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Self-interstitial atom clusters as obstacles to glide of $1/3\langle 1\,1\,\bar{2}\,0\rangle\{1\,\bar{1}\,0\,0\}$ edge dislocations in α-zirconium

R.E. Voskoboynikov [a,*], Yu.N. Osetsky [b], D.J. Bacon [a]

[a] *Materials Science and Engineering, Department of Engineering, The University of Liverpool, Liverpool L69 3GH, UK*
[b] *Computer Sciences and Mathematics Division, Oak Ridge National Laboratory, One Bethel Valley Road, P.O. Box 2008 MS-6138 Oak Ridge, TN 37831, USA*

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Abstract

Atomic-scale details of interaction of a $1/3\langle 1\,1\,\bar{2}\,0\rangle\{1\,\bar{1}\,0\,0\}$ edge dislocation with clusters of self-interstitial atoms (SIAs) in α-zirconium has been studied by computer simulation. Four typical clusters are considered. A triangular cluster of five SIAs lying within a basal plane bisected by the dislocation glide plane is not absorbed by the dislocation but acts as a moderately strong obstacle. A 3-D SIA cluster lying across the glide plane is completely absorbed by the dislocation by creation of super-jogs, and is a weak obstacle. Interaction of the dislocation with glissile SIA loops with perfect Burgers vector inclined at 60° to the dislocation glide plane shows that the process depends on the vector orientation. Defects of the two orientations are strong obstacles, and one, which initially forms a sessile segment on the dislocation line, is particularly so.

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1. Introduction

Strength, toughness and plasticity of structural metals are largely determined by dislocation behaviour, and the degradation of mechanical properties under exposure to irradiation is strongly influenced by the formation of point defect clusters, which are effective barriers for dislocations moving under stress. In the present report we consider the effect of self-interstitial-atom (SIA) clusters on the glide of edge dislocations in the prism slip system of the HCP metal α-Zr. Zirconium and its alloys are important because of their practical significance for the safe operation of modern commercial light water reactors [1]. Fuel cladding, for example, is made of Zr-based alloy and, being the barrier between nuclear fuel pellets and the surrounding environment, is subjected to high dose irradiation. This results in creation of point defects and their clusters by displacement cascades, and these are known to act as obstacles to dislocation motion and, in addition to raising the yield and flow stress [1], to cause flow localisation by dislocation channelling in prism and basal planes [2].

We present here the first results for the interaction with such obstacles of the $1/3\langle 1\,1\,\bar{2}\,0\rangle\{1\,\bar{1}\,0\,0\}$ edge dislocation gliding under increasing strain in a prism plane. We consider four typical but distinct SIA clusters. The nature of the atomic mechanisms are revealed, strain–stress curves are determined and the critical resolved shear stress (CRSS) at which a cluster is overcome by the dislocation is obtained. Two of the SIA clusters for this modelling are those found in recent extensive molecular dynamics simulations of displacement cascades in Zr [3]. In addition, two large clusters (117 SIAs) in the form of perfect dislocation loops with Burgers vector $\mathbf{b} = 1/3\langle 1\,1\,\bar{2}\,0\rangle$ making angle of 60° and 120° with **b** of the dislocation are considered. Perfect loops such as these

* Corresponding author. Present address: OCIAM, Mathematical Institute, 24–29 St. Giles, Oxford OX1 3LB, UK.
E-mail address: voskoboynikov@maths.ox.ac.uk (R.E. Voskoboynikov).

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are observed experimentally by TEM in neutron-irradiated Zr [1]. Obstacle effects on the $1/3\langle 1\,1\,\bar{2}\,0\rangle(0\,0\,0\,1)$ edge dislocation of the basal-slip system have also been modelled and the results are described in an accompanying paper [4].

2. Computer simulation method

The technique described in [5] based on the method in [6] has been adopted to conduct atomic-scale simulation of the edge dislocation with $\mathbf{b} = 1/3\langle 1\,1\,\bar{2}\,0\rangle$ gliding on a $\{1\,1\,0\,0\}$ prism plane. With the interatomic potential used [7,8], this dislocation does not dissociate on this plane and has a Peierls stress of 5.6 MPa [5]. Thermal effects are not considered here and so simulation of 0 K was carried out by relaxation using the conjugate gradients method. An interstitial cluster was introduced in the relaxed, dislocated model and the equilibration procedure repeated again. A resolved shear strain was then applied, increasing from zero in steps of 10^{-4}. After each step, the crystal was relaxed and the resultant applied shear stress was evaluated (see [5]). A local geometry approach [5] was adopted to visualize and identify the atomic structure of the dislocation core and defect cluster. A simulation was considered finished when the gliding dislocation overcame the cluster and the CRSS was taken as the maximum on the stress–strain curve. The model contained more than 3.2×10^6 free atoms and the distance between the periodic boundaries along the dislocation line, i.e. the spacing along the row of clusters, was 137 b, where b is the magnitude of **b**.

