Engineering Conferences International

ECI Digital Archives

Nanomechanical Testing in Materials Research and Development VII

Proceedings

9-30-2019

Effect of anisotropic elasticity on dislocation pile-ups at grain boundaries

Xiaolei Chen
Université de Lorraine, CNRS, Arts et Métiers ParisTech, France, xiaolei.chen@univ-lorraine.fr

Stéphane Berbenni
Université de Lorraine, CNRS, Arts et Métiers ParisTech, France

Christian Motz
Department of Materials Science and Technology, Saarland University, Germany

Thiebaud Richeton
Université de Lorraine, CNRS, Arts et Métiers ParisTech, France

Effect of anisotropic elasticity on dislocation pile-ups at grain boundaries

Xiaolei CHEN [1][2], Thiebaud Richeton [1], Christian Motz [2], Stéphane Berbenni [1]

cxl900705@gmail.com

[1] Université de Lorraine, CNRS, Arts et Métiers ParisTech, LEM3, F-57000 Metz, France

[2] Department of Materials Science and Technology (MWW) / Saarland University, Germany

Objectives:

The current context of miniaturization of objects involves the development of experimental and numerical multi-scale techniques taking into account the effects of internal lengths inherent to the microstructure (crystallographic slip)

- Analytical and numerical calculations of stresses due to different **dislocation pile-up** configurations in a **bi-crystal** considering or not grain boundary properties and **free surface** effects in the context of heterogeneous **anisotropic elasticity**
- Characterization by AFM of the slip behavior at grain boundaries of during compression tests on micron-sized **FCC bi-crystals** (Ni)
- Comparisons between the theoretical calculations and the experimental results for the height of slip lines due to a dislocation pile-up
- Estimation of the resistance of different **grain boundaries** and quantification of the contribution of anisotropic elasticity on **slip transmission**

Micromechanical calculations of dislocation and pile up stress fields in anisotropic bi-materials and tri-materials with/without free surfaces (LEM3)

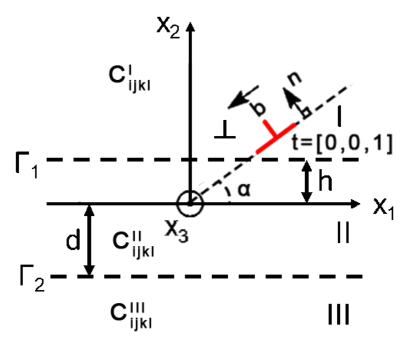
-- Two different methods of calculations based on Stroh's formalism [1] were used:

- Method of Choi [2] for tri-material configurations

➢ Use of standard analytic continuation arguments and alternating technique to satisfy boundary conditions at the two interfaces.

$$u_i = 2\mathrm{Re}\left[A_{ij} f_j(z_j)\right]$$

$$f_i(z_i) = \begin{cases} f_i^0(z_i) + f_i^{I0}(z_i) + \sum_{n=1}^{\infty} f_i^{In}(z_i) & z \in \mathrm{I} \\ \sum_{n=1}^{\infty} f_i^{n}(z_i) + \sum_{n=1}^{\infty} f_i^{IIn}(z_i) & z \in \mathrm{II} \\ \sum_{n=1}^{\infty} f_i^{IIIn}(z_i) & z \in \mathrm{III} \end{cases}$$



$\langle\Gamma_1, \Gamma_2\rangle$ represent grain boundary

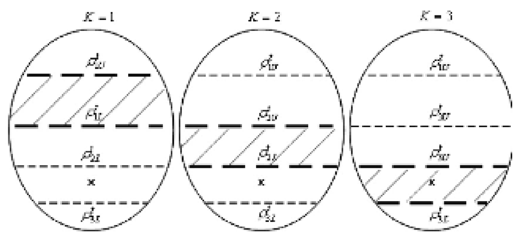
➢ Modeling compliant or rigid grain boundary in tri-materials: $c_{ijkl}^{\mathrm{II}} = \frac{\lambda}{2}\left(c_{ijkl}^{\mathrm{I}} + c_{ijkl}^{\mathrm{III}}\right)$

- Method of image dislocation density of Wu [3] for an infinite number of layers

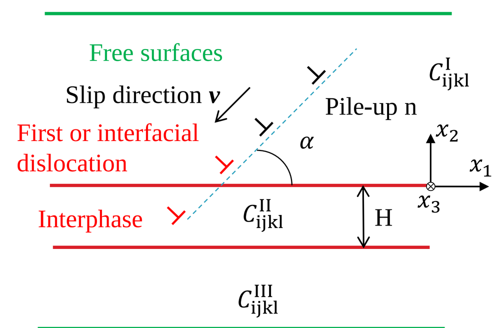
➢ Decomposition of a K-layer problem into K infinite homogeneous sub-problems.

