Journal of MATERIALS RESEARCH

Invited Paper
DOI:10.1557/s43578-020-00096-z

ADVANCED NANOMECHANICAL TESTING

FOCUS ISSUE

Dislocation–grain boundary interactions: recent advances on the underlying mechanisms studied via nanoindentation testing

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Received: 16 November 2020; accepted: 22 December 2020; published online: 19 January 2021

To comprehend the mechanical behavior of a polycrystalline material, an in-depth analysis of individual grain boundary (GB) and dislocation interactions is of prime importance. In the past decade, nanoindentation emerged as a powerful tool to study the local mechanical response in the vicinity of the GB. The improved instrumentation and test protocols allow to capture various GB–dislocation interactions during the nanoindentation in the form of strain bursts on the load–displacement curve. Moreover, the interaction of the plastic zone with the GB provides important insight into the dislocation transmission effects of distinct grain boundaries. Of great importance for the analysis and interpretation of the observed effects are microstructural investigations and computational approaches. This review paper focused on recent advances in the dislocation–GB interactions and underlying mechanisms studied via nanoindentation, which includes GB pop-in phenomenon, localized grain movement under ambient conditions, and an analysis of the slip transfer mechanism using theoretical treatments and simulations.

Introduction

The plastic behavior of metals is mainly governed by the motion of dislocations, whereas in polycrystalline materials, dislocation–grain boundary (GB) interactions strongly impact the mechanical response [1–10]. Grain boundaries are often considered to act as a stationary impediment to the dislocation motion, which substantially increases the yield strength of the polycrystalline materials due to dislocations pile-ups in the vicinity of the GB. According to the well-known Hall–Petch relationship [2], the yield strength of the polycrystalline material increases with decreasing the grain size, which also gave rise to the notion "smaller is stronger".

Grain boundaries are not alike and have a different character. However, the classical Hall–Petch model considered only an average hardening contribution by treating all GBs the same. To precisely predict the mechanical behavior of a polycrystalline material at a local scale, a quantitative understanding of the contribution of the individual GB character on the dislocation grain boundary interaction is required [11–13]. Depending upon the GB character, type of dislocations, grain orientation of the adjacent grains, and loading conditions, various interactions between dislocations and individual GB have been reported [14, 15].

i. Dislocations can pile-up or stored at the GB.
ii. Dislocations can be absorbed in the GB (without transmission of dislocations in adjacent or parent grain).
iii. Dislocations can be transmitted in the adjacent grain, with or without leaving a residual dislocation in the GB.
iv. Absorbed dislocations at the GB can be re-emitted in the adjacent grain with or without leaving a partial dislocation in the GB.

v. Absorbed dislocations at the GB can return to the parent grain with or without leaving a partial dislocation in the GB.

Depending upon the adjacent grain orientation, GB character, and the nature of the dislocations, among the above-mentioned dislocations–GB interactions, one or more events can occur at the same time [16–20]. However, due to the complex GB structure and evolving boundary conditions of the adjacent grains during the plastic deformation, reliable criteria for various dislocations–GB interactions are still missing [21].

In the literature, theoretical descriptions and numerical simulation of the interaction between dislocations and GBs have been attempted for a wide range of observation scales. In this regard, different methods like molecular dynamics simulations, discrete dislocation dynamics theories, and continuum crystal plasticity frameworks have been employed [22–27]. Moreover, slip transmission criteria at GBs have been formulated, which consider the misalignment between directional flows at the grains adjacent to a GB as well as the misorientation between slip directions and the normal of GB plane [15, 28–31]. Conventional continuum-scale frameworks are not capable of formulating the microforces imposed by a dislocation pile-up at the GB. Therefore, strain gradient crystal plasticity theories with the potential of incorporating a description of geometrically necessary dislocations (GNDs) have been recently developed [32–35].

To understand the underlying dislocation–GB mechanisms, a range of experimental approaches has been utilized. For example, the slip transfer across the GBs in bulk samples has been investigated via Tensile Testing Setup along with X-ray diffraction [36–38] and Scanning Election Microscopy (SEM) [39–42]. Digital image correlation combined with SEM has been used to investigate the strain along with slip transfer across the GBs [43–45]. The strain accumulation in the vicinity of the GBs also been studied via Electron Backscattered Diffraction (EBSD) [46–48]. To study the GB–dislocation interactions at the atomic scale, Transmission Electron Microscopy (TEM) has been utilized in the literature [14, 49–51]. A small dimension specimen's mechanical response is different as compared to the bulk material. Therefore, over the past decade, the micropillar compression (ranging from micron to sub-micron diameter) testing has gained significant interest [52–57]. The micropillar compression testing experiments have also been conducted to study the individual GB–dislocation interaction. These studies are mostly conducted on the face-centered cubic (FCC) metals [54, 58–61]. However, the first body-centered cubic (BCC) bicrystal pillar compression testing was reported recently [62], in which the micropillar compression testing was conducted on nominally 8 μm diameter Tantalum bicrystal and the slip transmission across three high-angle GBs is investigated.

Over the last decade, substantial advances in the nanoindentation (also known as instrumented or depth-sensing indentation) systems and new test protocols have opened new directions to study the small-scale mechanical properties [63–65]. For example, fast time constant (10's of μs) and high data acquisition rates (close to MHz) [66] allow to capture various events (e.g., slip transmission across the GB [67–70], phase transformation [71, 72], cracking [73–76], etc.) during nanoindentation in the form of strain bursts in the load–displacement curve. The steady advancement in the nanoindentation systems along with data analysis protocols made it a powerful tool to study the local mechanical response in the grain interior [77–81] and the vicinity of the individual GB [67–69, 82].

