Interaction of a dislocation pileup with {332} tilt grain boundary in bcc metals studied by MD simulations

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The sustainability and capacity of macroscopic deformation by polycrystalline metals and metallic alloys is controlled by the propagation of dislocation-mediated slip through grains. In this paper, the interaction of a pileup of $1/2\langle 111 \rangle$ dislocations with the {332} tilt grain boundary (GB) is studied as a function of temperature in three bcc metals: iron (Fe), chromium (Cr), and tungsten (W). The interaction results in the transformation of the crystal dislocation into GB dislocations. The {332} tilt GB absorbs the crystal dislocations of the pileup, neither the transmission nor reflection of dislocations was observed. The reaction product at the GB is determined by the crystallography of the GB and the features of the crystal dislocations involved, specifically, the orientation of the Burgers vector and the glide plane of the dislocation. In general, the decomposition results in the formation of a sessile GB dislocation with a riser that facets the GB and several elementary disconnections that glide away. In some cases, the riser increases its length with the number of dislocations absorbed and a new asymmetrical grain boundary of {112}/{110} type is created. For a given external shear stress, the number of dislocations absorbed depends on the orientation of the Burgers vector, glide plane of the pileup, and material.

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I. INTRODUCTION

The mechanical response of polycrystalline metals and alloys is defined by a number of physical processes such as generation of dislocations, dislocation glide, dislocation-dislocation interaction, and interaction of the gliding dislocations with grain boundaries (GBs) [1]. The initiation of micro yielding is controlled by the initiation of dislocation glide, their multiplication, and the interaction with strengthening defects, while sustainability and capacity of macroscopic deformation is defined by the propagation of dislocation-mediated slip through grains [2–4]. GB strengthening or the Hall-Petch strengthening mechanism [5,6] is based on the observation that GBs impede dislocation movement and that the number of dislocations within a grain have an effect on how easily dislocations can traverse grain boundaries and travel from one grain to another. Indeed, the multiplication of dislocations leads to the formation of pileups whose propagation is controlled by the grain boundaries. This is why the knowledge of the grain morphology and substructure is important information usually supplied as one of the main characteristic of the structural material. Experiments involving nanotwinned pure copper show that the presence of nanometer-thickness nanotwins offers an exceptional combination of strength and ductility [7,8], suggesting that specific GBs may improve not only strength but ductility as well. Kapp *et al.* [9,10] found that grain coarsening in cyclically deformed Ni is distinctively amplified in regions of shear localization, strengthening the concept of deformation driven boundary migration. To rationalize these results, the interaction of dislocation pileup

(DPU)—inevitable upon severe plastic deformation—with several symmetric tilt grain boundaries (STGB) in copper, aluminum, and nickel was studied [11–17].

The above-noted works employed direct atomistic simulations by molecular dynamics (MD) which provided rich details on local structural transitions occurring as the DPU impinges on the GB interface, and helped to extend the Lee-Robertson-Birnbaum criteria by accounting for local stress-field at the GB due to the pileup [11]. A practical implementation of MD was realized via a hybrid atomistic/discrete-dislocation model. With such an approach, MD was applied to study the possible events such as absorption of the head dislocation, reflection, transmission, or the total absorption of the pileup. However, the above-mentioned studies are essentially limited to investigation of face-centered cubic (FCC) metals, while body-centered cubic (BCC) metals represent an important segment of structural materials widely applied in transport, medicine, and energy sectors.

This paper presents the first part of an investigation where we apply the hybrid atomistic/discrete-dislocation model to investigate the interaction of the DPU with a number of tilt boundaries in several BCC metals, namely, iron (Fe), tungsten (W), and chromium (Cr). The choice of these metals is driven by their wide application in the energy sector, in particular as structural materials for nuclear and space applications. The work consists in three parts, which correspondingly present the (i) investigation and analysis of the interaction mechanisms, (ii) effect of the grain boundary structure, and (iii) the effect of temperature and loading rate on the interaction mechanism.

Considering all GBs simulated in the project, three different types of reactions were observed, such as, absorption, transmission, and reflection. The type of reaction varies from one GB to another but all of them begins by the initial absorption of the first dislocation from the pileup. Along with the reactions, several line defects associated with the GB were observed, namely, grain boundary dislocations (GBD). Among the GBD, the ones that step the interface are named disconnections. For convenience, in this study we follow the nomenclature: (1) elementary disconnection is a mobile disconnection with Burgers vector (B_v) parallel to the GB plane that glides along the interface; (2) other sessile disconnections are called GBD with core riser or simply “risers” if the dislocation character is implicit [18]. An elementary disconnection glides under an applied stress due to its dislocation nature. This glide is accompanied by GB migration due to the step of the boundary associated with the disconnection. Thus, the motion of glissile disconnections produces two effects, on the one hand, it accommodates plastic deformation and, on the other hand, the motion of the step transforms one part of bicrystal into another part (i.e., displacement of the GB interface in the normal direction) [19].

Following the notation introduced in [20], we denote the GBD that steps the GB along n planes of the upper crystal and m planes of the lower crystal as $\mathbf{b}_{n/m}$ (the elementary disconnections are $\mathbf{b}_{n/n}$). For completeness, we extend the notation to the B_v of the crystal dislocations of the upper crystal as $\mathbf{b}_{n/0}$. Using this notation, the values of n and m are conserved separately in the balance of B_v for any reaction considered (see reaction in Sec. III.A.1).

The initial absorption of the crystal dislocation can be divided into two groups. (1) Absorption and split into an elementary disconnection and a sessile GBD that does not step the interface [Fig. 1(a)]. (2) Absorption and split into several elementary disconnections and into a sessile grain boundary dislocation that steps the interface, i.e., GBD with core riser [Fig. 1(b)]. The reactions of the next upcoming dislocation of the pileup that follow the first absorption depend on the GB type. It can be either a full absorption with or without changes of GBD's B_v [Figs. 1(a) and 1(b)], or transmission/reflection [Figs. 1(c) and 1(d)]. The formation of dipoles of elementary disconnections occurs either at the GBD, acting as a source of disconnections, or at stress concentrations on the interface far from the GBD.

In this paper, we provide the details of the interaction mechanisms on the example of the $\Sigma 11(332)\langle 110 \rangle$ symmetric tilt grain boundary interacting with dislocations of $1/2\langle 111 \rangle$ type. Among the STGB with $\langle 110 \rangle$ tilt axis, the (332) GB structure presents a deep cusp in the GB energy—misorientation curve (e.g., 1039 mJ/m^2 in Fe [21]) thus it must be rather stable. This GB is the coherent boundary of the (332) twin, that is the conjugate of the (112) twin; the later presenting the deepest cusp of the GB energy (e.g., 262 mJ/m^2 in Fe [21]).

