

# A *Matlab* toolbox to analyze slip transfer through grain boundaries

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**Abstract.** Slip transmission across grain boundaries is an essential micromechanical processes during deformation of polycrystalline materials. Slip transmission processes can be characterized based on the geometrical arrangement of active slip systems in adjacent grains and the value of the critical resolved shear stress acting on the incoming and possible outgoing slip systems. We present a *Matlab* toolbox which enables quantification of grain boundary slip transfer properties and comparison with experiments. Using a graphical user interface, experimental grain boundary data can be directly exported as input files for crystal plasticity finite element simulation of bicrystal experiments.

## 1. Introduction

The micromechanical behavior of grain boundaries (GBs) is one of the key components in understanding heterogeneous deformation of metals [1]. An increasingly important issue in constitutive modeling is to include the GB micromechanical effects in order to improve the prediction of mechanical microstructure-property relationships [2]. To investigate the nature of the strengthening effect of grain boundaries, slip transmission across interfaces has been investigated through bicrystal indentation tests performed close to grain boundaries [3-7]. To better understand the role played by the GBs and to quantify the GB micromechanics, a *Matlab* toolbox including graphical user interfaces (GUI) was developed [8]. This toolbox also links experimental results to crystal plasticity finite element (CPFE) simulations.

## 2. Strain transfer across grain boundaries

Luster and Morris [9] proposed a criterion to describe slip transfer across a GB based on the geometrical alignment of adjacent slip systems at the GB, see Fig. 1. To analyze the conditions for slip transfer, the crystallography of the GB and its geometry has to be known. At least five degrees of freedom are required to characterize a GB [10]: three for the rotation between the two crystals (Euler angles  $(\varphi_1 \phi \varphi_2)$  for each crystal or misorientation axis/angle pair  $([uvw]/\omega)$ ) and two for the orientation of the GB plane (either the trace angle and the GB inclination or the GB normal). The grain orientation and trace angle can be measured by electron backscatter diffraction (EBSD) orientation mapping and the inclination can be evaluated by serial polishing or focused ion beam sectioning. The parameter,  $m'$ , and several other related parameters [1] such as the residual Burgers vector [11] and resolved shear stress based criteria are implemented in the toolbox.

## 3. Slip transmission analysis through the toolbox

A sample of Ti-5Al-2.5Sn (wt%) was prepared by mechanical grinding and polishing. The alpha/beta microstructure of the sample consists mainly of grains with a hexagonal structure [12]. It was characterized by EBSD and Fig. 2 displays the data in the *map GUI* component of the toolbox). Grain boundaries are color-coded to represent their maximum  $m'$  value taking into account basal and prismatic 1<sup>st</sup> order  $\langle a \rangle$ -slip systems, which are of importance for slip transmission in such alloys [12]. The visualization of the slip transmission parameter on EBSD maps makes the identification of interesting individual GBs convenient. A suitable bicrystal was identified, for which an intermediate potential for slip transmission was expected. The grain boundary #315 was selected and nanoindentation was performed close to

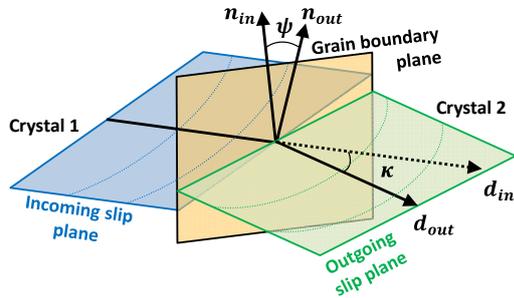


Fig. 1: Definition of  $m'$  [8], based on angle,  $\kappa$ , between incoming and outgoing slip directions,  $d_{in}$  and  $d_{out}$ , and angle,  $\psi$ , between slip plane normals,  $n_{in}$  and  $n_{out}$ .