Nanoindentation combined with advanced characterization techniques [like EBSD, Electron Channeling Contrast Imaging (ECCI), TEM, etc.] and simulations will lead to a better understanding of the underlying mechanisms of the individual GB–dislocation interactions, which is the main focus of the present review paper. The paper includes GB pop-in phenomenon ("GB pop-in phenomenon" section), localized grain movement under ambient conditions ("Stress-driven GB movement during indentation under ambient), and an analysis of the slip transfer mechanism using theoretical treatments and simulations ("Theoretical and numerical concepts for slip transfer" section).

Dislocations–grain boundary interactions studied via indentation

GB pop-in phenomenon

In nanoindentation testing, load on the indenter tip and displacement of the indenter tip into the material surface are continuously measured in real time. The load–displacement (LD) curve obtained from nanoindentation tests often shows displacement bursts, which are referred to as "pop-ins" (schematically shown in Figs. 1 and 2). The initial contact is elastic in nature and the first pop-in (Fig. 1b) observed at low load levels often depicts the elastic to the plastic transition of the material. At the pop-in dislocations that are nucleated and afterward, the material deforms elastic-plastically [83–86]. The stress required for the activation of dislocation sources depends on the dislocation density within the stressed region. Specifically, if the test specimen is not well prepared or has been pre-deformed, even for the same material, the initial pop-in load can vary strongly [76, 87]. Ohmura et al. [88] reported that the indentations conducted in the grain interior show the initial pop-in at a relatively larger load as compared to the indentation performed close to the GB. In this work, the authors proposed that the GBs can be an effective source of dislocations which results in the smaller initial pop-in load and size.

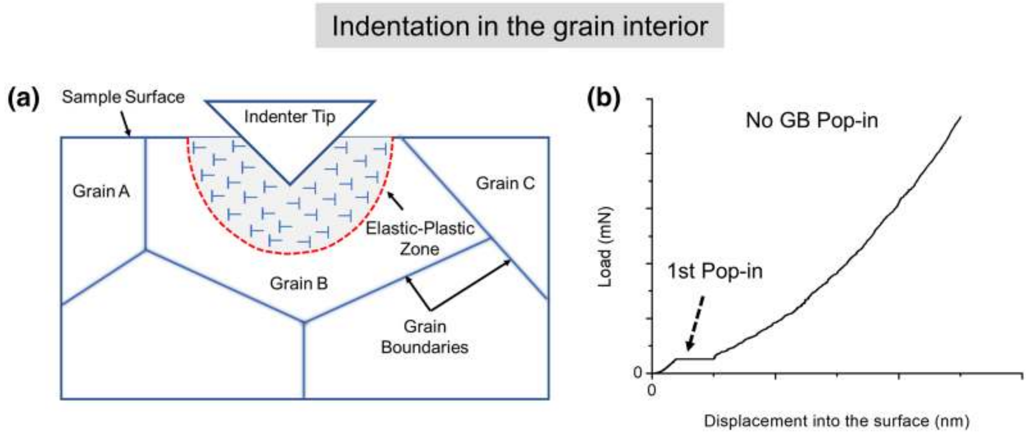

Figure 1: Schematic diagram of (a) an indentation performed in the grain interior, (b) LD curve showing only initial pop-in event.

