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PHYSIQUE – CHIMIE INGENIERIE

NANOSCIENCES – PHOTONIQUE – SCIENCES DES MATERIAUX & CARACTERISATION

Molecular dynamics studies of Cu-Mo nanostructured composites

PhD position for 3 years

Starting date: October 1, 2023

Keywords: theory and modeling, molecular dynamics, metallic nanolayers.

Subject: Recently, significant efforts have been devoted to the design of nanometric metallic multilayers (NMMs). These systems are constructed by stacking multiple nanometric (4 - 100 nm) layers of two metallic elements. They demonstrate exceptional properties resulting from the significant number of interfaces associated with their nanoscale layered microstructure. This project will focus on Cu-Mo NMMs, which consist of immiscible metals and display incoherent fcc/bcc interfaces (see [1] for a general introduction on NMMs). These Cu-Mo NMMs offer a combination of high thermal and electrical conductivity, and low coefficient of thermal expansion (CET). These properties can be tailored to meet specific requirements ("materials on demand") by controlling the Cu-Mo ratio, layer thickness, and texture. Additionally, they are excellent candidates to serve as heat sink in electronic devices. For instance, the nanometric structure of Cu-Mo NMMs allows for achieving an ideal CTE match with the base materials of miniaturized components, thereby enhancing their thermal management performance. The primary objective of this thesis is to provide a fundamental study of the specific mechanisms responsible for the unique properties exhibited by Cu-Mo nanolaminates. This study will be carried out in close collaboration with the researchers conducting experiments at EMPA.

Cu-Mo NMMs are expected to maintain their initial microstructure even when annealed at high temperatures. However, after annealing, the layered system transforms into a composite with Cu inclusions in Mo matrix. This transformation occurs in 3 stages: grain coarsening, thermal grooving and pinch-off of the layers. After annealing, the layered system became a composite with Cu inclusions in Mo matrix. By observing this phenomenon, we aim to determine whether a degraded material can retain its properties. The driving force originates from the interface energy, thermal properties of the components, and large stresses in the multilayers. Understanding the kinetics that lead to structural instability remains an open question crucial for interpreting experimental observations.

The PhD candidate will acquire the necessary tools to conduct molecular dynamics (MD) studies using LAMMPS software and analyze the MD data. Indeed, MD proves to be a valuable tool for investigating at nanoscale NMMs. The student will gain skills and competences related to modeling on the atomistic scale, data analysis, scripting for high-performance computing (HPC), programming, scientific work, writing, and publishing.

[1] A. Saenz-Trevizio and A.M. Hodge, Nanotechnology 31 (2020) 292002 (doi:10.1088/1361-6528/ab803f)

Context : The PhD is funded by the ANR DEFROST "Next-gen multi-material devices: designing of nanostructured Cu-Mo composites". The research work will be carried out in a multidisciplinary team in Dijon, with a sustained collaboration with GPM laboratory (Rouen, France) and the Laboratory for Joining Technologies & Corrosion (EMPA, Switzerland). Several scientific visits are planned in these two laboratories during the 3 PhD years.

Required knowledge: The candidate should demonstrate a strong motivation for programming and numerical simulation in the context of material studies. Additionally, a basic knowledge in materials science and/or statistical physics is required.

Contacts: CV and letter of motivation should be sent to Dr. O. Politano (olivier.politano@u-bourgogne.fr) and Dr. F. Baras (florence.baras@u-bourgogne.fr).