➢ Summing the contributions of the source (homogeneous) and all image dislocation densities in sub-problems 1, 2 and 3, respectively.

$$\sigma_{ij}(K, \rho_{JK}^t, x_1, \Delta x_2) = \int_{-\infty}^{\infty} 2\sum_{\alpha=1}^{3}\left(\xi_{K\alpha ij}^{tR} P(\Delta x_1, p_{K\alpha}^R \Delta x_2, p_{K\alpha}^I \Delta x_2) + \right.$$



➢ Dislocation positions in an equilibrated pile-up computed by an iterative relaxation scheme that minimizes the Peach-Koehler force on each dislocation [4]:



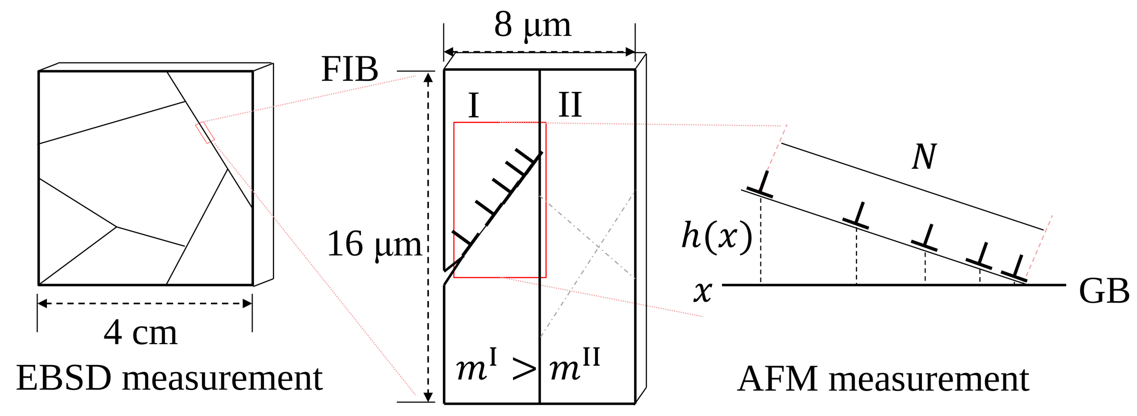
In-situ micromechanical experiments (MWW)

➢ Bi-crystals (Ni) made out of poly-crystalline sheets by FIB

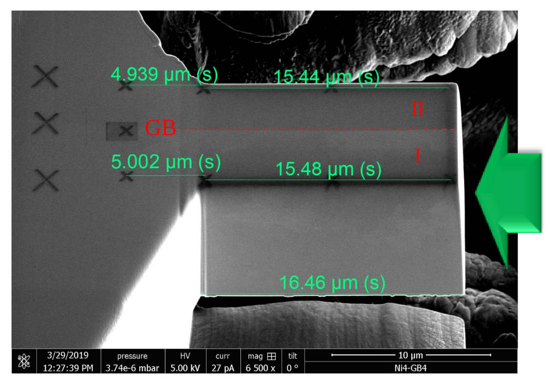
➢ Micro-compression tests to test dislocation – grain boundary interactions.

➢ Observations of bi-crystal plasticity using SEM, AFM and EBSD

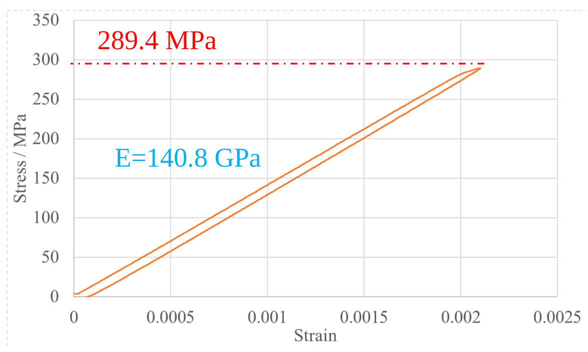
➢ From slip height h(x) determined by AFM, the number of dislocations N in the pile up is obtained and feeds the numerical pile up calculations.