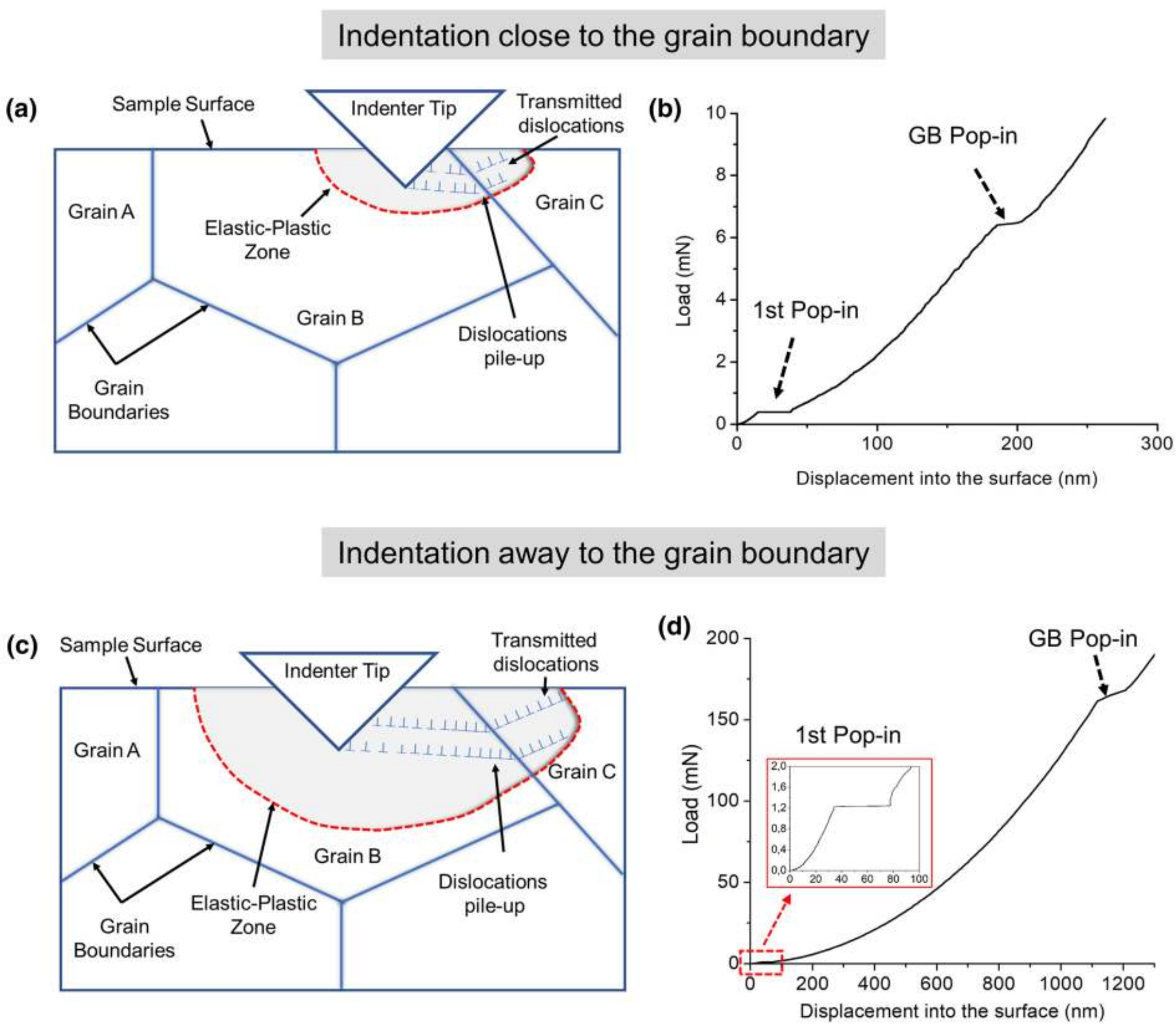

Figure 2: Schematic diagram of (a) an indentation performed very close to the GB, (b) representative LD curve of the indentation (a) showing GB pop-in at smaller load, (c) the indentation performed at a larger distance to the GB, and (d) representative LD curve of the indentation (c) showing GB pop-in at relatively higher load.

For the indentations performed in the grain interior, along with the first pop-in, often multiple secondary pop-ins at relatively higher loads have been reported on the LD curve. Such multiple pop-ins are possibly due to further activation of dislocation activity in the expanding plastic zone or other effects like cracking or phase transformation of material during indentation, as has been briefly mentioned in the introduction part.

If the indentation is performed close to the GB, in addition to the first pop-in, a single [70] or multiple secondary pop-ins [89] at relatively higher loads have been observed on the LD curve. These secondary pop-ins are related to the dislocation–grain boundary interactions and are referred to as "GB pop-ins".

The occurrence of the GB pop-in events is strongly influenced by the applied load, the distance of the indenter tip to the GB, misorientation between the adjacent grains, GB character, and the orientation of the indenter tip with respect to the GB [67–70, 82]. The influence of the distance of the indenter tip to the GB on the occurrence of the GB pop-in loads is schematically shown in Fig. 2. In Fig. 2, two cases for the occurrence of the GB pop-in events are schematically presented, assuming that only the distance between the indenter and the grain boundary is varied between Fig. 2a and c. The misorientation between the adjacent grains (grains B and C), GB character (GB between grains B and C), and the orientation of the indenter tip with respect to the GB is thus assumed to be the same. In the first case, the indentation is conducted very close to the GB, in grain B (Fig. 2a). In the second case, the indentation is performed at a much larger distance to the same GB, in grain B (Fig. 2c). Due to the larger indenter tip distance to the GB, dislocations need to travel more distance to reach the GB and then pile-up in the vicinity of the GB. After the critical stress is reached, the dislocations will transmit to the adjacent grain C and the GB pop-in event can occur at a much larger load (schematically shown in Fig. 2d) as compared to the indentation performed very close to the GB (Fig. 2b). It is also clear from the schematic Fig. 2a and c that the elastic–plastic zone below the indentation is much larger for the indentation performed far away from the GB as compared to the indentation performed very close to the GB.

Up to date, experimental observations of the GB pop-in have only been reported for BCC materials like Fe–0.01 wt% C [68], Fe–2.2 wt% Si [90], Fe–14 wt% Si [69, 89], Molybdenum [82, 89, 91], Tungsten [9, 70], Niobium [67], and the intermetallic $L1_2$ phase Ni_3Al [92]. Due to the lower Hall–Petch constant, in FCC metals, it is suggested that slip transfer phenomena are relatively easier as compared to BCC metals [67]. It seems that in BCC metals, other than FCC metals, slip transfer across the GB requires relatively high local stresses. The slip transfer causes then a relaxation of these stresses, which manifests itself in a GB pop-in and this is one possible reason, why GB pop-ins are mainly reported in BCC materials. Moreover, a GB hardening effect has been found showing an increasing hardness with a decreasing distance to the GB. However, there has been recently some debate in the literature on the GB hardening effect. Wo and Ngan [92] studies on Ni_3Al and Soer et al.[69] on Fe–14 wt% Si bicrystal did not observe appreciable GB hardening, while in another Fe–14 wt% Si [89] investigation, Soer et al. reported the GB hardening effect. Moreover, Wang and Ngan [67] work on niobium, Britton et al. [68] on Fe–0.01 wt% C, and recently Javaid et al. [9, 70] on tungsten clearly show a significant increase in hardness before the GB pop-in events. The absence of GB hardening effect in Ni_3Al [92] and Fe–14 wt% Si [69] could be related to the GB type or the used experimental conditions, so further clarification is required.