II. SIMULATION TECHNIQUE

The present atomistic calculations were performed using supercells containing two grains of bcc metal. The principal axes x , y , and z of the upper crystal (λ) were oriented along the

FIG. 1. Schematics of the dislocation reactions at the GB: (a, b) Absorption of the pileup dislocation (black) and split into sessile GBD (red) and several elementary disconnections (green) that step the interface several planes in both grains. (c) Transmission and (d) reflection with emission of elementary disconnections. The arrows indicate the sense of motion.

[1 $\bar{1}$ 3], [$\bar{1}$ $\bar{1}$ 0], and [3 $\bar{3}$ $\bar{2}$] directions, respectively, while for the lower crystal (μ) the axes were mirror reflected. Each simulation begins with a static relaxation, i.e., energy minimization, which was performed by applying periodic boundary conditions along the x and y directions and fixed boundaries perpendicular to the GB plane.

A hybrid atomistic/discrete dislocation model was applied to simulate the interaction of a grain boundary with a DPU [22]. Rather than using a concurrent coupling [23], the hybrid approach uses separate continuum and atomistic simulations that define mutual boundary conditions. The positions of continuum dislocations in a pileup are defined as a function of an externally applied shear stress and the positions of any dislocations in the atomistic region held fixed at the atomistically determined positions. The displacement field of the continuum pileup is then used to define displacement boundary conditions on the (much smaller) atomistic simulation cell. The atomistic region is then evolved by molecular dynamics at finite temperatures. An algorithm allows us to model the introduction of a DPU which is directed towards the GB through the application of a load in the system.

The MD simulation cell consisted of a symmetric bicrystal with an initially coherent symmetric tilt GB interface in the middle. Approximate dimensions of the cell size were $80 \times 4 \times 40$ lattice vectors along the corresponding directions with a total number of atoms $\sim 600\,000$. Periodic boundary conditions were imposed along the [$\bar{1}$ $\bar{1}$ 0] tilt axis, with fixed boundaries in the other two directions.

The pileups are introduced on the upper crystal along two {112} glide planes for edge dislocations and along a {110} plane for the mixed dislocation. The glide plane inclinations respect to the GB are about 29.5° and 100.02° for the two

FIG. 2. Snapshot of MD simulation of a GB with marked selected groups of atoms. Each group is a pair of regions lying below and above glide planes. See text for details. The insert shows an example of reaction with group no. 2 around it.

edge and 154.76° for the mixed dislocations, respectively. The bicrystals were relaxed using the conjugate gradient method and then atomic displacements corresponding to an initial σ_{app} were applied to all the atoms. The crystal was relaxed again and thermalized for 20 ps to achieve a desired initial temperature. The loading was realized by updating atomic positions of the fixed boundaries to mimic the increase of σ_{app} . The fixed integration MD time step taken was 1 fs for all runs.

With respect to the loading conditions, the following parameters were fixed: the number of dislocations in a pileup (15 units), the increment of the externally applied stress ($\Delta\sigma_{app} = 100$ MPa) and the maximum of the externally applied stress ($\sigma_{app, max} = 5.5$ GPa). For a given glide plane inclination, we consider, in turn, two dislocations with opposite sense of their Bv pointing away from the interface $\mathbf{b}_{n/0}$ and pointing towards it $\mathbf{b}_{-n/0}$. To understand the particular mechanisms of dislocation-GB interaction, we varied the simulation temperature from 150 K up to 600 K, thus enhancing or reducing the role played by thermal activation.

The interatomic interactions in iron were modeled by using the embedded-atom method (EAM) potential by Ackland *et al.*, fitted to reproduce properties of dislocation lines obtained from DFT [24]. The accuracy of the potential in the study of $\langle 110 \rangle$ tilt GBs was checked in [25]. In chromium it was used the potential by Bonny *et al.*, fitted to thermodynamic and point-defect properties obtained from DFT calculations and experiments [26]. As for tungsten, potential by M.C. Marinica *et al.* has been chosen. The potential is fitted to a mixed database, containing various experimentally measured properties of tungsten and ab initio formation energies of defects [27].

To assess the impact of the dislocation reactions on the local evolution of stress state, we allocated several groups of atoms, which were selected in the MD input script in LAMMPS [28], to record the forces and displacements during the simulation runs. As a result, the stress tensor is measured on seven pairs of groups of atoms (Fig. 2), as well as the stress state on all mobile atoms of the simulation box. The positions of the groups of atoms are chosen to provide relevant information

FIG. 3. Dichromatic pattern of (332) GB. Black sites (upper grain), white sites (lower grain). Bv of crystal dislocations: Edge = 1, 2, 5, and 6; Mixed = 7, 8, 9, and 10. Disconnections: 3 = $\mathbf{b}_{2/2}$ and 4 = $\mathbf{b}_{-2/-2}$ stepping the interface up and down, respectively. Red and blue vectors are translation vectors of λ and μ crystals: their difference is $\mathbf{b}_{-2/-2}$. The unit cells of both crystals are included.

on the DPU gliding, its reaction with the interface, and the possible outcomes. Group “1” is chosen along the glide plane of the initial DPU; group “2” is at the initial reaction site; groups “3” and “4” are along glide of mobile disconnections; groups “5”, “6,” and “7” are chosen along the glide planes of possible transmitted or reflected dislocations. Angles, at which glide planes in “5”, “6,” and “7” lie, are calculated based on ad hoc preliminary simulations. For the interactions presented in this paper, the relevant region is #2.

The interaction mechanisms related to crystallography are the same for the three metals considered. Thus, for the sake of brevity and clearness, we present in detail the results for Fe and compile the results of Cr and W in Tables I and II.