3. Results

3.1. Interaction with triangular SIA cluster in basal plane

Computer simulation suggests that nearly 10% of all SIAs created in displacement cascades agglomerate in triangular clusters of 4, 5 and 6 SIAs all lying in one (0 0 0 1) atomic plane [3]. Interaction of the dislocation with a 5-SIA cluster (15 atoms sharing 10 lattice sites) lying in a basal plane and intersected through its centre by the dislocation glide plane has been simulated. Fig. 1 shows (a) the initial configuration, (b) the stress–strain curve, and (c–f) several snap-shot visualisations taken from the computer modelling. Initially, there is a slight repulsion of the dislocation by the cluster that leads to an increase of the flow stress above the Peierls-stress value. With further straining the stress increases to point c on the stress–strain plot and the dislocation then enters the cluster with a stress reduction, see c and d on Fig. 1b and Fig. 1c and d. The dislocation line is then pinned by the cluster and bends as further strain leads to near-linear increase

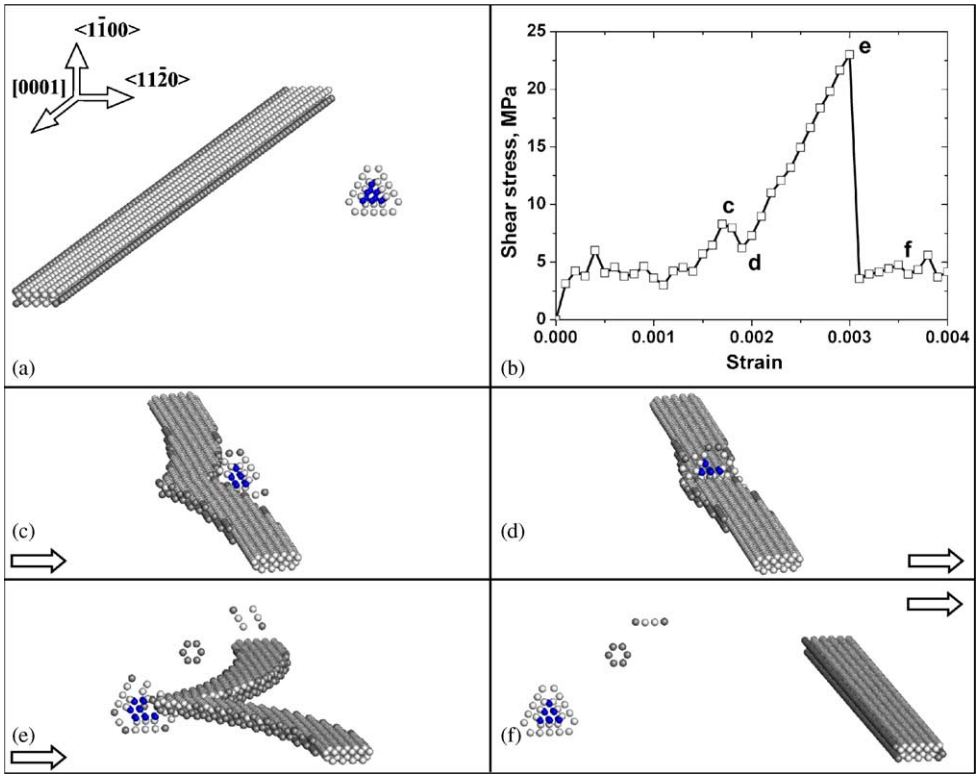

Fig. 1. Interaction of the edge dislocation with 5-SIA triangular cluster. In this and other figures, white, grey and black spheres correspond to 12, 10–11 and 6–8 first neighbours in FCC coordination, respectively. (a) Initial configuration; (c–f) typical configurations marked at strain–stress curve (b). The unmarked white arrow here and in other figure shows the direction of dislocation glide.