Wang and Ngan [67] also proposed a criterion for the occurrence of the GB pop-in events, based on an analysis of the size of the plastic zone with respect to the distance to the GB, the c/d-ratio. Here, c is the radius of the elastic–plastic boundary when the strain burst occurs, and d is the distance from the center of residual impression to the GB. They reported a c/d-ratio between 1.5 and 5 for various GBs and suggested that for a specific GB, this range should be narrow. Britton et al. [68] and Javaid et al. [70] also validated this criterion and found the c/d-ratio to be 1.2 and 1.6–2.7, respectively. Obviously, dislocations need to reach the grain boundary and local stresses require to rise in order to initiate a grain boundary pop-in event. The conditions for the occurrence of a GB pop-in will thereby strongly depend on the local stress state, which again can depend on additional parameters (like GB structure, indenter tip, inclination of the GB below the surface, indentation size effect, etc.) not considered in the c/d-ratio.

The GB pop-in events are believed to be associated with the dislocation transmission across the GB. The possible mechanism for such dislocation–GB interaction is that during the indentation process, dislocations are generated around and below the indentations. These dislocations travel toward the GB and form pile-up in the vicinity of the GB. Some dislocations may also be absorbed by the GB. On further loading, a critical stress will reach at which these absorbed, and pile-up dislocations transfer to the adjacent grain which leads to a sudden displacement burst (GB pop-in) on the LD curve. On the basis of in situ straining TEM observations [93], some studies [67–69, 94] believed that the dislocations absorption at the GB and their re-emission is the possible mechanism for the GB pop-in event. However, no direct experimental evidence of the linkage of the GB pop-in event with the absorption of the dislocation at GB and their re-emission has been reported in the literature.

Recently, Javaid et al. [70] reported a statistical analysis on the GB pop-in events in the coarse grain polycrystalline tungsten and also studied the three-dimensional dislocation structure at the GB pop-in events using a combination of sequential polishing and ECCI technique. They confirm that all set of Berkovich indentations performed in the vicinity of an individual GB (with misorientation of 57° between the adjacent grain) show the GB pop-ins. Javaid et al. [70] also confirm that at the GB pop-in events, the residual impressions were not touching the GB, which discarded the physical contact between indenter and GB as a possible mechanism for the occurrence of the GB pop-in. They stopped the indentations at the GB pop-in events and obtained various cross-sections using a sequential polishing technique [95]. The ECCI images on the sequential polished obtained cross-section clearly show the dislocation pile-up and transmission in the vicinity of the GB at the GB pop-in events. An exemplary image from this work is shown in Fig. 3.

In this three-dimensional investigation, Javaid et al. [70] also reported that Berkovich indenter tip orientation with respect to the GB strongly influenced the content of dislocation traveling toward the GB and transmitted in the adjacent grain. From the three-dimensional analysis, they clearly show that when the side of the Berkovich indenter was facing the GB, more dislocation content was observed near the GB in both grain A and B (shown in Fig. 3) as compared to the indenter tip facing the GB. They also relate the observed high transmitted dislocation content with the measured hardness values before the GB pop-in events. When the Berkovich indenter side was facing the GB, they observed higher transmitted dislocation in the adjacent grain (Fig. 3) as well as higher hardness values before the GB pop-in event as compared to the indentations where the Berkovich indenter tip was facing the GB. Recently, Jakob et al. [82] also reported that the orientation of the Berkovich indenter tip with respect to the same GB can strongly influence the measured hardness values.

To validate the linkage between the occurrence of the GB pop-in event with the absorption of dislocation at GB and their re-emission as the possible mechanism, further in situ nanoindentation and computational studies are required.

Stress-driven GB movement during indentation under ambient conditions

Under ambient conditions, GBs are considered as obstacles to the dislocation motion in the coarse grain (> 1 µm) polycrystalline metals. The well-known Hall–Petch relation is based upon this assumption. Recent studies [83, 96–102] on nanocrystalline materials suggest that the GBs cannot always be considered as static structures under ambient conditions. Such localized GB migration cannot be explained by using classical grain growth models [103] and, therefore, are distinguished as the stress-driven GB movement. Since the present review is largely focused on the indentation-based dislocation–GB interactions, only indentation studies revealing the localized GB movement will be reviewed in the preceding paragraph.

The stress-driven GB movement has been observed mostly in the ultrafine grain FCC metallic materials. For example, Minor et al. [83] performed the in situ TEM indentation experiments on the ultrafine grain aluminum (Al) and observed a significant GB movement at room temperature. They suggested that the inhomogeneous stress field below the indentation can possibly lead to such a localized stress-driven GB movement. Later, Soer et al. [104] also conducted similar experiments on