III. $\{332\}$ GB-DISLOCATION REACTIONS

In the (3-3-2)[$-1 - 10$] tilt GB, the only reaction observed has been the absorption of pileup dislocations. The absorption resulted in the transformation of crystal dislocations into GBDs with core riser (riser hereafter) and several elementary disconnections, $\mathbf{b}_{\pm 2/\pm 2}$ (vectors no. 3 and no. 4 in Fig. 3), that step the GB two planes either upwards or downwards, depending on the reaction $\mathbf{b}_{Xtal} = \mathbf{b}_{riser} + N\mathbf{b}_{\pm 2/\pm 2}$. The reaction is not unique and it is only restricted by the two conditions applicable to any GB-dislocation interaction. On the one hand, the reaction follows the conservation of Bv and, on the other hand, the GB defects are defined by the difference of broken symmetries of the crystals that form the interface [18,29]. These two conditions can be visualized in the dichromatic pattern (DP) [30] formed by the superposition of the lattice sites of both crystals superposed with the (3-3-2) plane in common, as presented in Figs. 3, 5, and 8. In the DP any lattice site of the common (3-3-2) plane can be taken as origin of translation vectors of both crystals, therefore any vector going from white site (μ crystal) to black site (λ crystal) represents a Bv of a GBD and the operations with Bv's are straightforward (example of vector no. 4 in Fig. 3: $\mathbf{b}_{-2/-2} = \mathbf{t}_\lambda - \mathbf{t}_\mu$). Moreover, the position of the Bv of GBDs relative to the common (3-3-2) plane indicates the step height of the GBDs. In the DP of Fig. 3 the λ crystal (black) includes the Bv's of the crystal dislocations that are studied. They are numbered as follows: 1, 2, 5, and 6 are edge dislocations and 7 to 10 are mixed dislocations (notice they link lattice sites of the black crystal). Vectors 3 and 4 are elementary disconnections. Following the notation introduced in [20], we denote them as 1 = $\mathbf{b}_{-2/0}$, 2 = $\mathbf{b}_{2/0}$, 3 = $\mathbf{b}_{2/2}$, 4 = $\mathbf{b}_{-2/-2}$, 5 = $\mathbf{b}_{-4/0}$, 6 = $\mathbf{b}_{4/0}$, 7 = 9 = $\mathbf{b}_{-1/0}$, and 8 = 10 = $\mathbf{b}_{1/0}$. The

TABLE I. Products of the reactions of $\mathbf{b}_{2/0}$ at 29.5 degrees. N absorbed is the number of absorbed crystal dislocations; T is the temperature (K); Bv is the Burgers vector of formed GBD with core riser; el. disc: number of accumulated $\mathbf{b}_{-2/-2}$; ID React.: Identification of GBDs Bv in Fig. 5(a) and Shear is the local shear stress necessary for the absorption (MPa).

N absorbed		1				2				3			
Mater.	T	Bv	el.disc.	ID React.	Shear	Bv	el.disc.	ID React.	Shear	Bv	el.disc.	ID React.	Shear
Fe	150	$\frac{1}{11}[\bar{4}\bar{4}\bar{1}]$	3	1	-	$\frac{2}{11}[\bar{3}\bar{3}\bar{2}]$	$3 + 7 = 10$	6	919	$\frac{1}{22}[\bar{1}\bar{7}\bar{1}\bar{7}\bar{1}\bar{5}]$	$3 + 7 + 6 = 16$	9	1436
	300	$\frac{1}{22}[\bar{7}\bar{7}\bar{1}]$	4	2	-	$\frac{1}{22}[\bar{1}\bar{3}\bar{1}\bar{3}\bar{5}]$	$4 + 5 = 9$	5	898	$\frac{1}{22}[\bar{1}\bar{7}\bar{1}\bar{7}\bar{1}\bar{5}]$	$4 + 5 + 7 = 16$	9	1172
	450	$\frac{1}{11}[\bar{4}\bar{4}\bar{1}]$	3	1	-	$\frac{1}{22}[\bar{1}\bar{3}\bar{1}\bar{3}\bar{5}]$	$3 + 6 = 9$	5	858	$\frac{1}{22}[\bar{1}\bar{7}\bar{1}\bar{7}\bar{1}\bar{5}]$	$3 + 6 + 7 = 16$	9	1019
	600	$\frac{1}{22}[\bar{7}\bar{7}\bar{1}]$	4	2	-	$\frac{1}{22}[\bar{1}\bar{3}\bar{1}\bar{3}\bar{5}]$	$4 + 5 = 9$	5	721	$\frac{1}{22}[\bar{1}\bar{7}\bar{1}\bar{7}\bar{1}\bar{5}]$	$4 + 5 + 7 = 16$	9	1001
Cr	150	$\frac{1}{11}[\bar{3}\bar{3}\bar{2}]$	5	3	-	$\frac{2}{11}[\bar{3}\bar{3}\bar{2}]$	$5 + 5 = 10$	6	890	$\frac{1}{22}[\bar{1}\bar{7}\bar{1}\bar{7}\bar{1}\bar{5}]$	$5 + 5 + 6 = 16$	9	1565
	300	$\frac{1}{11}[\bar{3}\bar{3}\bar{2}]$	5	3	-	$\frac{2}{11}[\bar{3}\bar{3}\bar{2}]$	$5 + 5 = 10$	6	848	$\frac{1}{22}[\bar{1}\bar{7}\bar{1}\bar{7}\bar{1}\bar{5}]$	$5 + 5 + 6 = 16$	9	1447
	450	$\frac{1}{11}[\bar{3}\bar{3}\bar{2}]$	5	3	-	$\frac{2}{11}[\bar{3}\bar{3}\bar{2}]$	$5 + 5 = 10$	6	839	$\frac{3}{11}[\bar{3}\bar{3}\bar{2}]$	$5 + 5 + 5 = 15$	8	1427
	600	$\frac{1}{11}[\bar{3}\bar{3}\bar{2}]$	5	3	-	$\frac{2}{11}[\bar{3}\bar{3}\bar{2}]$	$5 + 5 = 10$	6	841	$\frac{3}{11}[\bar{3}\bar{3}\bar{2}]$	$5 + 5 + 5 = 15$	8	1210
W	150	$\frac{1}{11}[\bar{3}\bar{3}\bar{2}]$	5	3	-	$\frac{1}{2}[\bar{1}\bar{1}\bar{1}]$	$5 + 6 = 11$	7	2026	-	-	-	-
	300	$\frac{1}{22}[\bar{7}\bar{7}\bar{1}]$	4	2	-	$\frac{1}{2}[\bar{1}\bar{1}\bar{1}]$	$4 + 7 = 11$	7	1918	-	-	-	-
	450	$\frac{1}{22}[\bar{5}\bar{5}\bar{7}]$	6	4	-	$\frac{1}{2}[\bar{1}\bar{1}\bar{1}]$	$6 + 5 = 11$	7	1276	-	-	-	-
	600	$\frac{1}{11}[\bar{3}\bar{3}\bar{2}]$	5	3	-	$\frac{1}{2}[\bar{1}\bar{1}\bar{1}]$	$5 + 6 = 11$	7	1352	-	-	-	-

TABLE II. Products of the reactions of $\mathbf{b}_{-2/0}$ at 29.5 degrees. N absorbed is number of absorbed crystal dislocations; T is the temperature (K); Bv is the Burgers vector of formed GBD with core riser; el. disc: number of accumulated $\mathbf{b}_{2/2}$; ID React.: Identification of GBDs Bv in Fig. 5(a) and Shear is the local shear stress necessary for the absorption (MPa).

