Atomistic study of athermal cross-slip and its impact on the mechanical properties of iridium

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Abstract

The mechanical behaviour of the face-centred cubic metal iridium is exceptional in that it undergoes brittle transgranular or intergranular fracture after extensive plastic deformation. We present a model for the origin of this behaviour that is based on the features of the cores of screw dislocations specific to this transition metal. Atomistic simulations performed using a bond-order potential find a planar core structure that corresponds to dissociation into Shockley partials and a metastable, non-planar core spread into two {1 1 1} planes. Stress-induced transformations between the two core configurations were studied and form the basis for a mechanism for cross-slip that requires neither thermal activation nor full constriction of the partials. The associated high rate of cross-slip leads to extremely intense forest hardening and a dislocation density that increases precipitously with plastic strain to the extent that brittle cleavage is a natural consequence.
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1. Introduction

The physical and mechanical properties of the face-centred cubic (fcc) transition metal iridium are in many ways exceptional. A refractory metal with a melting temperature of 2443 °C, iridium is highly resistant to oxidation and corrosion [1]. However, it is a material that undergoes both transgranular and intergranular fracture even at elevated temperatures [2–7]. The propensity for transgranular cleavage in both polycrystalline and single crystal iridium is particularly unusual since the fcc metals are regarded as prototypically ductile owing to their excellent and weakly temperature-dependent plasticity. In this paper, we will present a model for the origin of this behaviour that is based on the results of atomistic simulations of dislocation core structures performed using a recently constructed bond-order potential (BOP) [8–10].

Transgranular cleavage is a common low temperature failure mode in many metallic materials but not in elemental fcc metals. It is often attributed to the limited mobility of dislocations at low temperatures that then inhibits the operation of dislocation sources, leading to inadequate dislocation multiplication. Brittle failure then results because stress concentrations are not relaxed rapidly enough via dislocation mediated plasticity. The best known example is the body-centred cubic (bcc) metals [11], in which the mobility of screw dislocations is strongly temperature dependent owing to their non-planar core structures. Similarly, the limited mobility of dislocations at ambient and low temperatures is responsible for the brittleness of many intermetallic compounds. On the other hand, pure fcc

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metals, such as aluminium, nickel and the noble metals, all fail by plastic rupture even at very low homologous temperatures because in these metals dislocation mobility is high and not strongly temperature dependent. The fundamental reason for this behaviour is that dislocations in fcc metals possess planar cores confined to {111} planes owing to their splitting into Shockley partials. The Peierls stress of dislocations with such planar cores is very low and any temperature dependence of their yield stress arises mainly from external effects such as solution hardening.

In contrast with all other fcc metals, extremely pure single crystals and polycrystals of iridium undergo cleavage and/or brittle intergranular fracture at temperatures up to 500 °C. The primary cleavage planes are of {100} and {210} type [5,12]. Importantly, cleavage does not occur during elastic loading, as is the case in usual brittle materials, but instead occurs after a period of extensive, neck-free plastic deformation [13]. Hence, this behaviour cannot be attributed to a low mobility of dislocations that could be related, for example, to sessile non-planar cores. The plastic deformation conforms to the usual fcc octahedral slip systems [13], and dislocations are observed to dissociate into Shockley partials on the {111} planes in a manner consistent with all other fcc metals. Due to a very high stacking fault energy, the separation between partials, estimated by high-resolution transmission electron microscopy (HRTEM) observations, is only around 8 Å in the case of the screw dislocation [14]. However, such a narrow splitting is not unique to iridium. Similar and even smaller widths of splitting have been observed, for example, in aluminium [15]. Thus, crystallographically the plastic deformation is identical to that in all other fcc metals. The feature that does set iridium apart from other fcc metals is the extraordinarily high, homogeneously distributed dislocation density accumulated during plastic deformation [13].

Consequently, while the glide behaviour of dislocations in iridium is the same as in other fcc metals, dislocation storage and multiplication take place at a significantly higher rate, producing the unusually high dislocation densities observed. The main theme of this paper is the explanation of this very high rate of dislocation multiplication on the basis of the atomic-level properties of dislocations. Specifically, atomistic simulations of screw dislocations in iridium employing a BOP show that, in addition to a planar core structure, a metastable non-planar configuration exists that may serve as an intermediate configuration for cross-slip which then does not require thermal activation or full constriction of the partials in the primary plane [8,9]. Such cross-slip is driven essentially by applied stresses that help to reduce the width of splitting between partials. Hence, dislocation core structure transformations are the basis for athermal cross-slip that can occur at a high rate even at low homologous temperatures, in comparison with other metals with the fcc crystal structure. The rapid broadening of slip bands that result from high rates of cross-slip leads to pronounced forest hardening and high

rates of dislocation storage and multiplication. The high rate of dislocation storage is compensated by dislocation multiplication via a large number density of Frank–Read sources [16] generated via the double cross-slip mechanism [17]. We propose that in iridium the exceptional rate of dislocation storage and multiplication is ultimately responsible for cleavage since the density of stored dislocations may reach locally levels where the mean free path over which dislocations may glide becomes so small that stress concentrations cannot be relaxed by further plastic flow [8].

2. Atomistic simulation methodology

Interatomic bonding in the transition metals is dominated by the formation of angularly dependent, unsaturated d-bonds [18]. Hence, it is essential that the effects of angularly dependent bonding are captured accurately in the description of interatomic bonding in iridium. To this end, we have adopted the BOP formalism, a real-space, $O(N)$, semi-empirical tight-binding scheme [19–21]. The BOP formalism has been demonstrated to be eminently suitable for the atomistic simulation of extended defects in transition metals [22–24] and intermetallic compounds [25,26].

The construction of the BOP for iridium is described in detail in Refs. [9,10]. This BOP was tested extensively in order to assess its efficacy as a description of bonding in fcc iridium along with its transferability to structures with symmetries and coordinations very different from the fcc environment [10]. Calculations of the phonon spectra [27], energy differences between different crystal structures and the tetragonal and trigonal deformation paths [28,29] using the BOP were all in excellent agreement with experimental and/or ab initio calculated data. These tests showed that BOP is well transferable to structures with greatly reduced symmetry and different coordination [9,10].

In this study, all atomistic simulations of the screw dislocation employed a cylindrical block of atoms one Burgers vector thick and of radius 60 Å (2171 atoms). The axis of the cylinder was parallel to $[1\bar{1}0]$ and periodic boundary conditions were applied in this direction. The dislocation was introduced into the centre of the block by applying to all atoms the displacement field evaluated using the anisotropic elastic theory of dislocations [30].

The block was divided into three concentric regions. Atoms in the inner part of the block (region I) with radius 30 Å (1051 atoms) were relaxed using a molecular-statics method with forces calculated by the BOP. The relaxation proceeded until the force acting on any atom was less than 0.01 eV/Å while atoms in the outer part of the block (regions II and III, with thicknesses 12 and 18 Å, respectively [8]) were held at their initial positions. The coordinates of all atoms (regions I, II and III) in the block were updated self-consistently using Green's function boundary conditions (GFBCs) [31,32] once the inner region was fully relaxed using the incompatibility forces generated in region II. Around four iterations of atomistic relaxation followed