of defect properties but also reveal how the fundamental processes at the atomic scale are linked to macroscopic material behavior.

1. Introduction

Tungsten is a refractory transition metal with a half-filled d-band, which crystallizes in a body-centered-cubic (bcc) structure. It is a metal with the highest melting temperature (3680 K) and for this reason its main applications have been filaments for bulb lamps, electrical contacts, arc-welding electrodes, and heating elements in high temperature furnaces. Notwithstanding, two recent developments may broaden significantly the use of tungsten and elevate even further its technological prominence. First, tungsten is considered as one of the structural materials that will play an important role in the fusion reactor ITER project [1,2]. Second, recent advancements in nanoengineering have enabled tailoring of microstructure and production of ultrafine-grained and nanocrystalline tungsten with significantly enhanced mechanical behavior [3]. An important general drawback in structural applications is the fact that in tungsten the ductile-to-brittle transition occurs well above room temperature [4,5]. This transition appears to be controlled by dislocation mobility rather than by crack nucleation [6,7]. In addition, the mechanical properties of tungsten are strongly dependent on alloying, impurities and thermomechanical treatment [8], which is a common characteristic of bcc transition metals.

The plastic deformation and fracture of crystalline materials is, in general, controlled by extended defects, specifically dislocations, grain boundaries and other interfaces [9–13]. For example, it is now generally accepted that in bcc metals the strong temperature dependence of the yield and flow stress arises owing to the complex structure of the core of 1/2<111> screw dislocations. Moreover, this core structure is responsible for unusual dependencies of the flow stress on the orientation of the crystal with respect to the loading axes and breakdown of the Schmid law (for reviews see, e.g., [14–22]). Atomic level understanding of dislocation cores and their effects on dislocation glide, phenomena associated with formation and propagation of cleavage and/or intergranular cracks as well as investigation of the structure and properties of nanocrystalline materials, are typical problems that are studied by the atomic level computer modelling. Such studies have become widespread in materials science, as demonstrated by a recent handbook that summarizes a broad range of methods and specific investigations [23].

2. Models of atomic interactions

The principal precursor of all atomic level studies, in particular those involving systems composed of a large number of atoms that do not form an ideal lattice, is a reliable description of atomic interactions. The state-of-the-art first-principles methods based on the density functional theory (DFT), which require only a few fundamental physical constants as input, provide such a description most reliably. However, these rigorous calculations are limited either to ideal structures without any defects or to studies of periodic arrays of very closely spaced defects, owing to the application of periodic boundary conditions and feasible block sizes that contain couple of hundred of atoms at most. Studies of large and complex systems require approximations and simplifications when describing atomic interactions that may, however, obliterate some important features of bonding. For this reason, the most challenging aspect of materials modelling is the choice of the description of atomic interactions that correctly and with sufficient accuracy reflects the physics of bonding in any specific case, while at the same time it is computationally treatable for large systems of particles.

Methods describing interatomic forces that have been most broadly used in large-scale atomistic studies of metallic materials are the embedded atom method [24] and the Finnis–Sinclair (FS) potential [25]. These central-force many-body potentials are able to describe well

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simple and noble metals in which the bonding is almost nearly free-electron-like (NFE). However, in transition metals and intermetallic compounds based on transition metals, the bonding has a mixed NFE and covalent character. In these materials it is the filling of the d-band that controls the cohesion and hence the particular ground state structure [26,27]. This bonding, which is mediated by the d-electrons, is covalent in character so that the atomic interactions are non-central and depend on the angles between bonds. Nonetheless, empirical central-force potentials have been constructed for elemental bcc transition metals [28] and used, for example, in studies of dislocation cores [29,30]. These calculations detected a number of general features of dislocation cores and their response to applied stresses that can be expected in all materials with the bcc lattice. However, such simple models of atomic interactions fail to identify subtle differences in properties of specific materials.

Various approximate schemes that include non-central forces have been advanced in recent years. One of the most successful schemes are many-atom Bond-Order Potentials (BOPs) that give an exact representation of the bond energy within the chemically intuitive tight-binding (TB) approximation to the quantum mechanical electronic structure [27,31] and retain thus the angular character of bonding. The BOPs provide a direct bridge between the electronic level modelling, with its full treatment of the electronic degrees of freedom, and the atomistic modelling, where the electronic degrees of freedom have been coarse grained into many-body interatomic potentials. Apart from the quantum mechanical character, another significant advantage of BOPs is that modelling of extended defects, which requires a large number of atoms, can be performed in real space and the computational effort scales linearly with the number of atoms in the system, decreasing thus dramatically the computational time. These potentials have now been developed for tungsten [32] as well as other transition metals and their alloys [33,34].