N absorbed		1				2			
Material	T	Bv	el.disc.	ID React.	Shear	Bv	el.disc.	ID React.	Shear
Fe	150	$\frac{1}{11}[\bar{3}32]$	5	12	828	$\frac{1}{11}[\bar{7}71]$	$5 + 3 = 8$	16	1056
	300	$\frac{1}{22}[\bar{2}25]$	7	14	700	$\frac{2}{11}[\bar{3}32]$	$7 + 3 = 10$	18	946
	450	$\frac{1}{22}[\bar{5}57]$	6	13	705	$\frac{1}{11}[\bar{7}71]$	$6 + 2 = 8$	16	937
	600	$\frac{1}{22}[\bar{5}57]$	6	13	710	$\frac{2}{11}[\bar{3}32]$	$6 + 4 = 10$	18	707
Cr	150	$\frac{1}{11}[\bar{3}32]$	5	12	620	$\frac{1}{11}[\bar{7}71]$	$5 + 3 = 8$	16	959
	300	$\frac{1}{11}[\bar{3}32]$	5	12	582	$\frac{1}{22}[\bar{1}313\ 5]$	$5 + 4 = 9$	17	938
	450	$\frac{1}{11}[\bar{3}32]$	5	12	562	$\frac{1}{22}[\bar{1}515\bar{1}]$	$5 + 2 = 7$	15	941
	600	$\frac{1}{11}[\bar{4}4\bar{1}]$	3	10	505	$\frac{1}{22}[\bar{1}313\ 5]$	$3 + 6 = 9$	17	894
W	150	$\frac{1}{22}[\bar{7}71]$	4	11	1735	$\frac{1}{22}[\bar{1}515\bar{1}]$	$4 + 3 = 7$	15	2299
	300	$\frac{1}{22}[\bar{7}71]$	4	11	1767	$\frac{1}{11}[\bar{7}71]$	$4 + 4 = 8$	16	2215
	450	$\frac{1}{22}[\bar{7}71]$	4	11	1607	$\frac{1}{11}[\bar{7}71]$	$4 + 4 = 8$	16	2149
	600	$\frac{1}{22}[\bar{7}71]$	4	11	1587	$\frac{1}{11}[\bar{7}71]$	$4 + 4 = 8$	16	2128

Bv's of the mixed dislocations 7 and 9 (as well as 8 and 10) differ in the sign of the screw part, which does not contribute to step the GB.

The vectors $\mathbf{b}_{2/2} = \frac{1}{22}[\bar{1}\ 1\ \bar{3}]$ and $\mathbf{b}_{-2/-2} = \frac{1}{22}[\bar{1}\bar{1}\ 3]$ are the shortest in the DP and correspond to the elementary disconnections responsible for the displacement of the GB by gliding along it [19].

Considering the pileup of edge dislocations gliding along $\{112\}$ planes, there are two possible glide plane inclinations, namely, inclined to the GB at 29.5 degrees ($\mathbf{b}_{-2/0}$; $\mathbf{b}_{2/0}$) and inclined at 100.02 degrees ($\mathbf{b}_{-4/0}$; $\mathbf{b}_{4/0}$). The third dislocation has mixed character and approaches the GB along a $\{110\}$ glide plane inclined 154.76 degrees ($\mathbf{b}_{-1/0}$; $\mathbf{b}_{1/0}$). For each glide plane inclination, two dislocations with opposite sense of the Burgers vectors are considered because the interaction of the GB with the first dislocation of the pileup is a function of the sense of the Bv.

Like GBDs at the $\{112\}$ interface, the GBDs at the $\{332\}$ interface can act as a source of disconnections [31] under

certain conditions, as detailed below. The evolution of the Bv of the risers depends on the number of dislocations of the pileup that are absorbed.

We describe the observed interaction mechanisms, as they were visualized using OVITO software [32]. The reaction mechanism was studied by inspecting atomic configurations at each strain increment.

A. Pileup of edge dislocations with Bv inclined 29.5 degrees

The Burgers vectors of the edge dislocations of the pileup are $\mathbf{b}_{2/0} = \frac{1}{2}[\bar{1}\bar{1}\ 1]$ and $\mathbf{b}_{-2/0} = \frac{1}{2}[\bar{1}\bar{1}\bar{1}]$. This section is divided in two subsections where we detail the specificities of the interaction between the DPU and the interface for the two possible senses of the Burgers vector. It is shown how the outcome of the reactions involved is strongly dependent on the sense of Bv.

1. Dislocation with Burgers vector pointing away from the interface ($\mathbf{b}_{2/0}$)

Figure 4 shows the interaction of the GB with three dislocations of a pileup at 300 K in Fe. The first dislocation is attracted by the GB and is absorbed as shown in Fig. 4(a) (notice the second dislocation of the pileup at the upper right corner of the figure). In the reaction it is formed a GBD with a stepping up riser along the $(\bar{1}12)_\lambda$ (glide plane of the pileup) in the upper grain and the $(1\bar{1}0)_\mu$ plane in the lower grain. In this reaction, four $\mathbf{b}_{-2/-2}$ are emitted stepping down the GB and run away under the local stress. This reaction can be described as

$$\mathbf{b}_{2/0} = \mathbf{b}_{10/8} + 4\mathbf{b}_{-2/-2}, \quad (1)$$

where $\mathbf{b}_{10/8}$ is the Bv of the riser shown in the DP of Fig. 5(a) as #2; this vector goes from the eighth plane of the white crystal to the tenth plane of the black crystal. The sum of vectors is marked by a green circle.

Then, under an increase of the applied stress, the second and third dislocations are absorbed. The Bv's of the risers for each absorption are depicted and numbered in the DP of Fig. 5(a). The reactions observed on the three metals are

FIG. 4. Snapshots of the interaction of the DPU with the $\{332\}$ GB in Fe at $T = 300$ K. (a) After the absorption of the first dislocation of the pileup. (b) After the absorption of the second dislocation. (c) Before the absorption of the third dislocation. (d) After the absorption of the third dislocation.

FIG. 5. Dichromatic pattern with possible Bv's of GBDs with core riser for a different number of absorbed dislocations (a) $\mathbf{b}_{2/0}$ and (b) $\mathbf{b}_{-2/0}$. Black horizontal lines indicate the GB. Black arrows are Bv's of pileup dislocations. Arrows from black to white sites are Bv's of GB defects. Examples of reactions (green circles) are shown for (a) no. 2 and (b) no. 12.

detailed in Table I, where the Bv of the reaction, the accumulated number of disconnections emitted after each reaction and the number assigned in the DP are presented together with the local shear stress necessary for the absorption of the dislocation.

