



Full length article

Oxygen - Dislocation interaction in zirconium from first principles

Nermine Chari^{a,1}, David Rodney^b, Emmanuel Clouet^{a,*}^a DEN-Service de Recherches de Métallurgie Physique, CEA, Université Paris-Saclay, F-91191, Gif-sur-Yvette, France^b Institut Lumière Matière, CNRS-Université Claude Bernard Lyon 1, F-69622, Villeurbanne, France

ARTICLE INFO

Article history:

Received 14 March 2017

Received in revised form

2 May 2017

Accepted 3 May 2017

Available online 5 May 2017

Keywords:

Dislocation

Plasticity

Zirconium

Oxygen

Density functional theory

Hardening

ABSTRACT

Plasticity in zirconium alloys is mainly controlled by the interaction of $1/3 \langle 1\bar{2}10 \rangle$ screw dislocations with oxygen atoms in interstitial octahedral sites of the hexagonal close-packed lattice. This process is studied here using *ab initio* calculations based on the density functional theory. The atomic simulations show that a strong repulsion exists only when the O atoms lie in the dislocation core and belong to the prismatic dislocation habit plane. This is a consequence of the destruction of the octahedral sites by the stacking fault arising from the dislocation dissociation. Because of the repulsion, the dislocation partially cross-slips to an adjacent prismatic plane, in agreement with experiments where the lattice friction on screw dislocations in Zr-O alloys has been attributed to the presence of jogs on the dislocations due to local cross-slip.

© 2017 Acta Materialia Inc. Published by Elsevier Ltd. All rights reserved.

1. Introduction

Zirconium is a hexagonal close-packed (hcp) transition metal, which deforms mainly by glide of $\langle a \rangle = 1/3 \langle 1\bar{2}10 \rangle$ dislocations in $(10\bar{1}0)$ prismatic planes [1–3]. All experimental studies [3–13] point to a low-temperature behavior controlled by lattice friction acting on screw dislocations. This lattice friction is extrinsic in nature and arises due to interactions with interstitial solute atoms like oxygen, as indicated by the rapid increase of the critical resolved shear stress for prismatic slip in single crystals when the oxygen content increases [7–10]. Moreover, microscopic observations of deformed Zr alloys [10,14,15] show long rectilinear screw dislocations, whose mobility is therefore limited compared to other orientations.

By way of contrast, in pure zirconium, dislocations of all characters have similar mobilities [16] and the plastic behavior becomes almost athermal like in fcc metals for very low O contents (≤ 100 ppm in weight) [7,9]. The easy prismatic glide of screw dislocations in pure Zr is consistent with *ab initio* calculations, which show that screw dislocations have a ground state dissociated in a prismatic plane [15–18], with a small energy barrier opposing prismatic glide

and a corresponding Peierls stress below 21 MPa [18]. Screw dislocations in Zr can adopt other configurations with a core partly or totally spread in a first-order pyramidal plane [16,19,20]. These configurations however are of higher energy and contribute only to secondary slip, which is activated above room temperature.

Oxygen is therefore added to zirconium alloys for its strengthening effect at an average content between 600 and 1200 wppm Zr (0.3–0.7 at.%) and with a maximum accepted content of 2000 wppm (1.2 at.%) [21]. The same hardening of prismatic slip by O solutes has been reported in titanium [3,4,22–26]. However, unlike in Zr, an intrinsic lattice friction exists even in pure Ti, because in this metal, the screw dislocations glide by a locking-unlocking mechanism due to the fact that their ground state is dissociated in a first-order pyramidal plane [16].

The origin of hardening caused by an O addition in Zr and Ti is not clearly understood. A control of dislocation glide through their interaction with interstitial solute atoms, as described by Fleisher model [27], has been proposed [6,23,28], but it is not clear why such interaction would mainly affect the screw dislocations. Moreover, this interaction must involve dislocation cores [25,29], since no elastic interaction exists in an hcp crystal between an $\langle a \rangle$ screw dislocation and an interstitial solute atom in an octahedral interstitial site [4]. Other authors attributed the lattice friction to the presence of jogs on the screw dislocations, with an increase of the jog density with the O content [7,9,12,14]. *Ab initio* calculations in Ti [30] have evidenced a short range repulsive interaction between

* Corresponding author.

E-mail address: emmanuel.clouet@cea.fr (E. Clouet).¹ Present address: AREVA NP, 10 rue Juliette Récamier, F-69006 Lyon, France.

screw dislocations and oxygen atoms, which can lead to solid solution hardening and to the creation of jogs by local dislocation cross-slip.

The aim of the present article is to characterize the short-range interactions between $\langle a \rangle$ screw dislocations and O atoms in Zr in order to better understand the effect of O addition on the lattice friction in this metal. Since core effects are expected, we will use an electronic structure description of atomic interactions based on *ab initio* calculations. We first analyse the interaction of O atoms with the prismatic and pyramidal stacking faults involved in the various potential dissociations of the screw dislocation. Interaction of an oxygen atom with the three different stable and metastable configurations of an $\langle a \rangle$ screw dislocation is then investigated. Consequences of the repulsive interaction evidenced by these calculations are discussed in the last section.

