

Atomistic modeling of idealized equal channel angular pressing process

Supplementary Material

Aruna Prakash^{1*}

^{1*}Micro-Mechanics & Multiscale Materials Modeling (M⁵),
Institute of Mechanics and Fluid Dynamics,
TU Bergakademie Freiberg,
Lampadiusstr. 4, Freiberg, 09599, Germany.

Corresponding author(s). E-mail(s): arun.prakash@imfd.tu-freiberg.de;

Supplementary Material

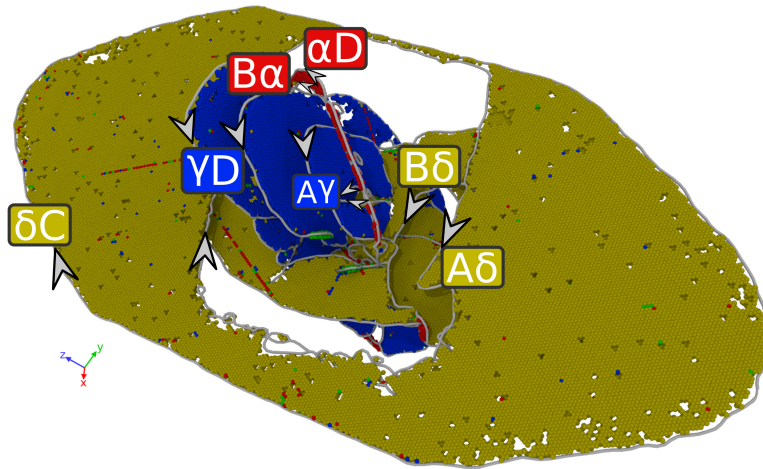
Supplementary movies

The following movies are included as part of supplementary material.

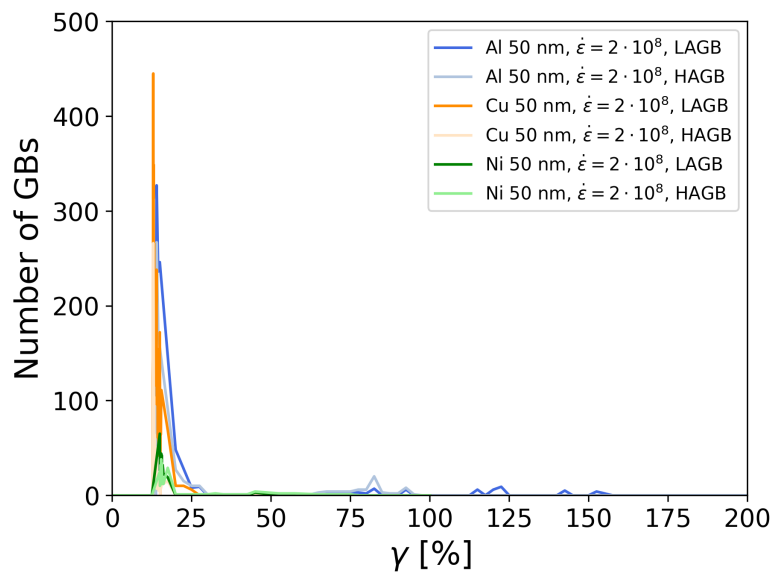
- **Movie M1:** Deformation of Al, 50 nm sample showing the dislocation activity for strain rate $\dot{\epsilon}_{xy} = 2 \cdot 10^8$.
- **Movie M2:** Deformation of Ni, 50 nm sample showing the dislocation activity for strain rate $\dot{\epsilon}_{xy} = 2 \cdot 10^8$.
- **Movie M3:** Deformation of Cu, 50 nm sample showing the dislocation activity for strain rate $\dot{\epsilon}_{xy} = 2 \cdot 10^8$.
- **Movie M4:** Deformation of Al, 100 nm sample showing the dislocation activity for strain rate $\dot{\epsilon}_{xy} = 2 \cdot 10^8$. Only the atoms classified as hcp by the common neighbor analysis algorithm are shown.
- **Movie M5:** Deformation of Al, 100 nm sample showing the dislocation activity for strain rate $\dot{\epsilon}_{xy} = 2 \cdot 10^9$. Only the atoms classified as hcp by the common neighbor analysis algorithm are shown.
- **Movie M6:** Texture evolution and deformation activity from the initial configuration until approx. 15% applied shear in cluster number 1 identified by ORISODATA.
- **Movie M7:** Texture evolution and deformation activity from the initial configuration until approx. 15% applied shear in cluster number 44 identified by ORISODATA.
- **Movie M8:** Texture evolution and deformation activity from the initial configuration until approx. 15% applied shear in cluster number 62 identified by ORISODATA.
- **Movie M9:** Texture evolution and deformation activity from the initial configuration until approx. 15% applied shear in cluster number 66 identified by ORISODATA.