Some remarks are as follows. The Bv number 7 in Table I, corresponding to tungsten, is $\frac{1}{2}[1\bar{1}\bar{1}]$. Although it is a lattice vector, it is not the Bv of a crystal dislocation because it is attached to the GB, it is the Bv of a GBD and is restricted to stay at the GB. The balance of Bv is indicated in the equation

$$2\mathbf{b}_{2/0} = \mathbf{b}_{26/22} + 11\mathbf{b}_{-2/-2}. \quad (2)$$

The indexes indicate that this riser is 26 planes of λ above the GB. To reduce the dimensions of Fig. 5, vectors 5, 6, and 7 have been shifted down by 11 planes (notice they are linked to square symbols) and vectors 8 and 9 have been shifted down by 22 planes [the periodicity of the coincident site lattice (CSL) along the z direction].

The Bv of the riser is calculated by Volterra operations, as the difference of two translation vectors from the upper and lower crystals, respectively, obtained from a Burgers circuit (see [20], for example). The vector is double-checked by calculating the Bv's as the difference of the initial crystal dislocation and the produced elementary disconnections. The decomposition of the Bv of the bulk dislocation is not unique; the reactions numbered from 1 to 4 in the DP of Fig. 5(a) are possible decompositions of the crystal dislocation that differ in the number of disconnections emitted. This is evidenced in Table I where the decomposition of the same Bv results in different number of elementary disconnections depending on the temperature and material.

As the reaction progresses and more dislocations get absorbed, the Bv of the riser evolves and its length increases. The labels from “5” to “7” indicated in the DP of Fig. 5(a) correspond to two absorbed crystal dislocations and labels “8” and “9” correspond to three absorbed crystal dislocations.

The maximum strain applied in all simulations has been the same for all materials and temperatures considered in this study, even though the total number of absorbed dislocations varies from two (in W) to three (in Fe and Cr).

Comparing the results of the absorption of each dislocation for the three temperatures studied we conclude that the mechanism of absorption of the pileup of dislocations by the (3-3-2) GB is independent of the temperature and material. For instance, the length of the riser after the absorption of the third dislocation in Fe is the same for all temperatures. This is because the total number of disconnections emitted is the same and consequently the Bv of the GBD associated to this riser is the same at the end of the full process, i.e., $\mathbf{b}_{38/32} = \frac{1}{22}[17\bar{1}7\bar{1}5]$

Although there is a unique mechanism for all materials and temperatures, the stress needed for the absorption of each dislocation is temperature dependent. Figure 6 shows the shear stress, measured locally within the interaction region (no. 2 in Fig. 2), necessary for the absorption of the dislocations for Fe [Fig. 6(a)] and Cr [Fig. 6(b)]. In the case of $\mathbf{b}_{2/0}$, only the stress necessary for the reaction with the second and third dislocations are plotted because the first dislocation is

FIG. 6. Shear stress, measured in the interaction region no. 2, for the absorption of the pileup dislocations $\mathbf{b}_{2/0}$ and $\mathbf{b}_{-2/0}$ vs temperature for (a) Fe and (b) Cr.

FIG. 7. (a) First dislocation of pileup after relaxation (no absorption). (b) First dislocation is absorbed under the stress of the second dislocation. (c) Second dislocation absorbed under the stress of the third dislocation.

attracted and spontaneously absorbed by the GB. As expected, the stress increases with the number of dislocations absorbed but for a given dislocation of the pileup there is a decrease of stress with increasing temperature, common for the three metals studied. This indicates that the process is thermally enhanced. For $\mathbf{b}_{-2/0}$, described below, the stress necessary for the first dislocation of the pileup to overcome the repulsion of the GB is included in Fig. 6 and Table II.

2. Dislocation with Burgers vector pointing towards the interface ($\mathbf{b}_{-2/0}$)

In this subsection we consider the complementary case, when the Bv of the dislocations points towards the GB ($\mathbf{b}_{-2/0} = \frac{1}{2}[\bar{1}\bar{1}\bar{1}]$); in this case the Bv of the elementary disconnections formed is $\mathbf{b}_{2/2} = \frac{1}{22}[\bar{1}\bar{1}3]$. The first relevant difference with the previous result is that there is no spontaneous absorption of the first dislocation because its interaction with the GB is repulsive.

Figure 7 shows the detail of the interaction of the GB with two dislocations of a pileup at 300 K in Fe. For the same total shear stress that was applied to the system for $\mathbf{b}_{2/0}$, the GB absorbs only two dislocations of the pileup. The essential difference with the $\mathbf{b}_{2/0}$ interaction is the orientation of the riser of the GBD; it is formed by the $(1\bar{1}0)_\alpha$ plane in the upper grain and $(\bar{1}\bar{1}2)_\mu$ plane in the lower grain. Now, the angle between the riser and the glide plane of pileup dislocations is bigger than 90 degrees impeding any possible glide of the pileup along it. So, after the absorption of two dislocations, the maximum external stress cannot overcome the repulsion between the third dislocation and the GBD.

The sequence of events is as follows. The first dislocation has been pushed by the pileup towards the GB against the initial repulsion of the GB. Figure 7(a) shows the equilibrium position of the first dislocation that is not absorbed by the GB and keeps its Bv. By increasing the shear stress (see the values in Fig. 6), the first dislocation is absorbed by the GB producing a GBD with the riser; it is shown in Fig. 7(b) for Fe. Table II indicates the Bv's of the GBDs as a function of temperature and material (from no. 10 to no. 14) that are shown in Fig. 5(b); accordingly, the number of $\mathbf{b}_{2/2}$ varies from 4 to 7. By increasing the shear strain, the second dislocation is absorbed with emission of $\mathbf{b}_{2/2}$'s. The Bv of the GBD and the number of disconnections is presented in Table II and the DP of Fig. 5(b). Bv's from #15 to #17 represent absorption of two crystal dislocations. Figure 6 shows the local shear stress necessary for the first and second dislocations to be absorbed.

FIG. 8. Dichromatic pattern with possible Bv's of GBDs with core riser for a different number of absorbed mixed dislocations. (a) $\mathbf{b}_{1/0}$ dislocation and the GBD associated (from no. 22 to no. 25). In the top in a green circle it includes the dislocations $\mathbf{b}_{4/0}$ and $\mathbf{b}_{-4/0}$ with the only GBD associated (no. 19). (b) $\mathbf{b}_{-1/0}$ dislocation and the GBD associated (no. 20 and no. 21). Black horizontal lines indicate the GB. Arrows from white to black sites are Bv's of GB defects. An example of reaction is shown on (a): $2\mathbf{b}_{1/0} = \frac{1}{11}[3\bar{3}\bar{2}] + [110] + 6\frac{1}{22}[\bar{1}\bar{1}3]$.