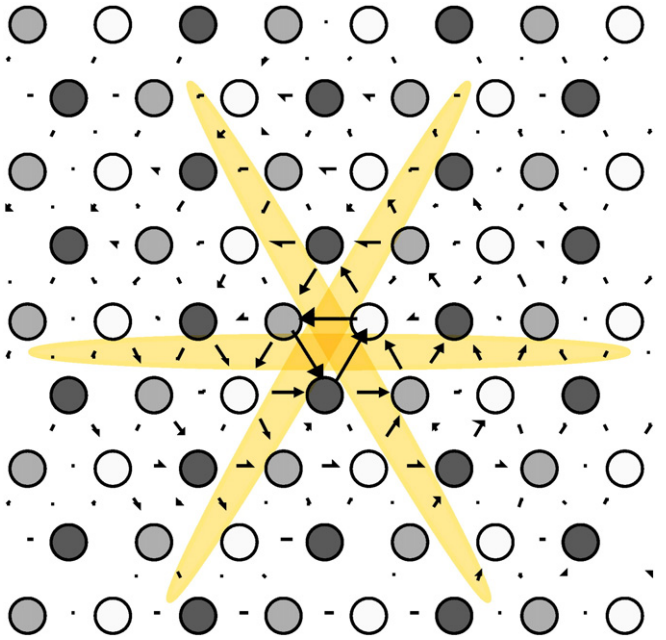

Fig. 1. Core structure of the 1/2<111> screw dislocation determined using BOP for tungsten [32]. The atomic arrangement is shown in the projection perpendicular to the direction of the dislocation line (the [111] axis), and circles represent atoms within one period; their positions in three successive (111) planes are distinguished by shading. The [111] (screw) component of the relative displacement of the neighboring atoms produced by the dislocation is depicted as an arrow between them. The length of the arrows is proportional to the magnitude of these components. The arrows, which indicate out-of-plane displacements, are always drawn along the line connecting neighboring atoms and their length is normalized such that the longest arrow is equal to the separation of these atoms in the projection.

3. Atomistic simulations of dislocations

As we mentioned already, earlier the distinguishing features of the plastic behavior of bcc metals are controlled by the structure and properties of the dislocation cores. As first suggested by Hirsch [35] and now firmly established by many experimental and theoretical studies (for reviews see [14–19]), dislocations controlling the characteristic features of the plastic properties of bcc metals are 1/2<111> screw dislocations. The most general reason is crystallographic: <111> is the direction of a three-fold screw axis in the bcc lattice and thus the structure of the dislocation parallel to this direction must possess such symmetry and is, therefore, intrinsically non-planar [36]. This further suggests that screw dislocations will be more difficult to move than dislocations of other orientations. However, crystallography alone does not determine into which planes of the <111> zone and in what manner the core is spread in space and, even more importantly, how such core responds to external loading. Capability to observe the atomic structure of the core directly is very limited [37] and a direct observation of the stress effects is not even feasible. Consequently, investigation of this phenomenon is an excellent topic for atomistic simulations.

A large number of atomistic simulations of dislocations in bcc metals have been made in the past using a broad variety of descriptions of interatomic interactions (for reviews see [16,20]). In all these studies the core was found to spread into three {110} planes. Two types of the core were found — in one case the core is spread asymmetrically into these three planes while in the other case it spreads symmetrically [38]. The equilibrium symmetrical configuration of the 1/2<111> screw dislocation core in tungsten calculated using recently constructed BOP [32] is shown in Fig. 1.

Analysis of the core structure is only the first step in studies of dislocations. The ultimate goal is understanding their glide behavior under the effect of external loads and determination of the stresses at which the dislocation starts to move as well as the actual glide plane. In a recent work Gröger and Vitek [39] presented a comprehensive atomic level study of the glide of 1/2<111> screw dislocations in tungsten. They showed that the breakdown of the Schmid law indeed originates at the atomic level. An explanation of this phenomenon has been provided based on calculations combining the shear stresses parallel and perpendicular to the slip direction. The atomistic simulations revealed that the critical resolved shear stress in the slip direction, at which the dislocation starts to move, depends sensitively on the shear stress perpendicular to the slip direction, which does not exert any force on the dislocation. The reason is that the shear stress perpendicular to the slip direction changes the symmetry of the dislocation core such that it either promotes or impedes the slip on the most highly stressed {110} plane. In general, when plastic deformation is affected by components of the applied stress tensor other than the Schmid stress, such behavior is defined as a non-associated plastic flow. In the setting of continuum mechanics it means that the yield function and the flow potential are not equal. Based on the results of atomistic simulations Gröger and Vitek [39] were able to formulate analytic yield criteria for continuum analyses of plasticity in both single and polycrystalline tungsten. The physical origin of the non-associated flow behavior is the complex response of the non-planar cores of screw dislocations to a general state of stress.

4. Atomistic simulations of grain boundaries

The microstructure of polycrystalline materials has a profound effect on their mechanical properties. Grain boundaries (GBs) can act as sinks and sources of dislocations, they can hinder motion of dislocations, or they can even become preferred sites of crack nucleation and subsequent fracture. For instance, during drawing and swaging tungsten wires and also wires made from other bcc metals develop a pronounced <110> texture [40,41]. The drawn wires show a preferred orientation, in which the <110> direction is parallel to the wire axis, and they are composed of a large number of highly elongated and curved grains