Microsc. Microanal. 27 (Suppl 2), 2021
doi:10.1017/S1431927621013350

# Tensile Deformation of Al Thin Films Studied by *In-situ* TEM and Molecular Dynamics Simulations

Lucia Bajtošová[1], Barbora Křivská[1], Jozef Veselý[1], Miroslav Cieslar[1], Jan Hanuš[1], Petr Harcuba[1] and Jan Fikar[2]

[1] Faculty of Mathematics and Physics, Charles University Prague, Czech Republic.
[2] Institute of Physics of Materials, Academy of Sciences of the Czech Republic Brno, Czech Republic.

Mechanical properties of nanocrystalline films with grain sizes smaller than 100 nm have recently been a subject of interest due to their wide applicability in micromechanical devices. Restricted dimensions of these films are a cause of properties deviating from the ones observed in bulk materials [1]. A combination of mechanical tests with direct observation of the material structure by *in-situ* transmission electron microscope (TEM) [2] can be combined with molecular dynamics (MD) simulation [3], a computer simulation method which allows prediction of individual atom motion from numerical integration of equations of motion.

DC magnetron sputtering was used to prepare 150 nm Al3%Mg thick films. The conditions of the deposition were following: working pressure 0.34 Pa, current ~100 mA and voltage ~5V. The film was sputtered on a glass substrate covered with polystyrene tape, which was then dissolved in toluene and acetone to obtain free standing samples. The film was *in-situ* annealed up to 640° C in TEM Jeol 2200FS, operated at 200 kV. Dog-bone shaped specimen were prepared in scanning electron microscope Zeiss Auriga using focused ion beam (FIB) and fixed onto Hysitron Push-to-Pull (PTP) device with stiffness 150 N/m. The specimens were deformed in TEM Jeol 2200FS by Hysitron PI 95 TEM PicoIndenter equipped with a flat punch and characterized by Automated orientation phase mapping.

Automated orientation phase mapping of the annealed 150 nm thick Al film revealed polyhedral columnar grains with sizes ranging from 20 to 200 nm. [110] texture in a direction perpendicular to the surface was observed. The samples were deformed in tension at strain rate $10^{-4}$ $s^{-1}$ with the active area simultaneously captured on camera in BF TEM mode (Fig. 1). Extensive contrast changes in individual grains signifying dislocation activity (Fig. 1b – marked by arrows) in the grain boundraries (GB) or grain rotations were detected along with minor in-grain dislocation activity short before the crack formation. The crack propagation started at 9% strain and stress 700 MPa and occurred along GB.

Large-Scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) [4] was used to perform the MD simulations. A polycrystal structure in an orthogonal box with dimensions x=200 nm, y=200 nm, z=200 nm was created using Atomsk software [5]. Periodic boundary conditions were employed in *x* and *y* directions. Six columnar hexagonal grains with [110] texture in z direction were created and deformed at strain rate $2.10^{9}$ $s^{-1}$ at 300 K up to 20% strain. Al MEAM potential was used to carry out the simulation. The simulation was repeated for the same polycrystal with modified size – thickness z = 500 nm and width x=400 and y=400 nm. The results were visualized by Open Visualization Tool (OVITO) [6] with the common neighbor analysis (CNA) and dislocation analysis (DXA).

The results of the simulation are shown in Fig 2. At 3% strain, one full dislocation was emitted from a GB, propagated through the grain (Fig 2. a,b) and was annihilated in the opposite GB. Aside from that, no in-grain dislocation activity was observed until 9% when two stacking fault planes bound by partial dislocations formed. Subsequently, tearing of the material along the GB perpendicular to the deformation

direction started (Fig 2. d). Most of the deformation at strains under 9% was carried out by a movement of dislocations inside GB. The deformation of polycrystal blocks with larges dimensions (200x200x500 $nm^3$ and 400x400x200 $nm^3$) yielded coincident results – dislocation movement inside GB, low in-grain dislocation activity and intergranular tearing at strains ~10% and strain 4.5 GPa.

