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Non-Schmid behavior of extended dislocations in computer simulations of magnesium

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Critical resolved shear stresses are studied by means of atomistic simulations for dissociated screw dislocation with Burgers vector $1/3[11\bar{2}0]$ in magnesium. Deviation from Schmid law is demonstrated for dislocation glide on basal and prismatic planes. It was shown that all stress components have influence on the critical resolved shear stress. The non-Schmid behavior is caused by changes of dislocation core width due to acting of non-glide stress components. In atomistic simulations, the critical resolved shear stress varies in the range of 0.2–6.7 MPa for basal slip and 25–55 MPa for prismatic slip depending on values of non-glide stress components. It is expected that such behavior can be partially responsible for scattering of experimental data for yield stress in magnesium.

1. Introduction

It is traditionally accepted that plastic deformation of materials obeys Schmid's law. The Schmid's law [1,2] tells that dislocation slip would occur when the shear stress resolved on the glide plane and in the glide direction reached a critical value, the critical resolved shear stress (CRSS). However, the cases of Schmid's law breakdown are also known. The most prominent example of non-Schmid behavior is slip in bcc metals, such as tungsten or molybdenum [3–5]. The CRSS is dependent on the stress components perpendicular to the Burgers vector for glide of 1/2[1 1 1] dislocation in bcc materials [6].The deviations from Schmid law are also observed in intermetallic compounds (e.g. Ni_3Al) [7–9] with $L1_2$ structure.

Twinning is another deformation mode, which in general obeys the Schmid law. However, the non-Schmid behavior of twinning in hcp metals was discussed recently in literature. Such behavior was reported for twinning in magnesium and its alloys [10–12]. A significant portion of twins with low Schmid factor was observed in hcp Zr [13]. Importance of non-Schmid stress on twinning nucleation mechanisms in magnesium was also mentioned [14].

The non-Schmid behavior of bcc metals is caused by non-planar dissociation of slip dislocations [15]. The effect of non-glide components of applied stress in bcc metals can be understood in the following way. Dislocation core dissociates in several planes producing partials connected by stacking fault segments. Such dissociation can be profitable from energetical point of view. Some of these partials can have Burgers vector components perpendicular to the initial Burgers vector of the dislocation. The sum of perpendicular components is zero. However, they can be affected by stress components perpendicular to the whole Burgers vector of dislocation. As results the dislocation motion is also affected by these components. Due to presence of dissociated dislocation similar scenario is also possible in close packed structures such as fcc and hcp. However, it is generally accepted that effect is not so large as in the case of bcc structure. For instance, Nabarro [16] considered deviations from Schmid law for screw dislocation in fcc structure. He concluded that reduction in CRSS caused by the dissociation of dislocation is almost negligible and deviations from Schmid law are unobservably small. On the other hand, the significant inclination from Scmid law was observed in Zn single crystals [17], where variation in the resolved normal stress resulted in a 30 percent drop in the resolved shear stress.

It is worth noting that hcp crystals reveal significant plastic anisotropy in contrast to fcc crystals. For instance, the ratio of CRSS for basal and non-basal slip can reach values of 1:80 [18–22] in magnesium alloys. Besides large variations can arise in the relative values of CRSS for different slip modes. It is sometimes accepted [19] that these variations can be originated from hardening phenomena. However, it is can be supposed that partially they can be

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caused by non-Schmid effect. The aim of present paper is to explore non-Schmid behavior of screw $1/3[11\bar{2}0]$ dislocation in magnesium by computer simulations. We would like to demonstrate the phenomenon for basal and prismatic slip and to open discussion about importance of non-Scmid effects in magnesium.

2. Methods

The calculations were performed by using of embedded atom method (EAM) potential developed by Sun et al. [23] and by using of LAMMPS [24] for simulation and OVITO [25] for visualization. Simulation block was oriented with its x-axis parallel to $[1\bar{1}00]$, y-axis parallel to $[000\bar{1}]$ and z-axis along $[11\bar{2}0]$ direction. The Sun et al. potential was selected from several widely used EAM potentials because it provides the best agreement of with DFT and experimental data for dislocation properties [26]. The calculation were performed with block size 1100 Å×1034 Å×6.36 Å. Several block sizes were tested in order to ensure that block is large enough to neglect the surface effects. The size of block in z-direction was taken as small as possible in order to minimize calculation efforts. However, it is taken larger than cut-off distance of interatomic potential in order to avoid self-interaction of atoms through periodic boundary conditions. Screw dislocation with dislocation line along z-axis was inserted in the center of simulation box by imposing of anisotropic elastic field obtained from analytical solution [27]. Periodic boundary conditions were applied in z-direction. Positions of atoms in outer layer of the block were fixed in x- and y-directions and energy minimization was performed in inner part of block in order to obtain relaxed dislocation core. Geometry of simulation block is sketched in Fig. 1.