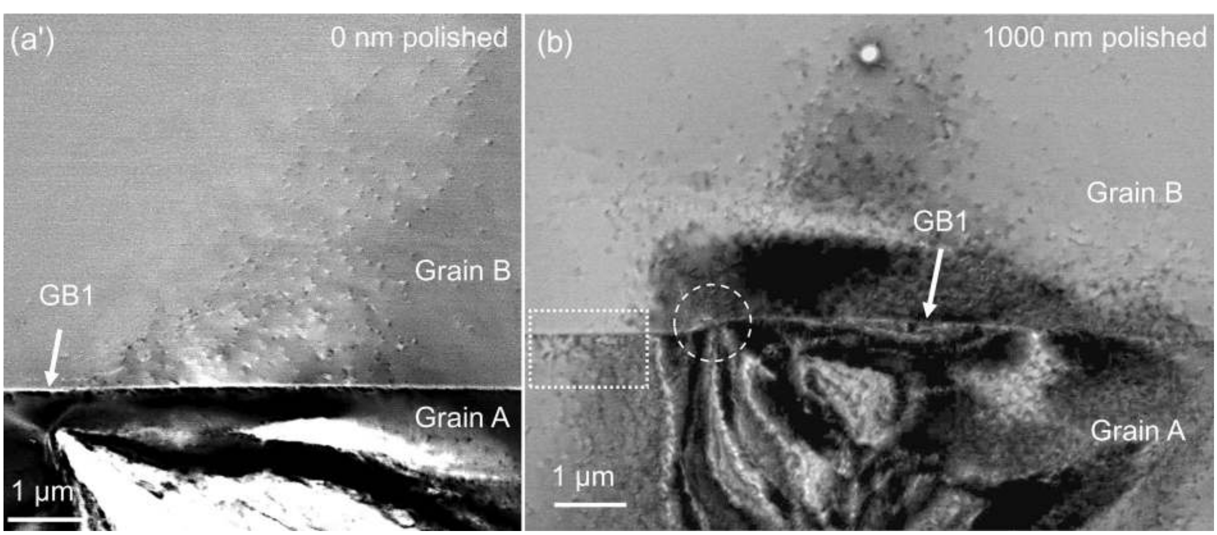

Figure 3: ECCI images of the indent (one side facing GB), (a) at the surface along, with inset region (b) showing dislocation pile-up in grain A (rectangular dotted area) and transmitted dislocation in grain A and B at—1000 nm [70].

the ultrafine grain Al and validated the extensive stress-driven GB motion from in situ TEM studies. In the same work, they also studied the aluminum–magnesium (Mg) alloy thin films via in situ TEM studies and observed that the high-angle GBs are effectively pinned by Mg solutes, whereas the low-angle GBs remained unaffected by the Mg solutes. The stress-driven GB movement is also demonstrated as grain growth in ultrafine grain Al thin films [96, 97]. Zhang et al. [98] conducted the in situ TEM indentation studies on nanocrystalline copper at ambient and cryogenic temperatures and observed rapid stress-driven grain coarsening below the indentation. Moreover, they observed that the grain coarsening under the inhomogeneous stress field was even faster at cryogenic temperature as compared to the ambient conditions.

Interestingly, all aforementioned stress-driven GB movement studies are conducted on ultrafine grained FCC metals and alloys. Recently, Javaid et al. [9] conducted the ex situ Berkovich nanoindentation experiments close to the different GBs of coarse-grained polycrystalline BCC tungsten. For multiple Berkovich indentations, they observed a significant localized GB movement inside the residual impression as well as below the indentation in the plastic zone (Fig. 4).

From their experimental observations, the authors differentiate three cases. In 1st case (Fig. 4a and d), no grain boundary movement is observed inside or below the indentation. In 2nd case, a significant grain boundary movement (indicated by XX*) is visible inside the residual impression (Fig. 4b) on the surface. However, below the indentation, the grain boundary becomes straight again (Fig. 4e). In the 3rd case, no grain boundary movement is noticeable inside the indentation (Fig. 4c) on the surface. The sequential polishing, however, revealed a clear grain boundary curvature (indicated by YY*) below the indentation (Fig. 4f). The driving force for such a localized grain boundary movement is believed to be high local dislocation density in the vicinity of the grain boundary. They also reported that the localized GB movement in tungsten is strongly influenced by the misorientation between the adjacent grain, distance of the indenter to the GB, the orientation of Berkovich indenter with respect to GB, and the applied load.

The stress-driven GB movement during indentation arises from the inhomogeneous stress field which leads to complex dislocation–GB interactions, which are not so easy to model. Cahn and Taylor [105, 106] proposed a unified theory of coupled GB motion, which shows reasonable agreement with the experimental work of Winning et al. [107, 108] performed on the Al bicrystal and also with Molecular Dynamics Simulations [106, 109]. However, to understand the underlying mechanisms during indentation-induced GB motion in detail, comprehensive three-dimensional in situ nanoindentation experiments along with modeling effort are further required.

Theoretical and numerical concepts for slip transfer

It is well accepted that misalignments at grain boundaries affect the ease of dislocation transmission. Therefore, geometric criteria, which take into account the misalignment between slip