By comparing Tables I and II, namely, comparing the reactions of $\mathbf{b}_{2/0}$ and $\mathbf{b}_{-2/0}$, we observe a slightly higher dependence on the material in the reaction with the latter. In this case, in Fe there is an emission of a higher number of disconnections, especially after the absorption of the first dislocation, indicating a better accommodation of the strain applied, compared to Cr and W.

B. Pileup of edge dislocations with Bv inclined 100.02 degrees

For the second glide plane inclination considered, the Burgers vectors of the dislocations of the pileup are $\mathbf{b}_{4/0} = \frac{1}{2}[\bar{1}\bar{1}\bar{1}]$ and $\mathbf{b}_{-4/0} = \frac{1}{2}[\bar{1}\bar{1}1]$. For the $\mathbf{b}_{4/0}$ Bv the interaction with the GB [Fig. 1(a)] requires a much higher stress. There is attraction and absorption of the first dislocation $\mathbf{b}_{4/0}$ of the pileup but after an increase of the shear along the glide plane of the dislocations of about 9.5 GPa, the second dislocation is not absorbed. The Bv of the GBD produced is shown in the DP of Fig. 8 (#19 inside a green circle). On the other hand, for the $\mathbf{b}_{-4/0}$ Bv there is no attraction between the first dislocation and the GB. If the dislocation of the pileup is pushed to the GB by increasing the shear stress, it reaches an equilibrium position and remains attached to the GB but it keeps its own Bv. The conclusion derived from these results is that the GB is a strong barrier for the glide of the pileup with this high incident angle.

C. Pileup of mixed dislocations with Bv inclined 154.76 degrees

The mixed dislocations interacting with the GB glide on a $\{110\}$ plane. The Burgers vectors of the dislocations of the pileup are $\mathbf{b}_{-1/0} = \frac{1}{2}[\bar{1}\bar{1}\bar{1}]$ and $\mathbf{b}_{1/0} = \frac{1}{2}[\bar{1}\bar{1}1]$.

For completeness, in our study of the mixed dislocation we considered the four vectors obtained by changing the sign of the edge part and the screw part, as indicated in Tables III and IV that correspond to Fe. In these simulations, the decomposition of the incident dislocation may change in plus or minus a disconnection as with the edge dislocation. Although the most frequent decomposition is related to the minimum magnitude of the Bv of the GBD, the thermal fluctuation or the local stresses may result in a different decomposition.

TABLE III. Products of reactions for the mixed ($\mathbf{b}_{1/0}$) in Fe. ID React.: Identification of GBDs Bv in Fig. 8.

Mater.	N absorbed	T	Bv Edge	Bv Screw	1		Shear	Bv Edge	Bv Screw	2		Shear
					el.disc.	ID React.				el.disc.	ID React.	
Fe		150	$\frac{1}{22}[\bar{3}\bar{3}\bar{2}]$	$\frac{1}{2}[110]$	3	22	504	$\frac{1}{11}[\bar{3}\bar{3}\bar{2}]$	$[110]$	$3 + 3 = 6$	24	483
		300	$\frac{1}{22}[\bar{3}\bar{3}\bar{2}]$	$\frac{1}{2}[110]$	3	22	510	$\frac{1}{22}[\bar{7}\bar{7}\bar{1}]$	$[110]$	$3 + 4 = 7$	25	471
		450	$\frac{1}{22}[\bar{3}\bar{3}\bar{2}]$	$\frac{1}{2}[110]$	3	22	506	$\frac{1}{11}[\bar{3}\bar{3}\bar{2}]$	$[110]$	$3 + 3 = 6$	24	352
		600	$\frac{1}{22}[\bar{3}\bar{3}\bar{2}]$	$\frac{1}{2}[110]$	3	22	506	$\frac{1}{11}[\bar{3}\bar{3}\bar{2}]$	$[110]$	$3 + 3 = 6$	24	375
		150	$\frac{1}{22}[\bar{4}\bar{4}\bar{1}]$	$\frac{1}{2}[\bar{1}\bar{1}\bar{0}]$	4	23	509	$\frac{1}{22}[\bar{7}\bar{7}\bar{1}]$	$[\bar{1}\bar{1}\bar{0}]$	$4 + 3 = 7$	25	469
		300	$\frac{1}{22}[\bar{3}\bar{3}\bar{2}]$	$\frac{1}{2}[\bar{1}\bar{1}\bar{0}]$	3	22	508	$\frac{1}{22}[\bar{7}\bar{7}\bar{1}]$	$[\bar{1}\bar{1}\bar{0}]$	$3 + 4 = 7$	25	412
		450	$\frac{1}{22}[\bar{3}\bar{3}\bar{2}]$	$\frac{1}{2}[\bar{1}\bar{1}\bar{0}]$	3	22	507	$\frac{1}{22}[\bar{7}\bar{7}\bar{1}]$	$[\bar{1}\bar{1}\bar{0}]$	$3 + 4 = 7$	25	377
		600	$\frac{1}{22}[\bar{3}\bar{3}\bar{2}]$	$\frac{1}{2}[\bar{1}\bar{1}\bar{0}]$	3	22	507	$\frac{1}{11}[\bar{3}\bar{3}\bar{2}]$	$[\bar{1}\bar{1}\bar{0}]$	$3 + 3 = 6$	24	327

When the edge part of the Burgers vector is pointing away from the interface ($\mathbf{b}_{1/0}$, Table III, lower frame in Fig. 9), two dislocations can be absorbed and the riser is along the glide plane, as for the edge $\mathbf{b}_{2/0}$.

Reversing the sign of the edge part ($\mathbf{b}_{-1/0}$, Table IV, upper frame in Fig. 9) only one dislocation can be absorbed. The angle between the glide plane and the riser is bigger than 90 degrees, it is the same one observed for the edge $\mathbf{b}_{-2/0}$ pointing towards the interface. The injection of a second dislocation only occurs at 900 K for a total shear stress of 5.7 GPa, indicating that the process is thermally activated.

Figure 10 plots the stresses presented in Tables III and IV. It is shown that the stress depends on the edge part of the dislocation, namely the orientation of the riser, but is almost independent of the temperature. Thus, the dislocation $\mathbf{b}_{1/0} = \frac{1}{2}[1\bar{1}\bar{1}]$ is attracted by the GB, it creates a riser along the glide plane and needs smaller local shear stress to be absorbed by the GB, allowing a second dislocation to be absorbed. The shear stress for the absorption of the second dislocation is smaller and it is dependent on the temperature, as shown in Fig. 10(b). It seems to indicate that the accommodation of two mixed dislocations leads to a better faceting of the GB because the screw component is a lattice vector; the GBD separates two identical interfaces.