2. Methods

Ab initio calculations are performed with the Pwscf code [31]. We use the generalized gradient approximation with the exchange-correlation functional of Perdew, Burke and Ernzerhof [32]. Zr and O atoms are modeled with an ultrasoft Vanderbilt pseudopotential, with 4s and 4p semi-core electrons included in the valence states of Zr. Electronic wave functions are described with plane waves with an energy cutoff of 28 Ry. A regular grid is used for the integration in reciprocal space, with $14 \times 14 \times 8$ k-points for the primitive hcp cell and an equivalent k-point density for larger supercells. The electronic density of state is broadened with the Methfessel-Paxton function, with a broadening of 0.3 eV. Atoms are relaxed until all atomic force components are below 10 meV/Å. The same set of *ab initio* parameters has already been shown to predict Zr lattice parameters and elastic constants in good agreement with experimental data [18] and to provide an accurate description of $\langle a \rangle$ screw dislocations in pure zirconium [16,18,19].

We checked that the most stable position for O atoms in the hcp Zr lattice is the octahedral interstitial site. Other interstitial positions – tetrahedral, basal tetrahedral and crowdion sites – have a higher energy (Table 1). The energy difference between these various interstitial configurations varies only slightly with the size of the supercell, showing that there is no complex long-range interaction between O atoms and their periodic images.

3. Oxygen interaction with stacking faults

$\langle a \rangle$ screw dislocations in Zr can adopt several configurations with either a planar or a non-planar dissociation in either a prismatic or a pyramidal-I plane, or a combination of both [16]. We therefore study the interaction of O atoms with the corresponding prismatic and pyramidal stacking faults [18–20], as a first step towards modeling the interaction of O atoms with screw dislocations.

Table 1
Energy of an O atom in a perfect hcp lattice for different configurations: octahedral (O) taken as the reference, tetrahedral (T), basal tetrahedral (BT) and crowdion (C). Results are given for different supercells defined by their number N_{sites} of lattice sites. The supercell is based either on the hcp primitive cell or corresponds to the cell used for dislocation modeling (cf. §4.1).

cell	N_{sites}	ΔE (eV)			
		O	T	BT	C
$3 \times 3 \times 2$ hcp	36	0.	0.90	0.93	1.82
$4 \times 4 \times 3$ hcp	96	0.	0.87	0.91	1.90
$5 \times 5 \times 4$ hcp	200	0.	0.84	0.87	1.91
$8 \times 5 \times 2$ dislo	320	0.	0.90	0.95	

3.1. Simulation setup

The interaction energy of an O atom with a stacking fault is defined as

$$E^{\text{int}} = E_{\text{SF-O}} - E_{\text{O}} - E_{\text{SF}} + E_{\text{bulk}},$$

where $E_{\text{SF-O}}$, E_{O} , E_{SF} , and E_{bulk} are the energies respectively of the cell containing both the O atom and the stacking fault, the cell with only the O atom, the cell with only the stacking fault, and the perfect hcp bulk cell. The same tri-periodic simulation cell is used for all four calculations, with only a shift equal to the fault vector added to the periodicity vector perpendicular to the fault plane for $E_{\text{SF-O}}$ and E_{SF} [18]. Only one fault and one O atom are introduced in the simulation cells. The O atom is placed in the already relaxed stacking fault and full atomic relaxations, without constraint, are then performed.

The lengths of the periodicity vectors are defined by three integers, n , m , and p . For the prismatic stacking fault, these vectors are $n/3 [1\bar{2}10]$, $m [0001]$, and $p [10\bar{1}0]$, and for the pyramidal fault $n/3 [1\bar{2}10]$, $m/3 [2\bar{1}\bar{1}3]$, and $p/3 [\bar{1}\bar{1}23]$. In both cases, the number of atoms in the simulation cell is $4nmp$. The integers n and m fix the surface of the stacking fault, and thus the fraction of solute atom per fault area, whereas p controls the distance between the fault plane and its periodic images. We have checked the convergence of the calculations with respect to these cell dimensions in Tables 2 and 3.

3.2. Prismatic stacking fault

The octahedral sites located in the fault plane (sites O_0 in Fig. 1a) are destroyed by the shear associated with the stacking fault. These sites become unstable positions for the O atom, which migrates during atomic relaxation to a nearby new octahedral site created by the fault. This site, labelled O_p in Fig. 1a, has a geometry close to an octahedral site in the body centered cubic (bcc) structure [33]. It is a stable position for the O atom, without any reconstruction of the fault, but the interaction energy is positive, and therefore repulsive (Table 2). This is in agreement with oxygen being an α -stabilizer since O is then expected to have a higher energy in the bcc than in the hcp structure. A similar result has been reported in Ti [30,33,34].

A slightly repulsive energy is also obtained for the octahedral sites located in the immediate vicinity of the fault plane (sites O_1 and O_2 in Fig. 1a) (see Table 2). There is therefore no attractive site and oxygen atoms can only increase the prismatic stacking fault energy in Zr.

3.3. First-order pyramidal stacking fault

The pyramidal fault also destroys the octahedral sites located in the fault plane (sites O_0 in Fig. 1b) and creates new bcc-like octahedral sites (sites O_p in Fig. 1b) that are stable insertion sites but with a repulsive interaction energy (Table 3), although slightly less

Table 2
Interaction energies (meV) of an oxygen atom with a prismatic stacking fault for different positions of the oxygen interstitial (see Fig. 1a). Calculations are performed for different $n \times m \times p$ cell sizes corresponding to the periodicity vectors $n/3 [1\bar{2}10]$, $m [0001]$, and $p [10\bar{1}0]$.

site	$4 \times 4 \times 3$	$4 \times 2 \times 4$	$2 \times 4 \times 4$	$4 \times 4 \times 4$	$5 \times 5 \times 4$
O_p	164	188	166	161	–
O_1	33	–	–	26	27
O_2	44	–	–	40	40

Download English Version:

<https://daneshyari.com/en/article/5436176>

Download Persian Version:

<https://daneshyari.com/article/5436176>

[Daneshyari.com](https://daneshyari.com)