the GB (see Fig. 3-a). A sphero-conical diamond tip with a nominal tip radius of  $1\ \mu\text{m}$  and a nominal cone angle of  $90^\circ$  was used and a maximum load of  $6\ \text{mN}$  was applied. The pile-up pattern developed around the indent is a function of the orientation of the crystal during axisymmetric indentation [13], and is in this case characteristic of basal and prismatic 1<sup>st</sup> order  $\langle a \rangle$ -slip activity [12]. The surface profile of the pile-up as measured by atomic force microscopy is given Fig. 3-b and the presence of a pile-up in crystal 2 probably indicates slip transmission. Analysis of slip transfer across this boundary was performed using the *bicrystal GUI* (see Fig. 3-c and 3-d). The result suggests that slip transmission occurs between the two crystals, with a prismatic 1<sup>st</sup> order  $\langle a \rangle$  slip to basal slip transfer along the profile P1, with a maximum  $m'$  value of 0.77. To further analyze the spatial distribution of crystallographic shear, the *preCPFE GUI* component was used to enable correlation of the experimental results with finite elements simulations.

#### 4. Stress state analysis using crystal plasticity finite element simulations

The *preCPFE GUI* has been created to enable rapid transfer of experimental data into simulation input files, so that a statistically significant number of indents can be assessed. A parameterized visualization of the bicrystal indentation model through the GUI allows tuning the geometry and finite element discretization and the size of the sample and the indenter, see Fig. 4-a. Once the 3D finite element model of the indentation process is set up, it is possible to generate a *Mentat procedure* file and a material configuration file using a *Python* routine [13, 14]. These input files are exported in order to carry out a fully automatic CPFE simulation of the bicrystal indentation using a flow rule based on Kalidindi's constitutive model available in *DAMASK* [15, 16]. Only prismatic 1<sup>st</sup> order  $\langle a \rangle$ , basal  $\langle a \rangle$  and pyramidal 1<sup>st</sup> order  $\langle c + a \rangle$  slip systems are considered and no inherent grain boundary resistance to slip is implemented. The constitutive parameters were identified from single grain indentation [13]. In this way the stress and strain fields close to the grain boundary can be rapidly quantified based on the precise experimental conditions, see Fig. 4-b and 4-c. Minor discrepancies between experimental and simulated pile-up patterns are observed. Transmission of prismatic  $\langle a \rangle$ -slip in crystal 1 to basal  $\langle a \rangle$ -slip in crystal 2 is observed, which confirms that strain transfer is mainly controlled by the geometric relationship of slip systems.

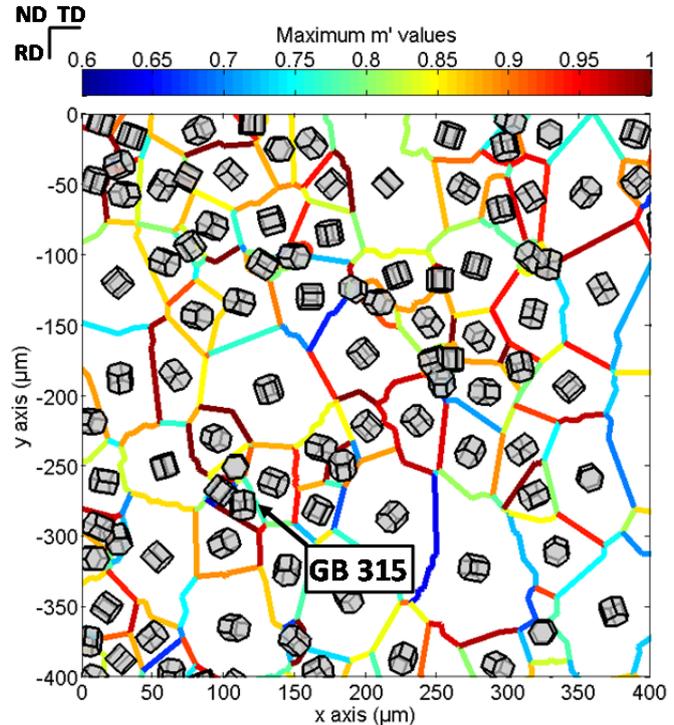


Fig. 2: EBSD orientation map of the Ti-alloy sample with grain boundaries color-coded by their maximum  $m'$  value (for basal and prismatic  $\langle a \rangle$ -slip systems).