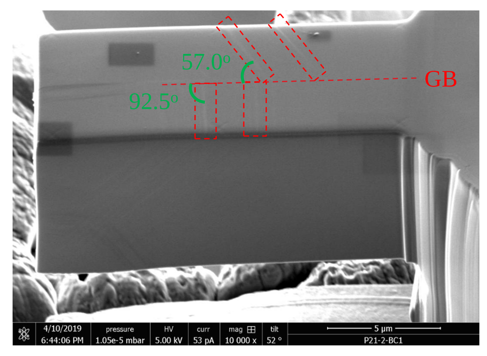
Experimental schema



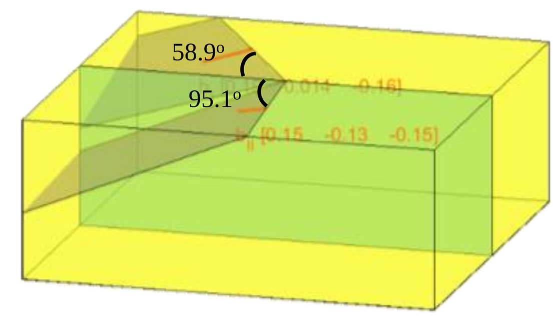
Size of the micro sample side surface: 8 µm * 8 µm



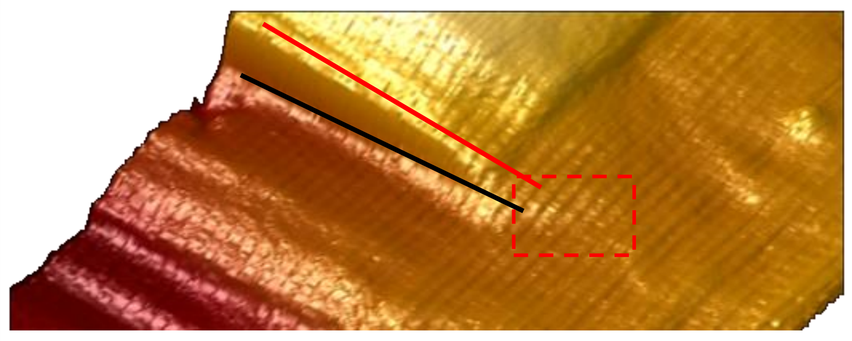
Stress-strain curve (calibrated by CPFEM)



