

# Core structure, dislocation energy and Peierls stress for $1/3 \langle 11\bar{2}0 \rangle$ edge dislocations with $(0001)$ and $\{1\bar{1}00\}$ slip planes in $\alpha$ -Zr

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## Abstract

Atomic-scale simulations of edge dislocations of the  $1/3 \langle 11\bar{2}0 \rangle (0001)$  and  $1/3 \langle 11\bar{2}0 \rangle \{1\bar{1}00\}$  slip systems have been carried out using a Finnis-Sinclair-type interatomic potential for  $\alpha$ -zirconium. The distribution of atomic displacements in the dislocation core shows that in this model the edge dislocation in the basal plane dissociates into two Shockley partials whereas the dislocation in the prism plane remains undissociated. The effective core radius and core energy are estimated, and dislocation response to increasing applied shear strain is investigated. The core properties and the critical stress for dislocation glide (Peierls stress) depend sensitively on whether the core extends or not.

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## 1. Introduction

Atomic-scale computer simulation of dislocations is an essential part of the modern multi-scale approach to predictive modelling of material service properties, particularly in relation to strength and plasticity. The results of such simulation provide detailed information about dislocation core structure, dislocation motion, and interaction with point defects, their clusters and other obstacles, and so give qualitative understanding of governing mechanisms. It also allows quantitative evaluation of the stress-strain curve, the critical resolved shear stress (CRSS) and dynamic and thermal effects. Furthermore, atomic-scale dislocation modelling of specific conditions (e.g.  $T=0$  K) can test analytical concepts of the elasticity theory of dislocations.

The primary topic of the present paper is atomic-scale simulation of two edge dislocations in the HCP metal  $\alpha$ -Zr. The dislocations have the same Burgers vector  $\mathbf{b} = 1/3 \langle 11\bar{2}0 \rangle$  but different glide planes, namely  $(0001)$  and  $\{1\bar{1}00\}$ . The CRSS for dislocation glide at 0 K (the Peierls stress), the dislocation core energy and the atomic displacements in the core region have been evaluated in order to contrast the effect of different slip systems. The information gained provides a background for investigation of the interaction of dislocations of the prism- and basal-slip systems with typical point defect clusters created by displacement cascades in radiation damage [1], the results of which are presented in accompanying papers [2,3].

## 2. Simulation technique and identification of the dislocation core

Simulations of the dislocations were carried out using an equilibrium short-range many-body interatomic potential for Zr [4,5]. In order to allow long-range (distance  $\gg b$ ) motion

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of the dislocation, periodic boundary conditions were employed along the direction of  $\mathbf{b}$  ( $x$ -axis) as well as the line direction ( $y$ -axis). Following the method described in [6], the initial unrelaxed model with an edge dislocation was created from two half-crystals  $z \geq 0$  and  $z < 0$  with  $x$  dimension  $(N+1)b$  and  $Nb$ , respectively. The lower half-crystal ( $z < 0$ ) is elastically elongated by  $b/2$  along  $x$  and the upper half is compressed by  $b/2$ : the two parts are then joined and relaxed to form a perfect dislocation with  $x$ - $y$  slip plane. Although the two half-crystals are strained by  $\pm b/2$ , the overall elastic deformation of a cell of size  $\sim 200b$  is small ( $< 0.25\%$ ). Furthermore, the dislocation glide plane coincides with the neutral stress axis of the model and the dislocation core is in a region of zero stress. It has been confirmed that effects of the boundary conditions can be neglected (see [6] for details). The model is bounded on the upper and lower  $x$ - $y$  faces by boxes of immobile atoms. The lower box is fixed whereas the upper one can be displaced rigidly to apply either a shear strain or stress to the cell of mobile atoms. In the present case, we simulated athermal properties ( $T = 0$  K) and so shear strain was applied (box displacement in the  $x$ -direction): the corresponding applied stress was computed from the force on the box from the inner region atoms after relaxation.

