PhD thesis 2022-2025

Title of the project: Metallic nanocomposites: an atomistic approach of microstructural evolution

Supervisor(s): Olivier Politano / Florence Baras

Laboratory: ICB/PMDM

Collaborations: V. Turlo (EMPA-Thun), C. Cancellieri (EMPA-Dübendorf, Switzerland)

Summary:

A nanocomposite (NC) is a multiphase nano-structured solid material. The properties of NC differ significantly from that of the component materials. The aim is to benefit from the respective properties to obtain tailored materials. For instance, a hard material with good electric performances. In this research project, we will consider nanometric metallic multilayers (N2MI) made up of alternating thin layers of two immiscible metals. Up to a given temperature, no solid-state phase transformations take place. Nevertheless, these N2MIs are intrinsically unstable due to multiple phase boundaries, in particular when the temperature increases.

This project aims at a profound understanding of the lack of structural stability during heat treatment. At elevated temperatures, N2MIs (e.g. Cu/Mo, Cu/Nb, Ag/Ni, Cu/W) are known to undergo structural changes resulting in the degradation of the initial laminated architecture. The degradation process is associated with the pinch-off of the layers followed by the spheroidization of residual layer-fragments. The morphological evolution upon elevated temperatures depends on the layer thickness as well on the initial microstructure (plain grain sizes, interphase orientations).

Molecular Dynamics (MD) is a valuable tool to study N2MIs, since the typical length (a few nanometers) corresponds precisely to the scale accessible in the simulation. MD actually describes the elemental mechanisms underlying the processes: atomic diffusion, creation of defects, mobility and segregation, … We will study the mechanisms occurring at the microscopic level to understand the influence of the interface orientation, the effect of mobility and defects, the formation of cracks and the creation of diffusion barrier. Along recent years, we have developed an extended expertise in nanometric metallic multilayers made up of miscible metals as the Ni-Al system [1,2].

Focus will be on Cu/W or Ag/Ni that have been studied experimentally [3,4]. The multilayer break-up proceeds by the formation of particles that grow at the expense of the multilayer. The driving force originates from the interface energy and large stresses in the multilayers. We will evaluate the influence of the atomic diffusion along the grain boundaries and interfaces on the formation of the particles. Our purpose is to determine the mechanisms responsible for the particle formation. We will also investigate the relative stability of some texture as reported in experimental observations by *in-situ* XRD diffraction.

This work will be conducted in close collaboration with EMPA researchers. They study experimentally the microstructural evolution in N2MI and develop modelling at mesoscale (phase field).

[1] F. Baras and O. Politano, Phys. Rev B 84 (2011) 024113

[2] A.S. Rogachev et al, Combustion Flame 166 (2016) 158-169

[3] K.O. Schweitz et al., The microstructural development of Ag/Ni multilayers during annealing, Phil. Mag. A80 (2000) 1867-1877.

[4] C. Cancellieri, et al., The effect of thermal treatment on the stress state and evolving microstructure of Cu/W nano-multilayers, J. App. Phys. 120, 195107 (2016)