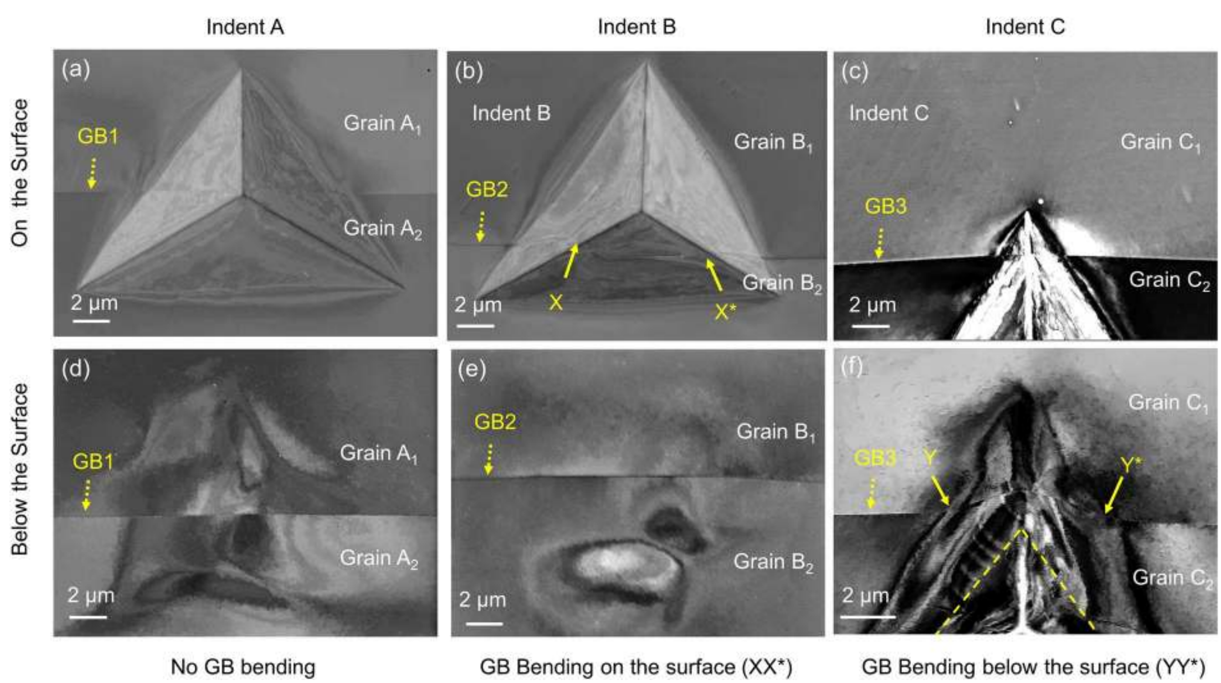

Figure 4: SEM and ECCI images of representative 2-μm-deep Berkovich indentations (a–c) on the surface and (d–f) below the surface obtained from sequential polishing [adapted with permission from Ref. [9]].

systems on both sides of a GB as well as the misorientation between the GB plane and slip systems, have been formulated. In the following, those slip transfer criteria are briefly discussed, see also Fig. 5. One of the earliest formulations were proposed in [28] as follows:

$$\tau_\beta = N^{\beta\alpha}\tau_\alpha, N^{\beta\alpha} = \left(\boldsymbol{m}_B^\beta \cdot \boldsymbol{m}_A^\alpha\right)\left(\boldsymbol{s}_B^\beta \cdot \boldsymbol{s}_A^\alpha\right) + \left(\boldsymbol{m}_B^\beta \cdot \boldsymbol{s}_A^\alpha\right)\left(\boldsymbol{s}_B^\beta \cdot \boldsymbol{m}_A^\alpha\right), \tag{1}$$

where the unit vectors $\boldsymbol{m}$ and $\boldsymbol{s}$ denote the normal vector of slip plane and the slip direction, respectively, and α and β stand for slip system numbers (Fig. 5). The resultant shear stress τ_β on the slip system β in the crystal B is here related to the counterpart shear stress τ_α on the slip system α in the crystal A. Considering the slip system α incoming toward the grain boundary, the outgoing slip system β is most probably activated when the associated factor $N^{\beta\alpha}$ is high enough. Here, the interaction factor $N^{\beta\alpha}$ is independent of the boundary inclination. It is worth noting that the contribution of the aforementioned factor needs in-depth discussions. As an example, when two slip planes on the sides of a GB are parallel to the GB plane, $N^{\beta\alpha}$ might equal to 1, however, if one of these slip planes becomes perpendicular to another one, $N^{\beta\alpha}$ could again yield 1 which leads to an unphysical interpretation.

Later, Luster and Morris [110] introduced a geometric compatibility factor m' by dropping the second term on the right side of Eq. (1).

$$m' = \left(\boldsymbol{m}_B^\beta \cdot \boldsymbol{m}_A^\alpha\right)\left(\boldsymbol{s}_B^\beta \cdot \boldsymbol{s}_A^\alpha\right) = \cos\phi \cdot \cos\kappa, \tag{2}$$

where ϕ is the angle between slip plane normals and κ is the angle between incoming and outgoing slip directions, which are illustrated in Fig. 5. Here, no contribution of grain boundary inclination is again seen. In a study of annealed polycrystalline Al foils with near-cube oriented grains [111], it was found that the slip transfer across GBs is very rare and is only evident when $m' > 0.97$. Moreover, a study of the slip transfer in Ti-6Al-4 V [112] shows that slip transfers might occur in a wider range of m' values when applied stresses increase, Fig. 6 in [112]. Performing the nanoindentation at the area of GBs in a polycrystalline niobium [67] indicates that the GB pop-in might be seen within the maximum load of 50 mN, when $m' > 0.93$. In a study of the correlation between intragranular slip transmissions and the GB misorientation in a polycrystalline Ni_3Al [92], good concurrences were found between the ease of transmission and high values of m' as well as between the difficulty in the transmission and $m' \leq 0.96$.

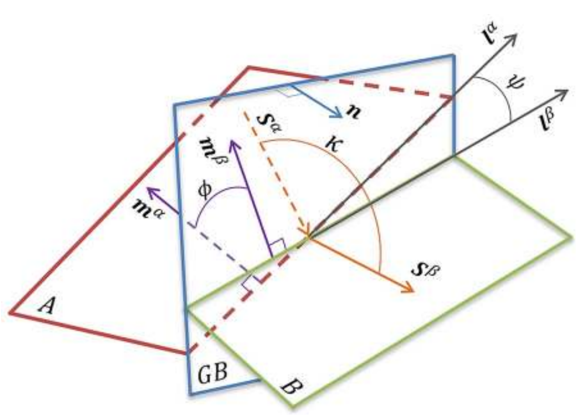

Figure 5: Two slip planes A and B adjacent to a grain boundary (GB) plane. $\boldsymbol{m}$ and $\boldsymbol{s}$ denote the normal vector of the slip plane and the slip direction, respectively. α and β stand for slip system numbers. $\boldsymbol{l}$ is the unit vector at the intersection line and $\boldsymbol{n}$ is the normal vector of grain boundary plane. Three angles ϕ, ψ, *and* κ depict the misorientation at the GB.