In this work and that of the accompanying papers [2,3], identification of the atomic structure of the defect regions was conducted using the local geometry approach where the number and position of the first neighbours are checked for each atom. Twelve neighbours in HCP coordination correspond to the perfect HCP structure, whereas nine atoms in HCP coordination of 12 first neighbours indicate an FCC arrangement. Eleven or ten first neighbours occur at the edge of partial

dislocations and lower coordination numbers can occur in the core of the  $1/3 \langle 11\bar{2}0 \rangle \{1\bar{1}00\}$  dislocation. Following Frank [7] (see also [8] or [9]), three different stacking faults can arise on the basal plane. Three atomic layers with nearest neighbours in FCC coordination define the extrinsic fault E, whereas one or two layers represent the  $I_1$  and  $I_2$  intrinsic faults, respectively.

### 3. Atomic displacements and structure of dislocation core

Figs. 1 and 2 show the core structure of the  $1/3[11\bar{2}0](0001)$  and  $1/3[11\bar{2}0](1\bar{1}00)$  edge dislocations, respectively, after conjugate gradients relaxation to minimise the potential energy. The former dislocation splits into two Shockley partials in the basal plane whereas the latter does not dissociate. The linear dimensions of the dislocation core can be extracted from analysis of the displacement of atoms originally in the plane  $z = 0$ , as shown in Figs. 3 and 4 for the basal- and prism-plane dislocations, respectively. Fig. 3 shows the distinctive features of atom displacements,  $\mathbf{u}(x)$ , in the core of a dissociated dislocation. (Note that only atoms of the upper half-crystal are treated here. If the displacements of atoms at the top of the lower half-crystal are subtracted from these displacements to give the displacement differences across the glide plane, they would exhibit the usual displacement discontinuity  $b$  (rather than  $b/2$ ) in  $u_x$ .) The component  $u_x(x)$  along the glide direction  $\mathbf{b}$  has two regions of high gradient at the position of the partials. Their exact location is determined by the extremum of

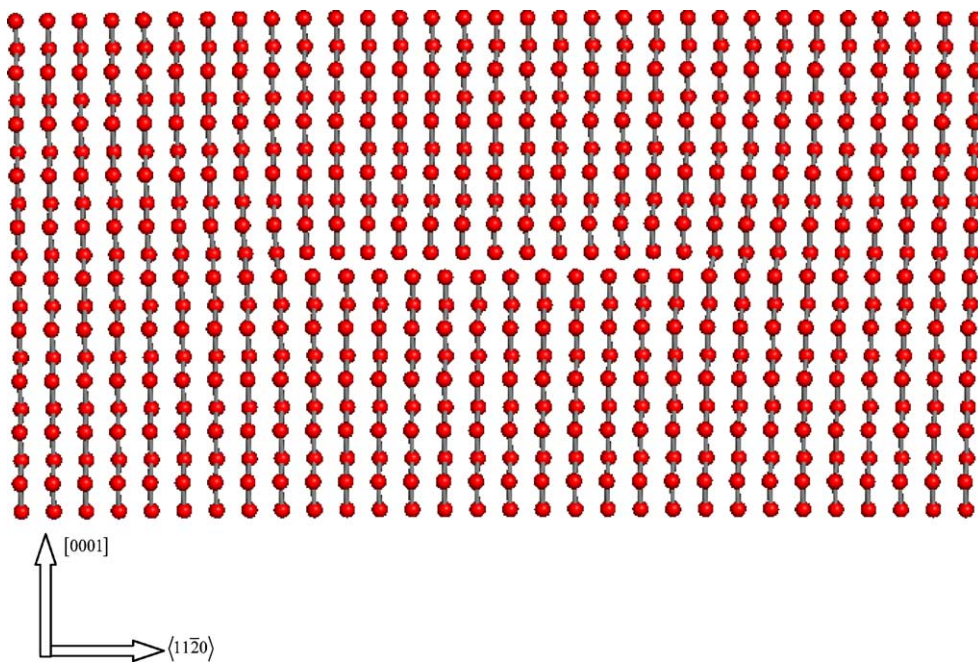


Fig. 1.  $[1\bar{1}00]$  projection of the core structure of the  $1/3[11\bar{2}0](0001)$  dislocation, which splits into partials on the basal plane. The  $(11\bar{2}0)$  planes perpendicular to  $\mathbf{b}$  are shown by sticks.

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