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Transitional grain boundary structures and the influence on thermal, mechanical and energy properties from molecular dynamics simulations

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ABSTRACT

The thermo-kinetic characteristics that dictate the activation of atomistic crystal defects significantly influence the mechanical properties of crystalline materials. Grain boundaries (GBs) primarily influence the plastic deformation of FCC metals through their interaction with mobile dislocation defects. The activation thresholds and atomic mechanisms that dictate the thermo-kinetic properties of grain boundaries have been difficult to study due to complex and highly variable GB structure. This paper presents a new approach for modelling GBs which is based on a systematic structural analysis of metastable and stable GBs. GB structural transformation accommodates defect interactions at the interface. The activation energy for such structural transformations was evaluated with nudged elastic band analysis of bi-crystals with several metastable 0 K grain boundary structures in pure FCC Aluminium (Al). The resultant activation energy was used to evaluate the thermal stability of the metastable grain boundary structures, with predictions of transition time based on transition state theory. The predictions are in very good agreement with the minimum time for irreversible structure transformation at 300 K obtained with molecular dynamics simulations. Analytical methods were used to evaluate the activation volume, which in turn was used to predict and explain the influence of stress and strain rate on the thermal and mechanical properties. Results of molecular dynamics simulations show that the GB structure is more closely related to the elastic strength at 0 K than the GB energy. Furthermore, the thermal instability of the GB structure directly influences the relationship between bi-crystal strength, temperature and strain rate. Hence, theoretically consistent models are established on the basis of activation criteria, and used to make predictions of temperature-dependent yield stress at a low strain rate, in agreement with experimental results.

1. Introduction

This section provides a brief literature review and overview of the multiple components of the study described in this paper. The research involves the modelling of the structure-property relationships of grain boundaries with atomic simulations.

Grain boundaries (GBs) significantly influence the thermo-mechanical properties of metals through their structural interactions as a source, sink and barrier to crystal defects such as dislocations and vacancies. The next sections present a brief review of the literature relating to computational modelling and GB effects.

1.1. Phenomenological modelling of grain boundary – defect interactions

Grain boundary (GB) engineering aims to enable the manufacture of metallic materials approaching theoretically optimal mechanical properties, based on microstructure-tailored designs [1]. There have been several recent breakthroughs to achieve ultra-fine grain sizes [2], highly-oriented GB structure [2–4], and carefully tailored networks of low energy GB structures [5]. Computer simulations have been critical for developing the scientific understanding of GB properties at the atomic scale which have established the basis for the breakthroughs in materials design with GB tailoring [6]. Coupled with the substantial progress since the late 1990s to refine the grain size and to control the GB

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structure and topology [7], the prospects for high performance, nano-engineered materials appear to be very good [1]. To obtain the significant gains possible with GB engineering, an extensive knowledge of structure-property relationships and defect mechanics at sub-micron scales is necessary [5,8].

Studying the relationship between crystal defect dynamics, grain boundary microstructure and material properties is experimentally difficult and costly at the sub-micron scales [5]. Extensive parametric testing at nano-micro scales is only possible using simulation methods, which should ideally be informed by fundamental atomistic interactions [9]. However, plastic deformation is more consistently defined by the combined motion and accumulation of millions of dislocations and their interactions with the meso-scale crystal structures, such as grain boundaries and precipitates [10]. Hence, it is critical to establish a multi-scale link to model atomistic effects in the meso- and macro scales.

Energy-based criteria are an ideal basis for constitutive modelling to overcome the time, temperature and length scale limitations of atomistic studies [11,12]. This is particularly true, because the internal energy is known to be a scale-independent characteristic of materials, which is the foundational principle of successful multi-scale models, such as the quasi-continuum method [9,13]. In polycrystalline metals, grain boundaries (GBs) form 3D networks which significantly influence the mechanical properties via interactions with crystal defects such as dislocations and interstitials [14,15]. In this study, we examine the thermal, stress and strain-rate effects, and determine if these correspond to the 'energetic activation' of defect - GB interactions. This study utilises the nudged elastic band (NEB) 'time-independent' technique, coupled with MD simulations, to evaluate the thermal activation parameters (i.e., activation energy) required for atomic processes [16,17]. Analytical models based on the resultant fundamental energy properties can be used to extrapolate simulation results to many temperature conditions and/or lower strain rates for important comparison with experimental tests [11,12,18–20].