Once analyzed the results for all dislocations, we conclude that the same crystallographic processes occur for the three bcc metals studied. The differences in the number of disconnections resulting in each absorption may be related to the core energy and Peierls stress of $\mathbf{b}_{2/2}$ that differ from one metal to the other. Occasionally, reactions with plus or minus

TABLE IV. Products of reactions for the mixed ($\mathbf{b}_{-1/0}$) in Fe. ID React.: Identification of GBDs Bv in Fig. 8 and the local shear stress (MPa) is plotted in Fig. 10.

Mater.	N absorbed	T	Bv Edge	Bv Screw	1		Shear
					el.disc.	ID React.	
Fe		150	$\frac{1}{22}[\bar{2}\bar{2}\bar{5}]$	$\frac{1}{2}[110]$	2	20	602
		300	$\frac{1}{22}[\bar{3}\bar{3}\bar{2}]$	$\frac{1}{2}[110]$	3	21	589
		450	$\frac{1}{22}[\bar{3}\bar{3}\bar{2}]$	$\frac{1}{2}[110]$	3	21	601
		600	$\frac{1}{22}[\bar{2}\bar{2}\bar{5}]$	$\frac{1}{2}[110]$	2	20	586
		150	$\frac{1}{22}[\bar{2}\bar{2}\bar{5}]$	$\frac{1}{2}[\bar{1}\bar{1}\bar{0}]$	2	20	587
		300	$\frac{1}{22}[\bar{2}\bar{2}\bar{5}]$	$\frac{1}{2}[\bar{1}\bar{1}\bar{0}]$	2	20	587
		450	$\frac{1}{22}[\bar{2}\bar{2}\bar{5}]$	$\frac{1}{2}[\bar{1}\bar{1}\bar{0}]$	2	20	583
		600	$\frac{1}{22}[\bar{2}\bar{2}\bar{5}]$	$\frac{1}{2}[\bar{1}\bar{1}\bar{0}]$	2	20	581

$\mathbf{b}_{2/2}$ may occur because, as shown in the DP of Figs. 5 and 8, the change of the Bv of the GBD, for a given number of dislocations absorbed, is mainly in orientation but small in magnitude.

Thus, the mechanism of the interaction of the $\{332\}$ GB with the pileup of $\frac{1}{2}(111)$ dislocations is essentially ruled by the crystallography with almost no influence of the temperature or material. Even though, for a given metal, the absorption is, in general, thermally activated and, especially in Fe, the threshold stress for absorption diminishes by increasing the temperature.

D. Behavior under shear stress of the GBDs created by absorption of crystal dislocations

The creation of GBDs has a crucial effect on the GB dynamic as the mobility of the interface can be enhanced or reduced with the subsequent effects on the plasticity. The GBDs created by absorption of dislocations described along the previous sections are stable GB defects (the absorption is not a reversible process) that cannot glide along the GB because their Bv is not parallel to the GB. Even though, these GBDs can move under certain conditions together with the GB.

Let us consider first the GBD far from the pileup. Under an external shear stress parallel to the GB, the GBD created by the absorption of $\mathbf{b}_{2/0}$ moves along its own riser accompanying the GB on its displacement in a shear-coupled

FIG. 9. Snapshots of the interaction of the mixed dislocation DPU with the GB. $\mathbf{b}_{-1/0}$: before (i) during (ii) and after (iii) interaction. $\mathbf{b}_{1/0}$: first dislocation is absorbed (i) before absorption of second dislocation (ii) and after absorption of second dislocation (iii): notice the riser is parallel to the glide plane.

FIG. 10. (a) Local shear stress along the glide plane for the absorption of the first mixed dislocation as a function of the temperature and the orientation of the Bv. (b) Shear stress for absorption of first and second $b_{1/0}$ dislocations.

GB migration. The process, generated by the glide of $b_{2/0}$ disconnections along the GB, is the same as for the (10-12) twin boundary in the hcp metals [33]. Thus, the GBD acts as a source of disconnection dipoles that move in opposite directions under the same shear stress. Under the applied stress, while one partner of the dipole glides along the GB, the other moves along the riser of the GBD in a conservative climb [34]. As a result, the whole GB moves by two planes for every dipole pair created. The same result is produced if a single disconnection sweeps the GB and climbs conservatively along the riser. Thus the displacement of the GBD is conservative (no atomic diffusion is needed) and it is reversed if the shear stress is reversed.

Let us consider that the GBD is the result of the interaction with a pileup of $b_{2/0}$ dislocations. When the sense of the shear stress favors the absorption of the pileup, it favors, as well, the glide of disconnections that move the GB down. If the sense of the shear is reversed after the absorption of few dislocations, the remaining dislocations of the pileup run away from the GB and the glide of disconnections, created at the GBD (or elsewhere) produces the displacement of the GB upwards, as described above.

The displacement of the GBDs created by the interaction with the other dislocations is not always conservative. For instance, the GBDs associated to $b_{-2/0}$ and $b_{4/0}$ pin the GB under a positive shear stress whereas they perform a conservative climb for a negative shear stress. A detailed study of the behavior of the GBDs under stress is in progress [35].

IV. DISCUSSION

The interaction of a pileup of dislocations with a GB is based on two different aspects, namely, (i) the geometrical aspect, i.e., the crystallographic structure of the dislocation and the GB, which is common to all materials of the same structure (bcc, in our study); (ii) the atomic interaction features, which are material dependent and which affect the energy balance, i.e., the external stress needed to inject dislocations into the interface, the local stresses needed to trigger the reactions, and Peierls stress to move elementary disconnections. An ambient simulation temperature also plays a role when thermal action assists in overcoming the energy/stress barrier for a reaction to proceed. The stress needed to create one elementary disconnection depends on the intrinsic properties of the material (combination of elastic constants, stacking fault energy and the resolved shear stress to move it). This

leads to the formation of a different number of elementary disconnections after the absorption of the first dislocation of the pileup and, consequently, different Bv of the riser (determined by the crystallography). The result of the absorption of the second and further dislocations of the pileup, i.e., the Bv of riser and number of elementary disconnections, depends on the material.

