Minicolloque n° CPR5 ☒ **Oral** ☐ **Poster**

An atomistic study of interface mobility and interdiffusion in Fe/Cr multilayers

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Interface mobility occurs alongside interdiffusion in equiatomic systems with an asymmetric miscibility gap such as Fe/Cr multilayers. These two phenomena lead to the decay of X-ray diffraction (XRD) satellite peak intensities, but the relationship between the decay rate and interdiffusion parameters is not clearly established. In this work, we study low-temperature interdiffusion and interface mobility in nanometric Fe/Cr multilayers using Atomistic Kinetic Monte Carlo (AKMC), and we aim to explain the XRD satellite peaks shift and decay from the atomic scale. The AKMC model [1] relies on a DFT-based vacancy diffusion model that successfully reproduces the phase diagram and high-temperature diffusion properties. We compare the evolution of concentration profiles in the Fe-rich layers and at the interfaces with annealed multilayers concentration profiles measured by atomic scale experimental techniques – Atom Probe Tomography (APT) and Scanning Transmission Electron Microscopy (STEM/HAADF). Interdiffusion in the Fe-rich layers and at the interfaces, as well as interface mobility, are well reproduced by the AKMC model. Experimental samples revealed unexpected dislocations and Fe inclusions in the Cr-rich layers, which could result in accelerated interdiffusion in the Cr-rich layers. The discrepancy found between simulated XRD profiles and the experimentally measured profiles will also be discussed. Moreover, we are developing an analytical model at the atomic scale to predict interface mobility in multilayers at different stages of annealing, and this model will be tested against both AKMC and experimental results.

[1] O. Senninger, Segregation and precipitation in Iron-Chromium alloys during thermal ageing and irradiation, Thesis Grenoble University (2013)

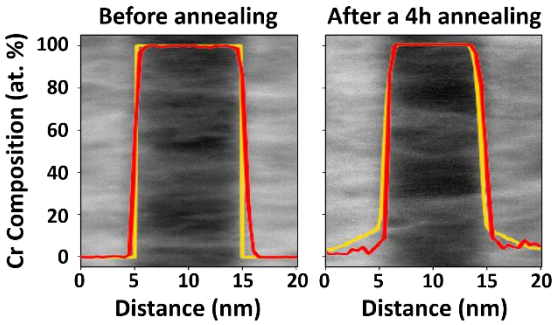

Figure 1 : Cr concentration profiles in Fe/Cr multilayers before (left) and after (right) a 4h annealing at 500°C measured by APT (red) and simulated by AKMC (yellow). The background image shows the Fe (light) and Cr (dark) layers obtained by STEM/HAADF. The asymmetry of the AKMC annealed profile and the resulting Cr-composition in the center of the Fe-rich layers are in good agreement with the measured APT profiles.