1.2. Activation energy for strongly mechanically driven phenomena

The influence of the thermo-kinetic properties and structural stability of GBs on the mechanical properties is closely related to the effect on the source, sink and barrier strength for crystal defects [5,21]. For example, highly non-equilibrium (high energy) GBs are known to be effective defect sources which has been observed experimentally [5] and studied with simulations [22,23]. In contrast, homogeneous defect nucleation will occur within the bulk before occurring in low energy twin boundaries [18,22].

Analytical methods have been used to establish powerful models based on the activation properties, to predict the threshold stress at a given transition temperature and strain rate [11]. Dislocation nucleation from the GBs is thought to dictate the elastic limit of polycrystals below grain diameters of approximately 0.1 μm, which is roughly the threshold size for the inactivation of Frank-Read sources [11,24]. Deng and Sansoz [12] used systematic MD simulations with twinned nanopillars to derive the activation parameters for dislocation interactions with twin boundaries and free surfaces in copper. Results compared favourably with prior NEB studies, used to derive models that proved useful for accurately predicting the strength and activation volume at significantly lower strain rates [11,18]. However, in prior atomistic studies the GB properties are assumed to be fully described by the resolved shear stress, misorientation angle [22,25–27] and inclination angle of the GB plane [28]. In contrast, the present study compares identically oriented and sized bi-crystals with many metastable Σ5(310) GBs to show effect of the grain boundary structure on the thermo-physical properties, independently from stress and size variables.

1.3. Outline

This paper presents an analysis of the relationship between the thermodynamic and mechanical properties of Σ5(310) GBs, based on atomic simulations of pure FCC aluminium. A systematic approach is used to evaluate the temperature and strain rate dependent properties from simulations. Analysis is based on a comparison of the mechanical properties of thermodynamically distinct metastable GB structures at several temperatures and strain rates. Constitutive models are established from the results, and used to predict performance at experimentally obtainable strain rates. Comparison with a prior experimental result in the literature is provided to demonstrate the effectiveness of predictions from the resultant model [16,29]. Hence, this paper provides a good 'proof-of-concept' that simulations can be used as a powerful tool to explain the energy properties of different GB structures and the influence of thermal and kinetic effects on the mechanical response.

In this study, the relationships between the GB structure, the thermal stability and the energy properties are evaluated for metastable GB structures. The thermo-kinetic effects of stable and metastable grain boundaries are presented, and used to explain the variability in the mechanical properties of different metastable bi-crystals of pure FCC Aluminium (Al), using molecular dynamics (MD) simulations. The paper involves three main parts. Firstly, a fundamental model is developed, which is capable of explaining the thermal stability of grain boundaries. Then, the fundamental athermal (0 K) mechanical properties and physical characteristics of GB structure are evaluated, and used to demonstrate a link between a mechanically driven (i.e., stress dependent) process and the temperature/strain-rate sensitivity. The paper concludes with a simulation-based assessment of the critical tensile stress for dislocation nucleation as a function of temperature and strain rate, and hence establishes a model linking the thermal, kinetic and mechanical properties.

2. Methodology

This section presents the approach used to study grain boundary–dislocation interactions with computational methods, and the methods to establish thermo-kinetic models for the GB structure – property relationships.

2.1. Molecular dynamics simulations with bi-crystals

Atomic simulations were performed using the LAMMPs programme [30], with two embedded atom method (EAM) and one modified (MEAM) potentials. These potentials were chosen for their effectiveness to simulate the Σ5 grain boundary energy and the stable and unstable stacking fault energy, which are important parameters for dislocation nucleation. The potentials will be referred to as EAM1 [31], EAM2 [32] and MEAM [33] in this paper.

Simulations were performed with bi-crystals of pure FCC aluminium, with tensile stress applied by assigning a constant uniaxial strain rate normal to the GB plane. The bi-crystals had a nominal 15 nm gap between the adjacent GBs and between the periodic simulation cell boundaries, which is consistent with prior bi-crystal simulations [22,23,28]. The Σ5(310) symmetric tilt GBs have the <010> tilt axis.

Fig. 1 provides a schematic of the bi-crystal geometry, dimensions and characteristic GB regions.

Multiple metastable bi-crystals were formed with EAM1, EAM2, and MEAM using the well-established rigid-body translation and iterative GB layer deletion procedure described in Ref. [34]. Using this method, 23 EAM1, 21 EAM2 and 25 MEAM bi-crystals were

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