MASTER INTERNSHIP M2 PPN (5 months)

2024-2025

Title of the project: Molecular dynamics simulation of Zr oblique angle deposition

Supervisor:

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Summary:

Vapor phase deposition (PVD) with the Oblique Angle Deposition (OAD) technique enables the elaboration of thin films with a tilted columnar microstructure. While this behavior is well known, the relationship between the incidence angle of the flux, the angle of the columns, and the angle of the crystallites, relative to the substrate reference frame, has been scarcely studied. This question is of primary importance when considering surface protection of artificial joint heads (e.g. hip or knee prosthesis) by PVD coatings to improve durability in service. As the hip joint head is a half sphere, the change in the geometrical configuration (distance, position, angle) will introduce morphological variations and consequently properties variations.

In the context of a previous work, Zr films were fabricated by OAD and characterized, particularly in terms of crystallite orientation. Two behaviors were observed: for low to medium incidence angles, the inclination of the main plane increases slightly, whereas for higher incidence angles, the crystallites tend to suddenly align with the column growth direction. Also, SEM observation showed that porosity increase with the substrate tilt angle, flux incidence angle and column tilt angle. In particular, flux angles lower than 45° the films are dense (less than 5 % of porosity) and provide good corrosion protection, however, for flux angles higher than 45° the film's porosity increases (up to 12-18 %) and deteriorates the corrosion protection.

In the framework of this master 2 project, we will study the deposition of Zr atoms on a substrate varying for different deposition angles. LAMMPS molecular dynamics code [1] and Ovito software [2] will be used to perform and analyze the simulations. We will first see if classical MD simulations will allow us to observe a variation of the deposited film morphology (column tilt angle, porosity) related with the angular distribution of the incoming particle flux. Secondly, we will quantify the intrinsic stresses in the deposited grains to understand the relation between the resulting microstructure with the anisotropic internal stress. The results will be compared with the experimental and theoretical approaches (Monte-Carlo modeling) that were developed to describe the deposition process [3].

References:

[1] A.P. Thompson *et al.*, LAMMPS - a flexible simulation tool for particle-based materials modeling at the atomic, meso, and continuum scales, Comp Phys Comm, 271 (2022) 10817.

[2] A. Stukowski, Visualization and analysis of atomistic simulation data with OVITO–the Open Visualization Tool, Modelling Simul. Mater. Sci. Eng. 18 (2010) 015012

[3] Khaoula Rahmouni, Aurélien Besnard *et al.*, In vitro corrosion response of CoCrMo and Ti-6Al-4V orthopedic implants with Zr columnar thin films, Surface and Coatings Technology, 436, (2022) 128310

Type of project (theory / experiment): theory and modelling, molecular dynamics

Required skills: A basic knowledge in materials science and statistical physics is required. A skill in numerical methods and computational languages is expected. The candidate will learn the necessary tools to develop molecular simulations with open-source software (LAMMPS). The scientific curiosity of the candidate will be appreciated.