Considering the role of grain boundary orientation, Shen et al. [29] proposed a modified geometric criterion accounting for the misorientation of intersection lines and slip directions as follows:

$$K^{\alpha\beta} = \left(\boldsymbol{l}_A^\alpha \cdot \boldsymbol{l}_B^\beta\right)\left(\boldsymbol{s}_A^\alpha \cdot \boldsymbol{s}_B^\beta\right) = \cos\psi \cdot \cos\kappa, \boldsymbol{l}_A^\alpha = \boldsymbol{m}_A^\alpha \times \boldsymbol{n}, \tag{3}$$

where $\boldsymbol{l}$ is the unit vector at the intersection line and $\boldsymbol{n}$ is the normal vector of the GB plane shown in Fig. 5. The angle ψ is between the intersection lines. The favored slip transfer is here the slip that minimizes the angles between the intersection lines and the slip directions [29]. Later, Shen et al. [17] concluded that emitted slip systems are successfully predicted if the geometric criterion (3) is accompanied by a criterion maximizing the resolved shear stress exerted on the emitted dislocations.

Moreover, the interaction between dislocations and grain boundaries were studied by Lee et al. [30, 31] based on in situ transmission electron microscope (TEM) deformation experiments, they proposed three criteria, the so-called Lee-Robertson-Birnbaum (LRB) criteria, determining which outgoing slip system will be probably activated during dislocation transmission. These criteria are introduced in the following, determining which outgoing slip system will be probably activated during dislocation transmission. These criteria are introduced in the following:

- First, a geometric condition is taken into account. It is to minimize the angle ψ between the intersection lines.
- Second, maximizing the resolved shear stress (RSS factor) which acts on the outgoing slip system and is induced by the incoming piled-up dislocations.
- Third, minimizing the residual grain boundary dislocation determined by the difference between Burgers vectors of incoming and outgoing dislocations.

In the early stages of slip transfer, the first criterion identifies an active slip plane. Then the second and third criteria

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determine active slip directions. Figure 4 in [15] details schematically the implementation of LRB criteria.

In the direction of formulating the slip transfer and force balances at a GB, a recent theory in the framework of strain gradient plasticity was proposed by Gurtin [113]. This GB theory accounts automatically for the grain misorientation and grain boundary orientation. As a key point in this theory, a GB free-energy as a function of GB Burgers vector production $\mathbb{G}$ was first proposed, $\mathbb{G}$ is given by:

$$\mathbb{G} = \sum_{\alpha} \left[\gamma_{\mathrm{B}}^{\alpha} \boldsymbol{s}_{\mathrm{B}}^{\alpha} \otimes \boldsymbol{m}_{\mathrm{B}}^{\alpha} - \gamma_{\mathrm{A}}^{\alpha} \boldsymbol{s}_{\mathrm{A}}^{\alpha} \otimes \boldsymbol{m}_{\mathrm{A}}^{\alpha}\right](\boldsymbol{n}\times),$$

$$|\mathbb{G}|^2 = \sum_{\alpha\beta} \left[\mathrm{C}_{\mathrm{AA}}^{\alpha\beta} \gamma_{\mathrm{A}}^{\alpha} \gamma_{\mathrm{A}}^{\beta} + \mathrm{C}_{\mathrm{BB}}^{\alpha\beta} \gamma_{\mathrm{B}}^{\alpha} \gamma_{\mathrm{B}}^{\beta} - 2\mathrm{C}_{\mathrm{AB}}^{\alpha\beta} \gamma_{\mathrm{A}}^{\alpha} \gamma_{\mathrm{B}}^{\beta}\right], \quad (4)$$

where A and B indicate adjacent grains to a GB and γ is the slip flow. $\mathbb{G}$ is affected by intra- and inter-grains moduli given by:

$$\mathrm{C}_{\mathrm{IJ}}^{\alpha\beta} = \left(\boldsymbol{s}_{\mathrm{I}}^{\alpha} \cdot \boldsymbol{s}_{\mathrm{J}}^{\beta}\right)\left(\boldsymbol{m}_{\mathrm{I}}^{\alpha} \times \boldsymbol{n}\right) \cdot \left(\boldsymbol{m}_{\mathrm{J}}^{\beta} \times \boldsymbol{n}\right) \quad (5)$$

Here, the generic labels I and J are replaced by A and B, if I = J denote the slip interaction intra-grains moduli and if I ≠ J represents the slip interaction inter-grain modulus which mimics Eq. (3). The resultant shear stresses acting on the slip systems as well as microforces induced by residual dislocations at the grain boundary are all related through a flow rule affected by inter- and intra-grain moduli.

Following the interaction modulus discussed in this section as well as the experimental works discussed in the previous sections, a numerical observation of the interaction between dislocation flows and GBs through nanoindentations applied at the area of a GB, is highly demanding in the field. In this regard, and referring to the continuum scale, strain gradient crystal plasticity frameworks with the potential of contributing a description of GNDs into traditional plasticity theories, are of high interest. These frameworks may provide an observation dislocation pile-up at GBs as well as a formulation of microforces acting at GBs. Moreover, in a combination of this framework with a GB theory such as the model proposed by Gurtin [113], the effects of geometric criteria, the role of shear stresses on the directional flows, and effects of residual burgers vectors at GBs are all taken into account.

