Master Internship

Can be followed by a PhD

University of Poitiers, Institut Pprime, France

Atomic scale simulations of nanotwinned gold thin films

Supervisors: **Sandrine BROCHARD and Julien DURINCK**

Keywords: twin, atomic scale simulations (molecular dynamics and statics), thin films

Context:

A twin is a portion of a crystal with a particular orientation, for example obtained by a reflection, with respect to a matrix with the same crystalline structure. Twins may appear during plastic deformation, crystal growth or recrystallization. During the last years, nanotwinned materials have been the subject of great interest due to their remarkable mechanical properties: they present large mechanical resistance, ductility and work-hardening capacities. Moreover, they have the same electrical resistivity as coarse grain crystals [1].

In this context, the "PtyMet" project aims at characterizing the stress field in nanotwinned thin films, and its impact on physical properties. We will combine experiments (X-ray diffraction and transmission electron microscopy) and simulations (molecular statics and dynamics) and focus on single-crystalline nanotwinned gold thin films prepared in our laboratory (figure 1 (a) and (b)).

From a numerical point of view, atomistic scale simulations are particularly well adapted tools for these studies. They include key materials properties such as the stacking fault and twin boundary energies, allowing precise descriptions of the defect configurations (e.g. dislocations, grain boundaries, twins, figure 1(c)). Furthermore, atomic scale simulations and experiments are now working on converging spatial scales.

Objective of the master thesis:

The aim of this stage is to establish via atomistic scale simulations the elastic strain field associated with different nanotwinned thin film microstructures. Equilibrium conditions will be determined using semi-empirical potentials, that are reliable for gold. In a first step, a simple configuration with a unique twin and periodic boundary conditions will be worked out. This will allow studying the impact of the twins' density and thickness. More sophisticated and larger systems will then be considered, with several twins having different orientations.

Associated PhD thesis:

This study will be continued with a PhD funded by the "PtyMet" project (main supervisor: Pierre Godard). This PhD will involve simulations and experiments. In particular, coherent X-ray diffraction patterns induced by the strain field given by the molecular statics results will be simulated and compared with experimental ones. It is also foreseen to study the deformation of the different nanotwins configurations with molecular dynamics.

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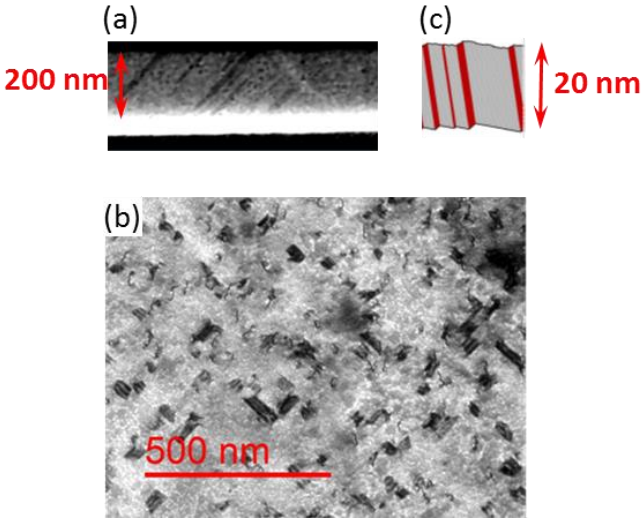

Figure 1: nanotwinned thin films
(a) Scanning electron microscopy image (cross-section) of a gold thin film. The dark areas cutting the film are twins.
(b) Transmission electron microscopy (plane view) of a 50 nm thick gold thin film. The dark rectangles are twins.
(c) Image from an atomic scale simulation (molecular dynamics) of an aluminium film strained to 6.3% [2]. Twins, nucleated at the surface, are highlighted in red.

[1] Lu et al., *Science* **304**, 422 (2004).
[2] Béjaud et al., *Computational Materials Science* **145**, 116 (2018).

Dates: the internship is available from February to September 2020, with a vacation period in August.

Funding: the wage is defined according to the collective agreements on salary scales for internship in France, about 550€ per month.

Working laboratory: Institut PPRIME (https://www.pprime.fr) – Futuroscope-Chasseneuil (15 km from Poitiers city, France)

Required skills/qualification: the applicant has to be in final year of Master and/or engineering school with a background in solid-state physics or materials science. He/she should show a strong interest in computer simulations. Atomic-scale simulations skills, especially in molecular dynamics, will be an asset.

Application: send a CV and a cover letter to the contacts below before December 2019.

Contact:

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