Note: In the movies M1 – M5 showing the deformation of the samples, the simulation box flips after 50% shear. This is a technicality in LAMMPS required to run simulations efficiently, since a large tilt requires a large volume of communication to acquire ghost atoms around a irregular-shaped subdomain of the processor. For more details, the reader is referred to the documentation of the LAMMPS package.

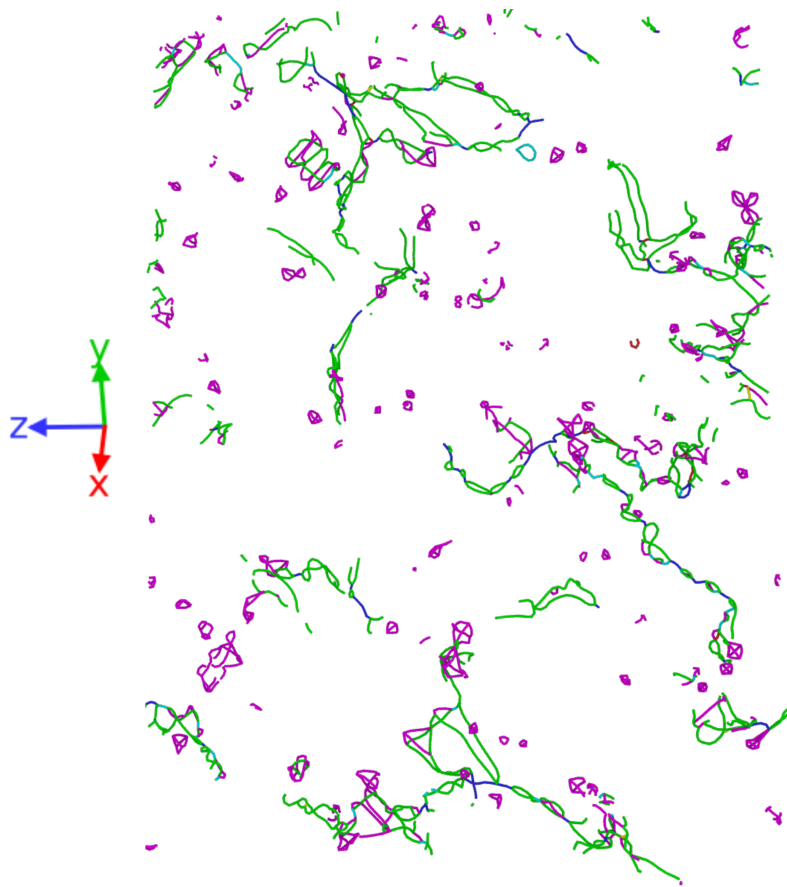
Supplementary figures



Supplementary Figure 1: Expansion of a partial dislocation loop creating a stacking fault in its wake. Shown here is defect configuration after approx. 12.7% shear in the Cu 50 nm sample. Only atoms classified as hcp are shown here. Atoms are colored according to the $\{111\}$ planes they belong to. For more details on the color code, the reader is referred to fig. 3 in the main article.



Supplementary Figure 2: Distribution of low angle (LAGB) and high angle (HAGB) grain boundaries in all 50 nm samples.



Supplementary Figure 3: Dislocation cell structure in a slice of 5 nm in the Al 50 nm sample after approx. 165% shear.