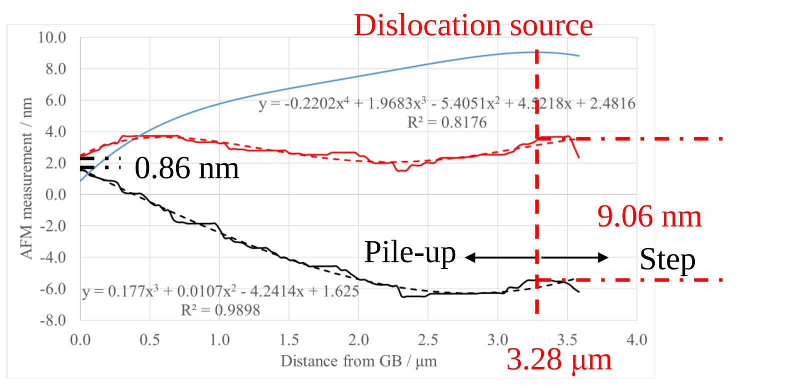
Slip lines analysis by SEM



Slip systems with maximum Schmid factor

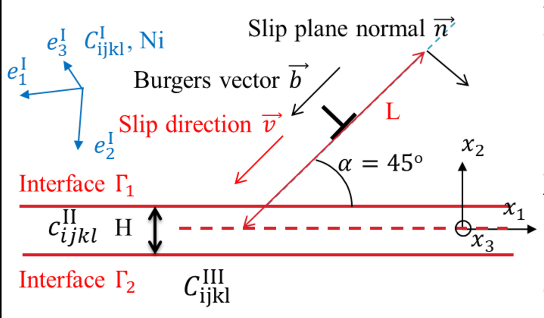


AFM measurement of slip lines, a weak slip transmission is observed

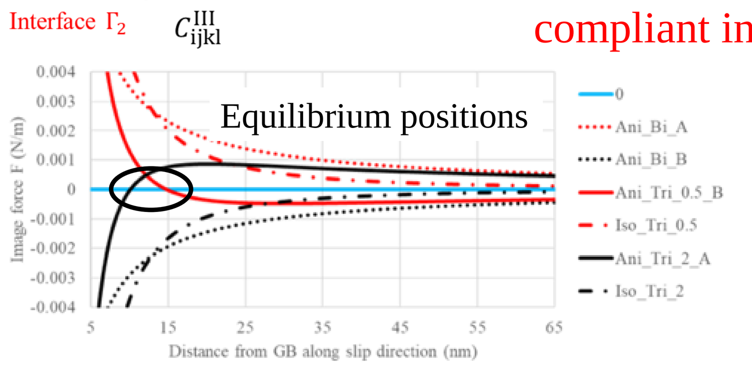


Polynomial fit of AFM measurement and calculation of the number of dislocations assuming single slip

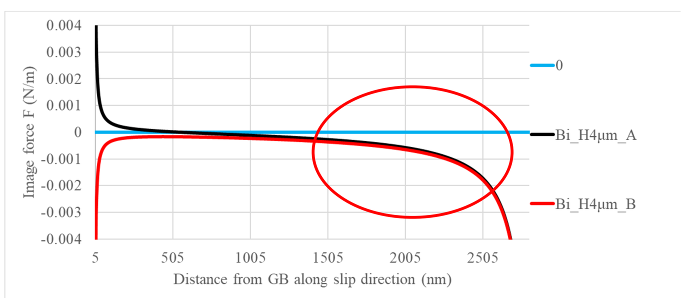
Application: effect of misorientation, GB stiffness and free surfaces on image force along slip direction [5]

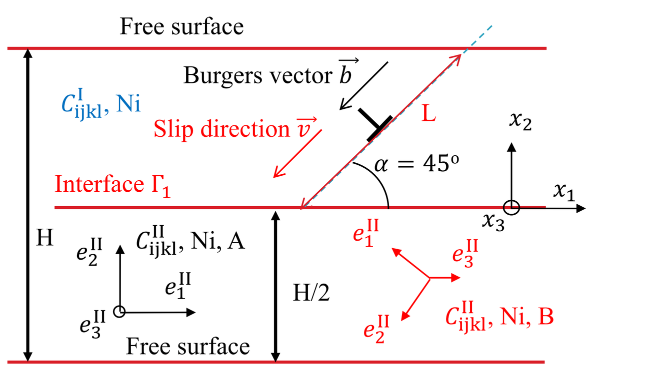


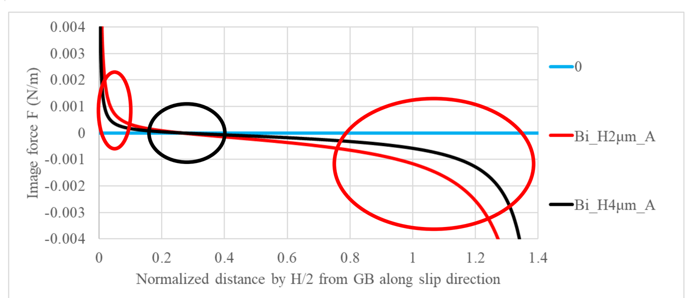
Fixed orientation of crystal I ($\varphi_1 = 45^o, \Phi = 324.7^o, \varphi_2 = 135^o$); Attractive orientation A ($\varphi_1 = 0^o, \Phi = 0^o, \varphi_2 = 0^o$) of crystal III and stiff interphase (λ = 2.0); Repulsive orientation B ($\varphi_1 = 90^o, \Phi = 45^o, \varphi_2 = 45^o$) of crystal III and compliant interphase (λ = 0.5)



Short distance effect of interphase: about 60 nm; Long distance effect of misorientation; Important to equilibrate leading dislocation in pile-up.



