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Grain boundary self-diffusion in ^{56}Fe/^{57}Fe multilayers by in situ neutron reflectometry

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For the stability of nanostructured materials, grain boundaries (GBs) can be controlled by the grain size. When the diffusion length $L_d=(2Dt)^{1/2}$ is small compared to δ (~0.5 nm), the GB width, the volume diffusion at low temperature is slow compared to the GB diffusion (type-C regime), D being the volume diffusivity and t the isothermal annealing time. We studied self-diffusion active at the GBs at temperatures 150°, 175°, 200° and 225° C (consequtively for 600 min each) from the change of the ^{57}Fe isotopic fraction monitored *in situ* by neutron reflectometry on the sub-nanometer length scale on Pt(4 nm)[^{56}Fe(x nm)/^{57}Fe(x nm)]$_4$/Si with (x=4 and 8), in a dedicated furnace at REFSANS of HZG at FRM II in TOF mode. The samples of different thicknesses represent different average grain sizes without their evolution within a sample [1]. *In situ* experiments is expected to follow the dynamics more efficiently and therefore the mixed interface width has been mapped with time at short intervals.
Specular profiles, extracted from the 2D detector maps, were analyzed by the Fitsuite code (www.fs.kfki.hu) simultaneously at each temperature as a function of momentum transfer vector Q and annealing time t to extract the GB diffusion coefficient. The regular diffusion (decaying Bragg peak) regime starts above 200° C. We find an increase in the intensity of the first Bragg peak at lower temperatures which is probably related to initial smoothening of the interfaces of the as-prepared state of the multilayer. We plan to analyze this aspect further from the corresponding off-specular scattering in the near future.

[1] J. Gong et al, RSC Adv. 7, 9573 (2017)

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