Temperature dependence of plastic deformation in FCC alloys – A large-scale molecular dynamics study

Stefan J. Eder[1,2)*], Manel Rodríguez Ripoll[1)], Philipp G. Grützmacher[2)], Daniele Dini[3)], Carsten Gachot[2)]

[1)]AC2T research GmbH, Austria
[2)]Institute for Engineering Design and Product Development, TU Wien, Austria
[3)]Department of Mechanical Engineering, Imperial College London, UK
*Corresponding author: stefan.eder@ac2t.at

In this work, we attempt to separate the respective influences of composition, mechanical pressure, and temperature on the irreversible microstructural changes occurring in the near-surface region of CuNi alloys in a sliding contact with a rough hard counterbody. Based on a large-scale molecular dynamics parametric study, we quantify and discuss aspects such as twin formation, grain refinement and coarsening, as well as shear layer formation in light of the stresses induced by the sliding process. Finally, we present highly time-resolved visualizations of dislocation activity at key moments capturing the deformation and the evolution of the sliding interface.

Keywords: microstructure, EBSD, FCC alloys, molecular dynamics, sliding contact

1. Introduction

The mechanical behavior of a material is greatly influenced by its microstructure. In FCC alloys, the stacking fault energy is one of the most important material parameters that determines the onset of twinning and thus the first evidence of plastic deformation. At low temperatures, plastic deformation is dominated by dislocation glide, while dislocation climb becomes more prominent at elevated temperatures; this in turn leads to macroscopic softening.

2. Methods

Our molecular dynamics (MD) simulations were performed using the open-source code LAMMPS [1]. The polycrystalline model measures 85x85x40 nm³, contains approximately 25 million atoms, and was prepared as explained in ref. [2], see Fig. 1. Boundary constraints were applied to the lower 3 Å of the model, where a "sacrificial layer" of 10 nm grains was attached to the "working layer" of 40 nm grains so none of the occurring mechanisms would be externally constrained. The rough rigid counterbody was moved across the surface of the sample at a sliding velocity of 80 m/s at a slight angle with the *x*-axis to prevent roughness features from coming into repeated contact with their own sliding marks.

3. Results and Discussion

Using time- and depth-dependent heat maps, we can quantify aspects of plastic deformation such as twin formation, grain refinement and coarsening, as well as shear layer formation [3]. These are then discussed in connection with the stresses in sliding direction within the base body induced by the sliding process. Via several data distillation processes in which dimension after dimension can be eliminated, the influences of mechanical pressure, temperature, and alloying content on plastic deformation can be summarized in a set of 2D maps that can be used by surface engineers when designing and optimizing tribological interfaces.

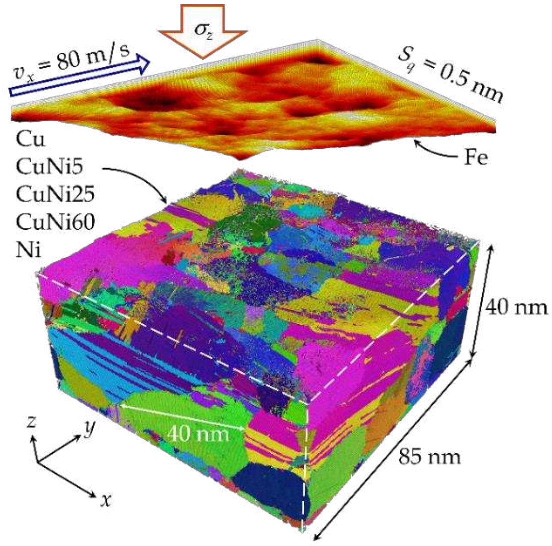

Figure 1: Exploded-view sketch of the CuNi base body and rough rigid counterbody after sliding under high mechanical load.

4. Acknowledgments

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5. References

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