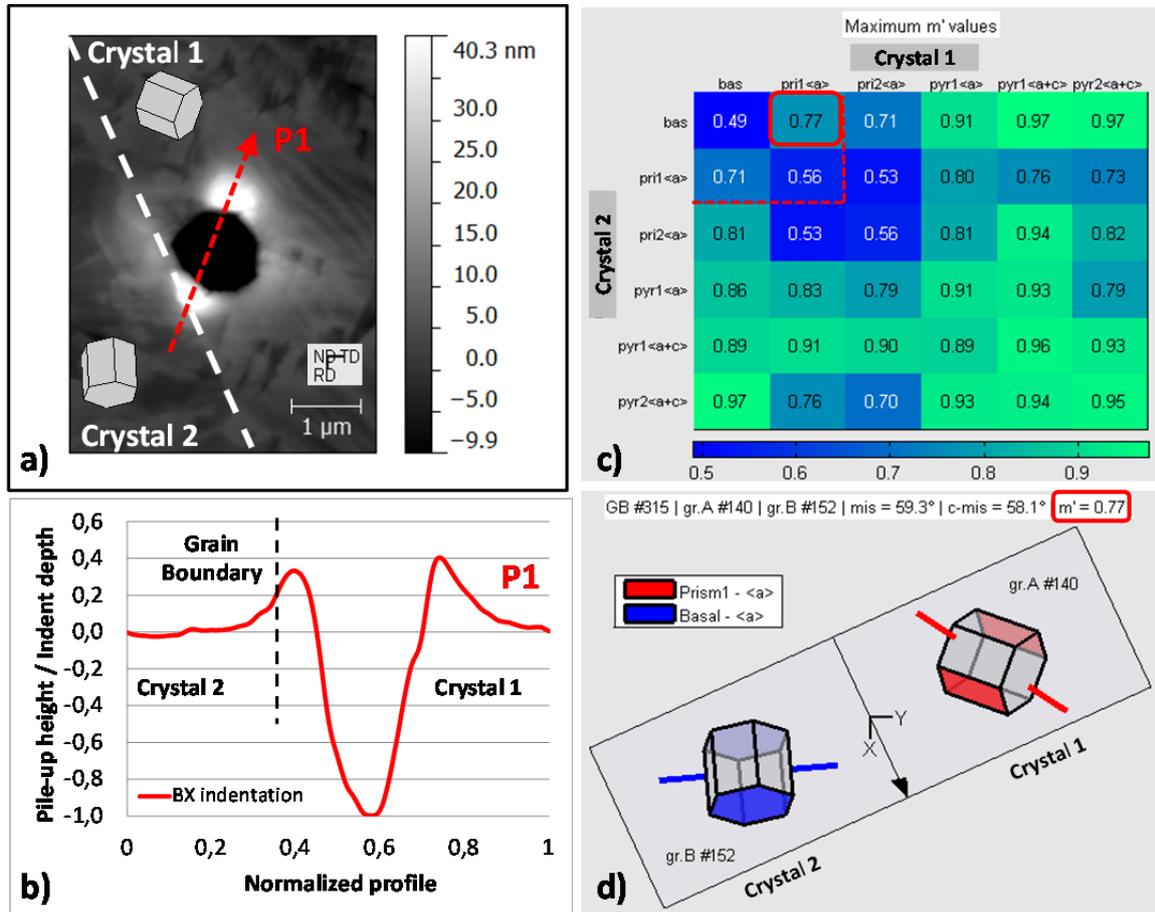


Fig. 3: a) Topography of a cono-spherical indent in Ti alloy, close to GB #315; b) line profile P1 of the pile-up; c) matrix of maximum  $m'$  values for bicrystal #315; d) Plot of the bicrystal #315 highlighting basal and prismatic  $\langle a \rangle$ -slip systems and corresponding surface slip traces of the systems associated with the maximum  $m'$  value.

## 5. Conclusion and Outlook

A software toolbox and three GUIs (*map*, *bicrystal* and *preCPFE*) were developed to analyze strain transfer across grain boundaries. By a combination of spherical indentation close to GBs with EBSD mapping, grain boundary slip transmission was characterized in Ti-5Al-2.5Sn (wt%). Preliminary results suggest that slip transfer in  $\alpha$ -titanium is mainly controlled by the geometrical alignment of adjacent slip systems at the boundary. The toolbox enables a reduction of possible sources of error in the analysis by visualization and a standardized workflow with automated data conversion. The slip systems for bcc, fcc and hcp structures and several slip transfer criteria are implemented to quantify the potential for slip transmission at GBs. The toolbox is interfaced with a *Python* package to generate CPFE simulation input files for single and bicrystal indentation testing, which is readily extendible to other experiments such as polycrystal tensile tests, micro-cantilever bending, and micropillar compression.

