Computer simulations of FCC alloys subjected to dry sliding as basis for a near-surface deformation mechanism map

Stefan J. Eder[a,b,*], Manel Rodríguez Ripoll[a], Ulrike Cihak-Bayr[a], Daniele Dini[c], and Carsten Gachot[a,b]

a) AC2T research GmbH, Viktor-Kaplan-Straße 2/C, 2700 Wiener Neustadt, Austria
b) Institute of Engineering Design and Product Development, TU Wien, Getreidemarkt 9, 1060 Vienna, Austria
c) Department of Mechanical Engineering, Imperial College London, South Kensington Campus, Exhibition Road, London SW7 2AZ, UK
* *corresponding author*

We study the microstructural response of five FCC CuNi alloys subjected to sliding with large-scale molecular dynamics simulations. The initial grains measure approximately 40 nm in diameter to ensure that plasticity is not dominated by grain boundary sliding, so our polycrystalline aggregate exhibits dislocation pile-up, twinning, and grain refinement analogous to polycrystals with much larger grains. We analyze the depth-resolved time development of the grain size, shear, twinning, and the stresses in the aggregate to produce a deformation mechanism map for CuNi alloys. This map captures the predominant microstructural phenomena occurring for a given composition and normal pressure, and will aid engineers in optimizing materials/surfaces to work within a required operating range. We compare tomographic visualizations of our atomistic model with focused ion beam images of the near-surface regions of real CuNi alloys that were subjected to similar loading conditions.

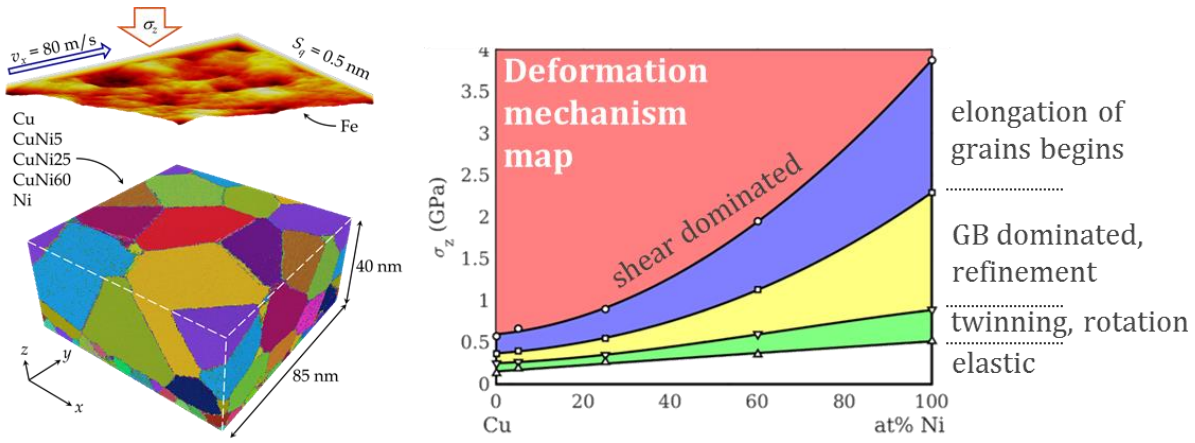

Figure 1 --- Left: MD setup of the polycrystalline CuNi alloy system containing 25 million atoms. Right: The deformation mechanism map derived from a pressure and composition dependent analysis of grain refinement, shear layer formation, twinning, and the stress distribution in the sample. The white data points are distilled from the MD results, and the fitted curves separate regions that are dominated by different deformation mechanisms.