The migration of dislocations was studied by application of glide shear strain to the block in small steps ($\Delta\varepsilon = 0.00001$) and subsequent minimization of block energy by dumped dynamics (fire algorithm implemented in LAMMPS). The calculation were performed at 0 K and dislocation was considered as straight line. The glide stress components are σ_{zy} for basal slip and σ_{zx} for prismatic slip. We use here the same convention for notation of stress components as Ref. [27], i.e. σ_{ij} acts in the direction i and in the plane with normal along j. Constant non-glide stress was applied before application of glide stress to the block. The critical resolved shear stress was measured at different levels of applied non-glide stress. Different non-glide components of stress were considered. The σ_{xy} and σ_{xx} are completely non-glide and produce zero stress on both basal and prismatic slip systems. However, σ_{zx} and σ_{zy} can also play roles of non-glide stresses. If the dislocation glides on basal plane, the σ_{zx} component tries to cross-slip it to prismatic plane. The same is valid for prismatic plane and σ_{zy} stress component.

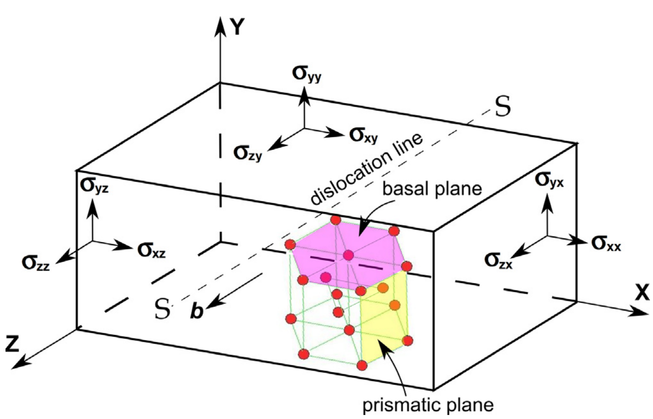

Fig. 1. Geometry of simulation block.

3. Results

3.1. Dislocation core structures

Fig. 2 shows γ-surfaces for basal (0 0 0 1) and prismatic $(1\,\bar{1}\,0\,0)$ planes. The γ-surfaces were produced by cut of crystal on the corresponding plane and the subsequent shift of one crystal part relative to another one. The relaxation of atomic position is allowed in the direction perpendicular to the cut. The γ-surfaces present dependence of energy on the shift. Minima on the γ-surface indicate positions of stable stacking fault on the corresponding plane. It can be seen from Fig. 2 that such minima are present on both γ-surfaces allowing dislocation dissociation on both planes. Corresponding energy of stacking faults are $\gamma = 0.296\ \mathrm{eV/nm^2}$ for basal I2 fault and $\gamma = 0.835\ \mathrm{eV/nm^2}$ for prismatic fault. Due to lower energy of basal stacking fault, the dislocation core dissociates in

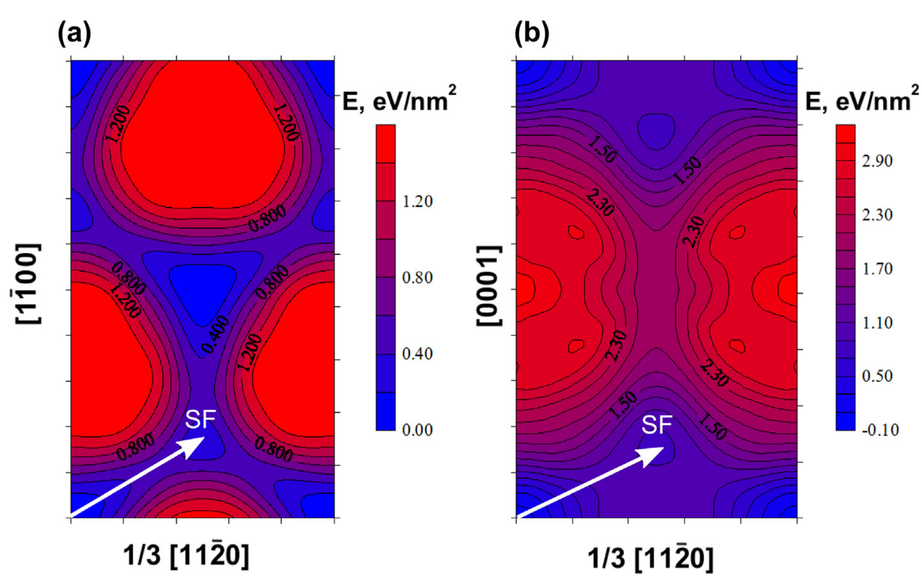

Fig. 2. γ-surfaces for (0 0 0 1) (a) and $(1\,\bar{1}\,0\,0)$ planes (b).