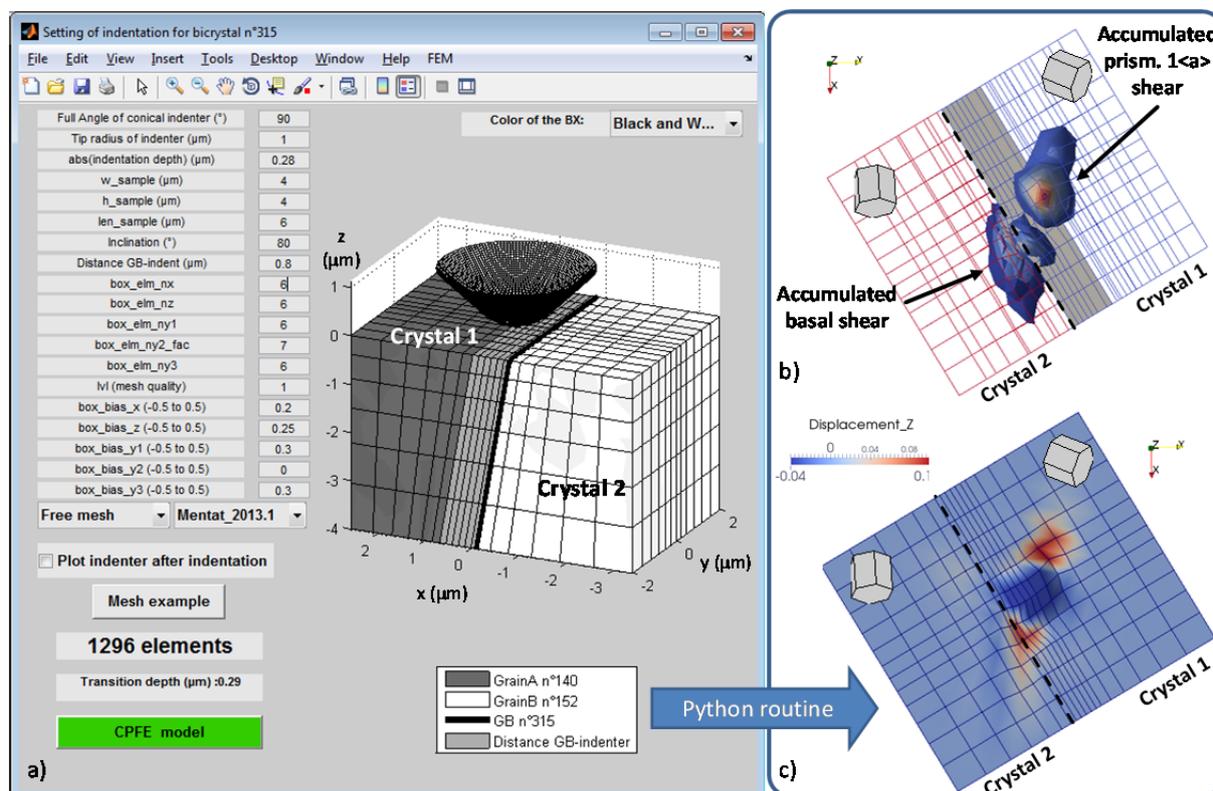


Fig. 4: a) View of the *preCPFE* GUI to optimize the mesh for bicrystal indentation experiment and generate simulation input files. b) Isosurfaces of basal shear in crystal 2 transmitted from prismatic slip activity around the indent in crystal 1. c) Topography of the simulated indent at GB #315.

## Acknowledgements

Supported by the Materials World Network program (DFG ZA 523/3-1 and NSF-DMR-1108211). We acknowledge useful discussions with Y. Su, P. Eisenlohr and M. Crimp.

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