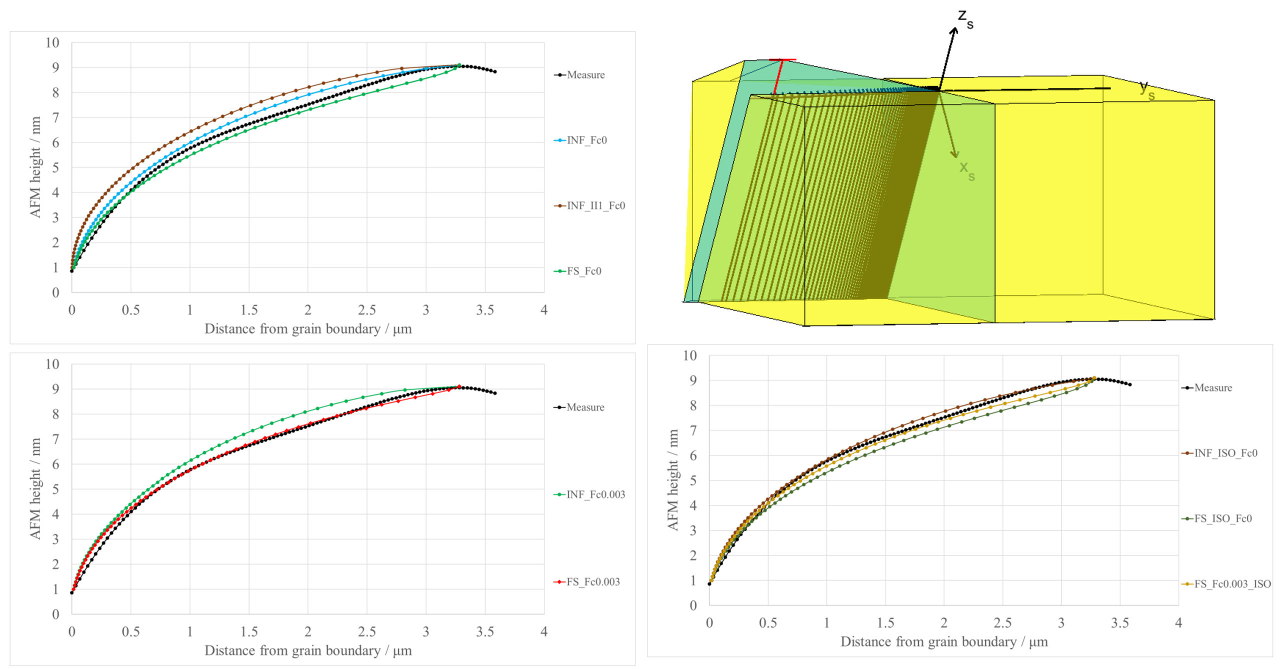




Free surfaces always attract dislocations; Size effect; Normalized equilibrium positions are close

Application: slip step heights due to a dislocation pile-up in heterogeneous anisotropic elasticity

- $H = N \times b_{unit} \times |b_s^{\mathrm{Ni}}|$, $b_{unit} \times |b_s^{\mathrm{Ni}}| = [0.15, -0.13, -0.15]$nm
- $N_T \approx 6$, $N_S \approx 61 \rightarrow N_P \approx 55$ with $\sigma_{ext} \approx 289.4$ MPa, λ=1, H=0.9nm
- A dislocation locked at $L = 3.28\ \mu m$ as dislocation source
- An interfacial dislocation of 6 b locked in GB to account for transmitted dislocations



Simulation considering grains misorientation, free surfaces, critical force for dislocation glide (F_C=0.003 N/m, 12 MPa for Ni) and transmitted dislocations across to GB fits very well with AFM measurement of dislocation pile-up heights.

Outlook

➢ Direct observations of discrete dislocations by ECCI

➢ Use molecular dynamics simulations to study the elastic stiffness of GB

➢ Use molecular dynamics simulations to study dislocation-GB interactions at atomic scale

➢ Estimate GB strength and improve slip transmission criteria

References :

[1] A. N. Stroh, "Dislocations and Cracks in Anisotropic Elasticity," Philos. Mag., 3, 625–646 (1958).

[2] S.T. Choi, Y.Y. Earmme. Elastic study on singularities interacting with interfaces using alternating technique Part I Anisotropic trimaterial. Int. J. Solids Struct. 39, 943-957 (2002).

[3] H.Y. Wang, M.S. Wu, H. Fan, Image decomposition method for the analysis of a mixed dislocation in a general multilayer. Int. J. Solids Struct. Vol. 44, Issue 5, 2007, P 1563-1581

[4] Wagoner, R.H. Calculating Dislocation Spacings in Pile-Ups at Grain Boundaries. MTA. 12, 2015-2023 (1981) .

[5] Chen, Xiaolei & Richeton, Thiebaud & Motz, Christian & Berbenni, S. (2019). 164. 141-156. 10.1016/j.ijsolstr.2019.01.020.