To the best of authors' knowledge, there is no study of GB pop-in based on continuum theories in the literature. Although there is one three-dimensional simulation of nanoindentation tests [114] based on a strain gradient theory, where a flat punch is indented close to a GB, and the effects of low- and high-angle GBs on the external load–displacement data are captured and reported in Fig. 10 in [114]. It is worth highlighting that a conventional crystal plasticity theory along with a series of geometric slip criteria have been recently implemented in a MATLAB toolbox called STABIX [115]. By employing this toolbox, Su et al. [116] investigated the effect of grain boundaries on the topography of the indented area at a range of variation of m' detailed in Eq. (2). Figure 9 in [116] compares the numerical and experimental observations. It was concluded that the difficulty in the slip transfer across GBs is pronounced at the GBs corresponding to poorly aligned slip systems and consequently, associated with the low values of m'.

Focusing on the smaller scales than the continuum level, a discrete dislocation study by Lu et al. [117] has recently investigated a bicrystal indented at the area of a GB. Figure 8 in [117] is reproduced here in Fig. 6 and shows two plateaus in the force data which are associated with displacement bursts at the order of 10% of burgers vector magnitude ($b = 0.25nm$) given in Table 1 in [117]. These relatively small plateaus in force–displacement data, were therein referred to as the effect of GB pop-in. Lu et al. [117] envisaged that performing this simulation in a larger dimension might pronounce the observations as seen in experiments. For the sake of completeness, it could be here mentioned that molecular dynamics simulations

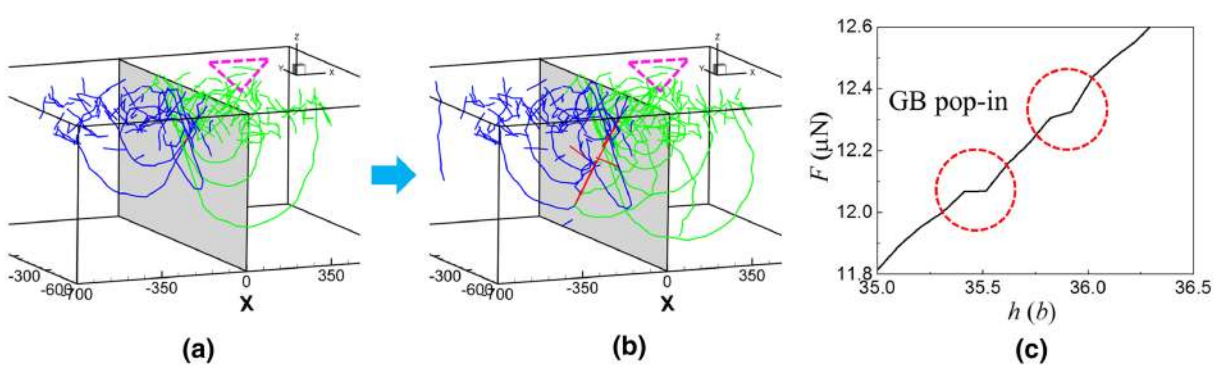

Figure 6: (a) Dislocation structure before penetration, (b) dislocation structure after penetration, and (c) load–displacement data around the moment of penetration. Adapted with permission from Ref. [117].

of nanoindentation in the vicinity of grain boundaries have also been endeavored in [118–120].

Summary and conclusions

Grain boundaries play a paramount role in the deformation of polycrystalline materials, specifically dislocation–grain boundary interactions lead to different deformation mechanisms, which need to be studied in detail. Using nanoindentation, the localized plastic deformation in the plastic zone allows probing the individual grain boundary–dislocation interactions for a wide variety of grain boundaries and materials. In the present article, recent advances on dislocation–individual grain boundary interactions studied via nanoindentation testing are reviewed, which are mainly focused on the experimental studies on the occurrence of the GB pop-in events, localized GB movement under ambient conditions, and an analysis of the slip transfer mechanism using theoretical treatments and simulations.

The occurrence of the GB pop-in events on the LD curve is strongly influenced by the distance of the indenter from the GB, misorientation between the adjacent grains, GB character, and the applied load. The GB pop-in events are believed to be associated with the dislocations absorption at the GB and their re-emission in the adjacent grain. It is, however, unclear why the GB pop-in is experimentally mainly observed for BCC metals. One open question is related to the local stresses acting on the GB, causing the occurrence of such a yield event for the specific grain boundaries.

There is clear evidence, from the three-dimensional analysis of the dislocation structure just after the GB pop-in, that dislocations pile-up at the GB and are then transmitted in the adjacent grain [70]. Furthermore, localized GB movement on and below the residual impression in tungsten have been reported, which is not considered as a usual deformation phenomenon for refractory metals at room temperature [9]. This localized GB movement under ambient condition is believed to occur due to the inhomogeneous state of stresses during the nanoindentation. On the other hand, for GB pop-in events, the dislocation absorption at the GB and their re-emission in the adjacent grain is reported to be the possible mechanism. For the slip transfer mechanism, several criteria have been theoretically developed. However, further experimental effort is needed for a wide range of grain boundaries and deformation conditions. New computational approaches at various length and time scales are also required to understand the complex interaction between the plastic zone of an indentation and individual grain boundaries. The local mechanical response at the grain boundary pop-in is thought to be an important parameter, which together with simulations will help to further understand the complex GB yield phenomena.

Acknowledgments

H.P. and K.D. acknowledge the support by the German Research Foundation (DFG) for research grant Po_ 2242/3-1 and Du 424/16-1.

Funding

Open Access funding enabled and organized by Projekt DEAL.

Data availability

Data will be made available on reasonable request.

Compliance with ethical standards

Conflict of interest On behalf of all authors, the corresponding author states that there is no conflict of interest.

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