Projet en laboratoire et/ou stage EUR Master 2
2019-2020

PROPOSITION DE STAGE M2 CDM

Titre : **Numerical studies of thin Co-Mo films** (Etude numérique de films minces de Co-Mo)

Responsable(s) : V. Vignal - O. Politano

Laboratoire : ICB ï Equipe M4OxE

Collaborateurs : H. Krawiec (AGH University, Poland), F. Baras (ICB, Manapi)

Lieu du stage : Equipe M4OxE

Description sommaire du sujet :

Nanocrystalline alloys produced by electrodeposition have excellent mechanical properties. They can undergo severe plastic deformation and they have high hardness and good resistance to wear. Other studies have shown that these alloys also have specific physical-chemical properties (such as magnetic, electronic, catalytic and optical properties). Therefore, they can find applications in many industrial sectors: biology, energy, nano- technologies, aerospace.

In particular, Co-Mo nanocrystalline coatings are characterized by high hardness and high thermal resistance. They have good magnetic properties and are good catalytic electrodes for hydrogen evolution reaction. These properties make these coatings promising materials for various applications. However, recent experiments performed at ICB have shown a higher tendency to the oxidation of the Co-Mo compared to pure Co or Mo. One suggests that oxidation of the alloy is significantly promoted with the combination of crystallites with size close to 2 nm and a mixture of Co and Mo. These two elements crystallize in two different systems: hexagonal close-packed structure for Co and body-centered cubic structure for Mo. Therefore distortions exist in the atomic lattice of the Co-Mo nanocrystalline coating which may promote oxidation.

This project aims at studying the properties of nanocrystalline Co-Mo by numerical simulations. Among all the simulation techniques available, Molecular Dynamics (MD) seems a perfect tool as the crystallites size observed experimentally in Co-Mo alloys (i.e. few nm) corresponds well to the length scale accessible by atomistic simulations. The systems will be simulated by using LAMMPS software (http://lammps.sandia.gov) and the interatomic potential developed by Zhou et al. (Phys. Rev. B, 69 (2004) 144113) for many metals and alloys.

MD will be used to study the mechanical properties of polycrystalline Co-Mo deposited on a Co substrate. In a preliminary approach, we validated the interatomic potential by computing some well known properties (melting temperature, elastic constants, lattice parameters, defect energies,é) of the pure Co, Mo and Co-Mo phases.

During this work, we will study the epitaxial relationship and the adhesion of Co-Mo thin film on Co or Mo substrates. The mechanical properties of the Co-Mo layer will be characterized as a function of the crystallite size with polycrystalline nanolayers.

Caractère du sujet (expérimental/théorique) : Numerical simulations

Connaissances requises particulières : Theory and modeling, molecular dynamics

Formation souhaitée de l'étudiant : The candidate will learn the necessary tools to develop molecular simulations with open source software (LAMMPS). Basic knowledge of Matlab/Octave will be appreciated.