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An atomistically informed kinetic Monte Carlo model of grain boundary motion coupled to shear deformation

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ABSTRACT

The shear coupled motion of grain boundaries (GBs) is modelled by using two different atomistic simulation techniques: molecular dynamics (MD) and kinetic Monte Carlo (KMC). MD simulations are conducted to identify the elementary mechanisms that take place during the coupled motion of GBs. This process is described on the one hand, in terms of the geometrical approach of the dislocation content in the boundary; and on the other hand, by the thermodynamics of the dislocation passage, shown as a thermal activated process. Relevant MD output is extended into a KMC model that considers the GB migration as a result of a sequence of discrete rare events. The independent motion of each structural unit forming the boundary conforms a single event, having a rate per unit of time to move to the next stable position computed according to the transition state theory. The limited time scale of classical MD is overcome by KMC, that allows to impose realistic deformation velocities up to 10 μm/s.

1. Introduction

Grain boundaries play an important role in determining the mechanical properties of nanocrystalline (nc-) materials (Hirth, 1972), e.g. enhancement of the initial resistance to yielding in nc-aggregates by the presence of GBs (Wulfinghoff et al., 2013). Several investigations have been carried out in order to understand the GB structure (Farkas, 2000), thermodynamics (Mishin et al., 2010) and related deformation mechanisms (Bieler et al., 2009; Dahlberg et al., 2013).

In particular, atomistic simulations have provided a further insight into the microscopic mechanisms and fracture nucleation at interfaces under applied mechanical loads. Shear behaviours of GBs have been studied in detail, and grain boundary (GB) motion coupled to shear deformation has been evidenced to be an important mode of plastic deformation, as a dominant behaviour or competing with other GB mechanisms in a wide range of temperatures, such as GB sliding (Du et al., 2010; Schäfer and Albe, 2012; Warner et al., 2006) or dislocation mediated slips (Sansoz and Molinari, 2005; Tschopp and McDowell, 2008; Spearot et al., 2007; Ohashi et al., 2009).

Basically this mechanism is described through the coupling of the GB to mechanical loads which in turn induces a shear deformation in the crystal region swept by the motion. Stress-induced GB migration was first observed in symmetrical low-angle GBs (LAGBs) in Zn bicrystals (Li et al., 1953). Read and Shockley (1950) determined the mechanism of this motion to be due to the collective glide of the array of parallel edge dislocations forming the LAGB. This mechanism was limited to boundaries with low tilt angle where the core of individual dislocations could be resolved. However, this model has been

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extended to high- angle GBs (HAGB) in the case of metals. Goryaka et al. (2009) confirmed experimentally the coupled motion of GBs for both low- and high-angle symmetrical tilt GBs with a misorientation angle within 0–90 in Al bicrystals. Also, computer simulations evidence that the coupling between normal boundary motion and the rigid translation of the adjacent grains can occur for HAGBs (Cahn et al., 2006; Frolov, 2014; Huang et al., 2014). The coupling effect was proposed to be a generic property of many atomically ordered GBs in the unified approach reported by Cahn and Taylor (2004) and confirmed over a large catalogue of 388 GBs (Homer et al., 2013).

To date, GB shear-coupled motion has been subjected to several studies to explore the impact of this mechanism in the mechanical properties of nc- materials, as well as its relation to other deformation processes (Tucker et al., 2010; Rajabzadeh et al., 2014; Goryaka et al., 2011; Berbenni et al., 2013a). The major challenge relies on the multiscale modelling, as discussed by Berbenni et al. (2013b) where a complete micromechanical model based on molecular dynamics (MD) simulations is proposed. Taupin et al. (2014) describe the shear coupled boundary migration in a continuous manner by using an elasto-plastic theory of disclination and dislocation fields, and results are found to be in good agreement with atomistic simulations and experiments.

In this paper, we continue to investigate the dynamics of this phenomenon within a multiscale framework for its comprehensive understanding. Two different atomistic simulation techniques are used throughout this work. On the one hand, MD simulations are used to identify the elementary mechanisms of GB migration, and on the other hand, we have extended the outcome of MD simulations to a kinetic Monte Carlo (KMC) model. KMC models the shear coupled motion of GBs based on the thermodynamics of the dislocation motion, in terms of individual resolved cores forming the GB. The main goal is to be able to reproduce the MD simulation results at a reduced computational cost by means of KMC. We apply this multiscale approach in bicrystals containing one individual [0 0 1] symmetrical tilt GB in Ni in a range of misorientation angles between 0° and 90°.

The structure of the present paper is the following. In Section 2 a complete description of the dynamics of coupling and the geometric characterization of GBs are introduced. MD simulations are carried out in different temperature regimes and reported in Section 3. To reach our final goal of extending the MD output, the main concern before moving to KMC is to validate such output. Due to the lack of experimental data, in Sections 3.2 and 3.3 simulated values are compared in detail to theoretical models previously illustrated. The minimum energy path of the shear-coupled GB motion is computed using the nudged elastic band method in Section 3.4, which is the most relevant input in the KMC method. Within the multiscale approach, the latter is proposed in Section 4. Numerical examples of KMC are presented in Section 4.2, where results are contrasted to previously shown MD results.

2. Dynamics of shear-coupled motion of grain boundaries and coupling modes

The simple model proposed by Ivanov and Mishin (2008) assumes the coupled GB motion as a motion through a periodic landscape. Following this approach, the system has a set of equivalent stable states which are separated by an energy barrier. At 0 K, in the absence of any external force applied, the GB is trapped in a particular equilibrium position. By applying a shear stress through imposing a parallel velocity ($v_{\parallel}$), the GB is elastically deformed and when a critical value τ_c^0 is reached, the relevant barrier vanishes to zero and the GB makes a transition by increments of H. This normal motion of the GB occurs simultaneously with the rigid-body translation of the adjacent grains (S), producing a permanent shear deformation of the lattice and the subsequent drop of the stress. The ratio $\beta = S/H$ is called coupling factor, discussed later. The first stress relaxation is followed by a new elastic loading step until the critical stress is reached again, and the GB makes another step, see Fig. 1, identified as a stick–slip behaviour.

At finite temperature, the GB could move before the critical stress is reached. Thermal fluctuations assist the GB to overcome the energy barrier, so critical stress τ_c is then expected to decrease with temperature. This decreasing is intensified as temperature increases, and at a fixed $v_{\parallel}$ the peak stress is expected to be linear in $T^{2/3}$ as (Ivanov and Mishin, 2008):

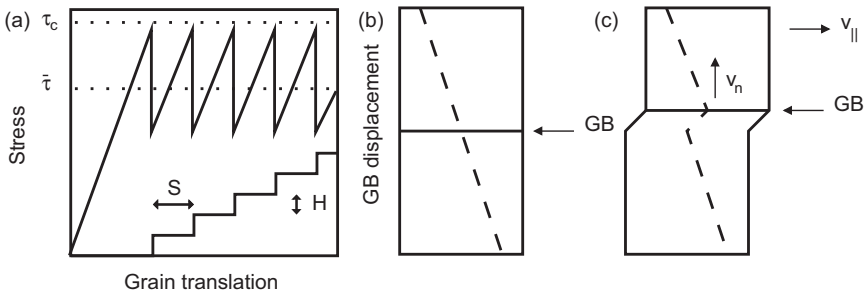

Fig. 1. Stick–slip behaviour. (a) In a perfect coupled motion, the normal motion of GB by increments of H is accompanied by rigid translation of the grains by increments of S. After each jump of the GB to the next stable position the stress drops. (b) Initial configuration of the system and (c) sheared lattice.