Acta Materialia 124 (2017) 633–659

Contents lists available at ScienceDirect

Acta Materialia

journal homepage: www.elsevier.com/locate/actamat

By invitation only: overview article

Ab initio modeling of dislocation core properties in metals and semiconductors

D. Rodney [a, *], L. Ventelon [b], E. Clouet [b], L. Pizzagalli [c], F. Willaime [d]

[a] Institut Lumière Matière, CNRS-Université Claude Bernard Lyon 1, F-69622 Villeurbanne, France
[b] DEN-Service de Recherches de Métallurgie Physique, CEA, Université Paris-Saclay, F-91191 Gif-sur-Yvette, France
[c] Institut Pprime, CNRS-Université de Poitiers, F-86962 Chasseneuil Futuroscope, France
[d] DEN-Département des Matériaux pour le Nucléaire, CEA, Université Paris-Saclay, F-91191 Gif-sur-Yvette, France

ARTICLE INFO

Article history:
Received 31 May 2016
Received in revised form
29 August 2016
Accepted 27 September 2016
Available online 21 October 2016

Keywords:
Dislocation
Plasticity
Alloys
Semiconductors
Density functional theory

ABSTRACT

Dislocation cores, the regions in the immediate vicinity of dislocation lines, control a number of properties such as dislocation mobility, cross-slip and short-range interactions with other defects. The quantitative modeling of dislocation cores requires an electronic-level description of atomic bonding. *Ab initio* quantum mechanical calculations of dislocation cores based on the density functional theory have progressed rapidly thanks to the steady increase in computing capacities and the development of dedicated numerical methods and codes. Our aim in this overview paper is, after a description of the methodology regarding in particular the boundary conditions, to review the new and unexpected results obtained on dislocation cores from first principles, including the identification of unforeseen stable and metastable cores and the quantitative evaluation of both interaction energies and energy pathways, in pure metals and alloys of different crystallography (FCC, BCC, HCP) as well as semiconductors. We also identify key challenges to be explored in this rapidly growing field.

Contents

* Corresponding author.
E-mail address: David.Rodney@univ-lyon1.fr (D. Rodney).

http://dx.doi.org/10.1016/j.actamat.2016.09.049
1359-6454/

1. Introduction

Crystal plasticity is an inherently multi-scale process starting at the atomic scale where dislocation cores, the regions in the immediate vicinity of dislocation lines, control a number of local properties, including the selection of glide planes and corresponding dislocation mobility, cross-slip and nucleation processes [1–5].

While the elasticity theory of dislocations [6–8] describes very accurately the long-range stress and strain fields produced by dislocations, an atomic-scale description is required to describe reconstructed regions like dislocation cores. Historically, the first model of a dislocation core involved an elasto-plastic framework, the well-known Peierls-Nabarro model [9,10], where the atomic-scale description was limited to the dislocation glide plane. Later, full atomistic calculations of dislocation cores [11] were performed using interatomic short-ranged pair potentials, almost simultaneously in face-centered cubic (FCC) [12–14] and body-centered cubic (BCC) metals [15,16]. Since then, empirical and semi-empirical potentials have been applied to a very large variety of dislocations in metals and alloys, intermetallic compounds, semiconductors as well as covalent and ionic crystals (seminal works include Refs. [17–24]). Interatomic potentials are very useful to study large-scale processes at finite temperatures, but they remain of limited predictability regarding the detailed structure of a dislocation core. A famous example is the long-term debate about the core structure of screw dislocations in BCC metals, which is predicted by interatomic potentials in two different forms, symmetrical and asymmetrical, depending on the details of the potential parameters [23,25–28].

To be quantitative and predictive, an electronic-level description of atomic bonding is required, as provided by *ab initio* quantum mechanical calculations performed within the density functional theory (DFT) [29]. The first calculations of a dislocation core concerned semiconductors [30–32], partly because electronic structure calculations in semiconductors require less computing resources than in metals. However, metals were soon considered: BCC [33], hexagonal close-packed (HCP) [34,35] and finally FCC [36]. Initially limited to pure metals, current studies also consider alloying effects.

Ab initio calculations are very computationally demanding and allow to simulate only a few hundreds of atoms. As a result, the calculations are mainly limited to straight infinite periodic dislocations. But even then, the lateral dimensions do not exceed a few nanometers, such that, given the long-range stress and strain fields produced by a dislocation, interactions with the boundary conditions are inevitable. These interactions affect the dislocation energy and possibly even its core structure. Therefore, *ab initio* calculations of dislocations, more than any other defect or simulation method, require a very careful choice of the boundary conditions. Fortunately, a large effort has been devoted this past decade to either develop adapted boundary conditions [37–39] or control and remove boundary condition effects, notably their elastic contribution [40,41].

Ab initio calculations of dislocation cores have recently made very rapid progress, because of the combined increase in computing power, progress in methodology particularly regarding boundary conditions and progress in scientific computing through the development of efficient workpackages like the Vienna Ab initio Simulation Package (VASP) [42], the PWSCF package, which is part of the QUANTUM ESPRESSO integrated suite of codes [43], and the SIESTA [44] and ABINIT [45] packages.

Our aim in this overview is to highlight the unique input *ab initio* calculations have brought to the modeling of dislocation cores and identify the outstanding challenges that remain in this rapidly growing field. After a description of the methodology (Sec. 2), we will consider the modeling and understanding of dislocation core properties in both metals and semiconductors. We will start with FCC metals (Sec. 3) where cores are probably the simplest but remain challenging for *ab initio* calculations because of their large dissociation. We will then address BCC metals (Sec. 4), where cores are more compact but show an intricate relation with the crystallography and applied stress. Following, we will consider HCP metals (Sec. 5), where several metastable cores have recently been identified. Finally, we will address semiconductors (Sec. 6), where the existence of the shuffle and glide systems, as well as charge effects in compound elements, induce a large variety of cores with complex structures.