In conclusion, a relatively good compliance between the experimental observations and the simulation results was reached. Neither the change of sample thickness from 20 to 50 nm, nor the change of grain size from 10 to 20 nm did significantly affect the simulation results. The tensile strength predicted in the simulation was several times higher than the experiment result [7].

References:

[1] A Tajik, H Jahed, InTech, p. 435.
[2] KS Kumar *et al*, Acta Materialia **51**(2) (2003), p. 387.
[3] FF Abraham, Advances in Physics **35**(1) (1986), p. 1.
[4] S Plimpton, J. Comp. Phys. **117** (1995), p. 1.
[5] P Hirel, Computer Physics Communications **197** (2015), p. 212.
[6] A Stukowski, Mater. Sci. Eng. **18** (2010), p. 015012.
[7] Authors would like to acknowledge the support from Grant Agency of Charles University under the project 574120.

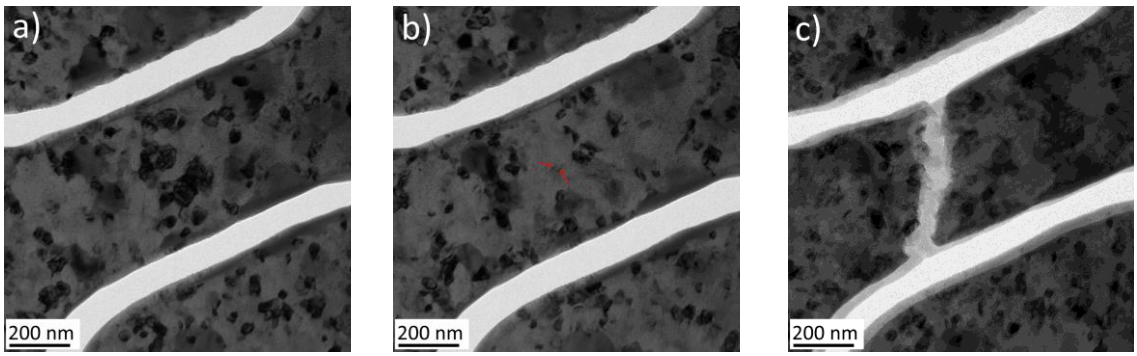


**Figure 1.** TEM images from *in-situ* tensile deformation experiment a) 0%, b) 6%, c) after rupture.

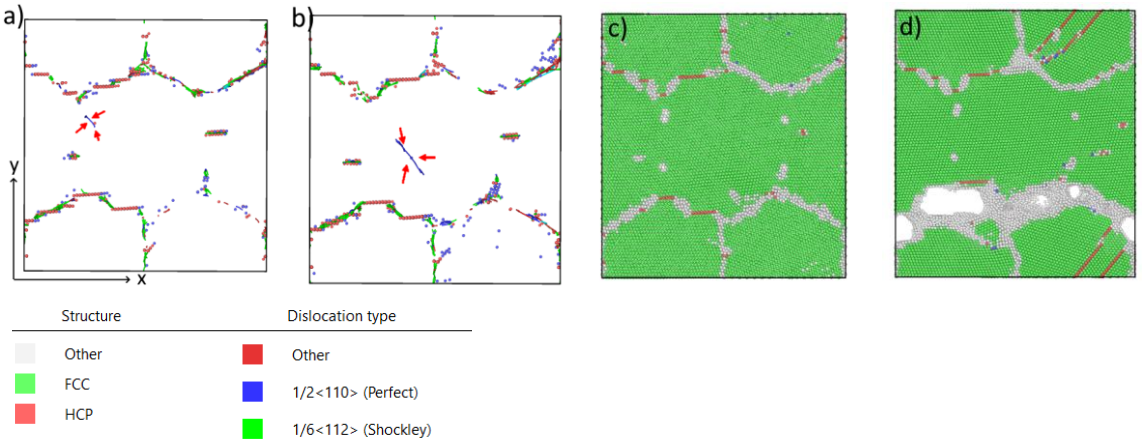


**Figure 2.** Visualization of MD simulation a) DXA 3%, b) DXA 6%, c) CNA 7%, d) CNA 11% strain.

https://doi.org/10.1017/S1431927621013350 Published online by Cambridge University Press