In this work, the maximum external stress is fixed for all simulations (5.5 GPa). This controls the maximum number of dislocations to be absorbed by the GB, which depends on the material, but, for a given material, does not depend on temperature. Through the performed MD simulations we observed that the same crystal dislocation acts differently depending on the sense of the Bv, which determines the reaction, in particular the riser of the GBD, either stepping up or down the GB. The same property occurs in hcp structures, for instance, in the interaction of the (10-12) twin with crystal dislocations [18]. The reaction with the edge dislocation $b_{2/0}$ steps the GB up, i.e., the riser of the GBD is along the glide plane of the incident crystal dislocation $(\bar{1}12)_\lambda / (1\bar{1}0)_\mu$ which favors the absorption of the following dislocations. The continuous absorption of dislocations leads to the formation of a new asymmetric GB interface of $\{112\}/\{110\}$ type, which continuously grows as more bulk dislocations are supplied. Thus the GB becomes faceted due to the interaction with the dislocation pileups created inside the grain. The scenario changes by changing the sign of the Bv of the pileup ($b_{-2/0}$). In the later case, the riser is almost perpendicular to the glide plane of the pileup, preventing the accommodation of the pileup along the riser. Even though, a smaller facet $\{110\}/\{112\}$ is produced in the GB. If the edge dislocation forms an angle with the GB of 100 degrees, the absorption is not favorable and the GB is a strong obstacle for the glide of the dislocation. When the pileup is formed by mixed dislocations, with glide plane $(1\bar{1}0)$ inclined at 154.76 degrees, the orientation of the riser of the produced GBD depends on the sign of the edge part of the dislocation. The riser is $(1\bar{1}0)_\lambda / (1\bar{1}2)_\mu$, parallel to the glide plane, for the $b_{1/0}$ but its orientation is not parallel to the glide plane for $b_{-1/0}$. Again, the observation of the resistance against the absorption for the mixed dislocation is consistent with the orientation of the riser, being the dislocation $b_{1/0}$ absorbed with a smaller shear stress; in this case, a second dislocation is absorbed.

The effectiveness of the GB to accommodate plastic deformation depends on the activated slip system. Thus, the mixed dislocation is absorbed at the lowest shear stress, as shown in Fig. 10, followed by the edge dislocation at 29.5 degrees ($b_{2/0}$) and, finally, the GB is a strong obstacle for the glide of the edge dislocation with glide plane almost perpendicular to the GB. The three metals studied keep the same behavior. Figure 6 and Tables I and II allow a comparison of the shear stress of each metal. Figure 6 shows quite similar stress values for Fe and Cr, but plotting the shear stress normalized by the shear modulus ($\mu(\text{Fe, Cr, W}) = (73, 108, 179) \text{ GPa}$, [22,36]), we can discern the differences. Thus, Fig. 11 presents the values in units of the shear modulus to absorb the second and third dislocations of the $b_{2/0}$ pileup (the first is spontaneously absorbed) versus temperature. The stress to absorb the second dislocation is almost independent of the temperature for Cr and W, but it decreases by increasing the temperature for Fe.

FIG. 11. Shear stress (normalized with the shear modulus) necessary for the absorption of a pileup with glide plane at 29.5 degrees of the GB.

The injection of the third dislocation requires a higher stress that significantly decreases by increasing the temperature in both Cr and Fe. The same tendency occurs with the absorption of the second dislocation of the pileup of mixed dislocations, as shown in Fig. 10. Therefore, the strength of the (332) GB is highest in Fe followed by W and the weakest is Cr. If the resolved shear stress is measured in shear modulus units, voids also, as well as (332) GB, act as significantly stronger obstacles in Fe than in W, as reported by Osetsky in a recent paper [36].

V. SUMMARY AND CONCLUSION

We studied in detail the interaction of $\frac{1}{2}\langle 111 \rangle$ dislocation pileups with $\Sigma 11(332)$ GB in different materials with bcc structure using a hybrid atomistic-continuum simulation model.

In this grain boundary, only the absorption of the dislocations was observed independently of the material and temperature. The crystal dislocation decomposes into a sessile GBD with core riser and mobile elementary disconnections.

The configuration of the GBD depends on the orientation and sense of the incident dislocation. Thus the riser of the GBD may be either oriented along the glide plane of the pileup developing a new asymmetrical $\{112\}/\{110\}$ GB or may be almost perpendicular to the glide plane. The formation of these facets is enabled thanks to the specific dislocation-GB interaction. The formation and growth of new GBs, as a result of the extensive plastic deformation, is well known to occur experimentally—the phenomenon is called grain refinement, which takes place in the third stage of the plastic deformation in metals. If the riser is almost perpendicular to the glide plane of the pileup, then the dislocations suffer repulsion and, for a fixed external stress, the GB absorbs a smaller number of dislocations.

The elementary disconnections formed during the interaction glide away and displace the GB in a conservative manner. The Burgers vector of the GBD is not parallel to the GB and therefore cannot glide along it, but, under the appropriate conditions of shear stress and orientation of the dislocation pileup, the GBD may perform a conservative climb and could

follow the GB in a shear-coupled GB migration. The study of the shear-coupled (332)GB migration is currently in progress [35]. The influence of the temperature in the absorption of dislocations depends on both, the material and the particular interaction.

The main conclusions are summarized as follows.

1. The crystallography of reactions. All observed reactions are analyzed and quantified in terms of constituents (i.e., dislocations taken place in the reaction process and its outcome). In all reactions there is full absorption of the entrant dislocation that transforms in grain boundary dislocations. Since the reactions accomplish the conservation of the Burgers vector, each particular dislocation-GB interaction is also analyzed using the dichromatic pattern. It is shown that the usage of dichromatic pattern provides an efficient tool to comprehend the reaction process as well as to predict the reaction processes for other GBs.

2. The reaction at each metal. All materials were studied in equivalent loading conditions. Even though, the maximum number of dislocations absorbed depends on the metal. In fact, the capacity of the GB to absorb dislocations depends on the underlying interatomic model (i.e., specific material properties). Thus, some particular atomic-level aspects specific of each metal, such as dislocation core structure, stacking fault energy, and GB core structure, determines the local shear stress needed for the process to occur.

3. The effectiveness of the GB to accommodate plastic deformation depends on the activated slip system. Thus the mixed dislocation is absorbed at the lowest shear stress followed by the edge dislocation at 29.5 degrees ($\mathbf{b}_{2/0}$) and, finally, the GB presents the highest strength for the glide of the edge dislocation with glide plane almost perpendicular to the GB.

4. The stress required to inject the dislocation into the GB plane depends on the slip system and is different for the three metals studied. According to the stresses applied, the (332) GB is stronger obstacle in W than in Fe and Cr. However, presenting the same data in units of shear modulus (μ), the GB in Fe is significantly stronger than in W, being the GB in Cr the weakest.

5. The influence of the temperature in the stress is also different for the three metals. For the pileup of edge dislocations, the stress to absorb the second dislocation is almost independent of the temperature for Cr and W but it decreases by increasing the temperature for Fe. The injection of the third dislocation requires a higher stress that significantly decreases by increasing the temperature on both, Cr and Fe. The same tendency occurs with the absorption of the second dislocation of the pileup of mixed dislocations.

6. Continuous absorption of dislocations on the studied GB leads to the formation of a new asymmetric GB interface of $\{112\}/\{110\}$ type which grows as more and more bulk dislocations are supplied. The formation of this interface is enabled thanks to the specific crystallography of the dislocation-GB interaction.

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