From alloy behavior to deformation twinning and beyond: MD simulations and machine learning for tribological insights

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Understanding the deformation behavior of alloys under tribological conditions is critical for designing materials with tailored mechanical properties. Molecular dynamics (MD) simulations provide an atomistic perspective on these mechanisms, offering a powerful approach to investigate microstructural evolution under extreme conditions (see Fig. 1).

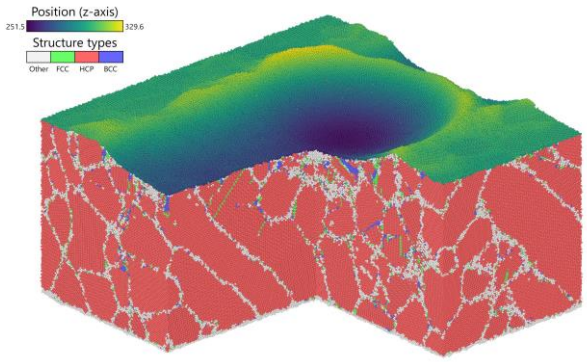

Figure 1. Large-scale scratch test simulation of acicularly grained titanium, showing microstructure and surface topology.

In polycrystalline CuNi alloys, for example, MD simulations involving tens of millions of atoms have allowed us to uncover the depth- and time-dependent evolution of grain refinement, twinning, shear deformation, and stress distributions during sliding [1]. These results have been synthesized into deformation mechanism maps, validated against experimental focused ion beam (FIB) microscopy images of near-surface regions subjected to similar loading conditions. Such maps are valuable tools for predicting the tribological behavior of alloys and identifying optimal compositions for reducing friction and wear, even under sliding conditions at ballistic speeds [2]. Building on this foundational work, we tackled the specific problem of identifying and tracking deformation twins, which are key features influencing mechanical performance in many metallic systems. While existing methods allow for the detection of twin boundaries, they often require extensive manual intervention and lack the ability to track twins over time. To address this, we developed a computational tool integrated into the OVITO visualization and analysis platform. This tool automates the detection of coherent twin boundaries, validates their structural orientation, links related twins, and tracks their evolution during MD simulations [3]. Applied to a copper single crystal under shear loading, the tool successfully identified the genesis, propagation, and interactions of deformation twins over multiple time steps (see Fig. 2). These capabilities offer unprecedented opportunities for studying the temporal dynamics of deformation twinning in a wide range of materials.

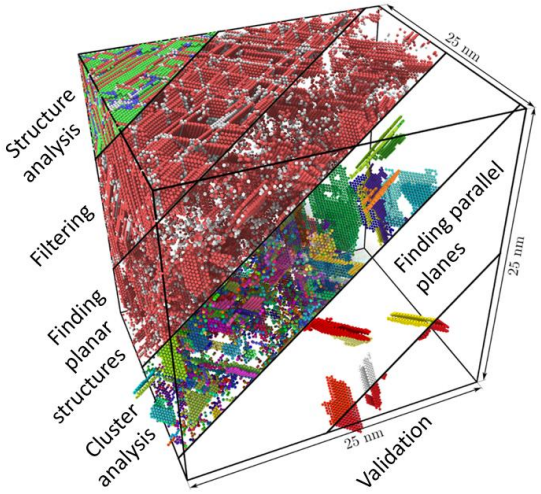

Figure 2. Workflow for twin boundary identification, pairing, and temporal tracking in a copper single crystal.

As we look to the future, our work is shifting toward leveraging machine learning (ML) techniques to further accelerate insights and expand the applicability of MD-based studies. The vast amounts of data generated by MD simulations—ranging from atomic coordinates to metadata on alloy composition, temperature, pressure, and sliding conditions—are ideally suited for ML-driven analysis.

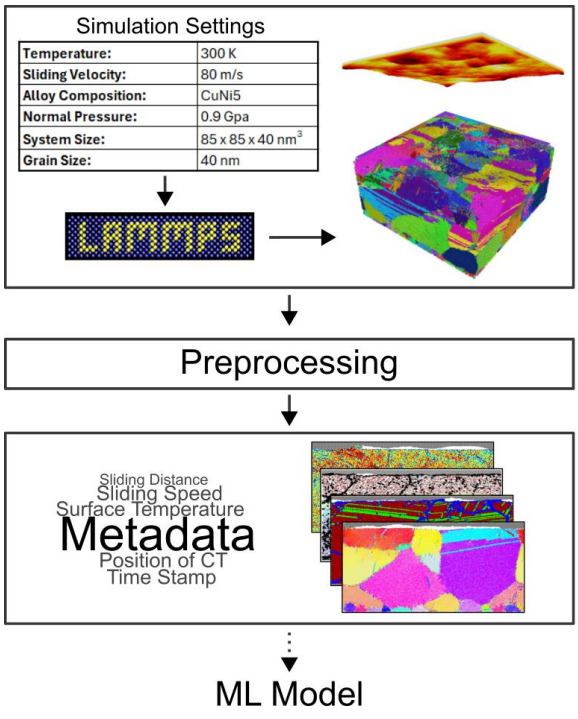

Figure 3. Data preparation pipeline for machine learning-assisted MD simulation analysis, including simulation setup, data preprocessing, computational tomographs, and metadata for ML models.

Our goal is to train ML models capable of predicting dominant deformation mechanisms across various alloy systems, effectively automating the creation of deformation mechanism maps and tribological Ashby charts. By pre-processing MD data into computational tomographs and combining it with state-of-the-art ML architectures (see Fig. 3) such as convolutional neural networks (CNNs) and transformers, we aim to streamline the analysis pipeline and make predictions applicable to a broader range of alloy classes [4].

This integration of MD simulations with ML techniques represents a significant step forward in materials science and tribology. By enabling faster, data-driven predictions of tribological performance, it reduces the reliance on computationally expensive simulations and supports the design of sustainable, high-performance alloys. Moreover, the insights generated through this approach hold potential for optimizing alloy design in industrial applications, from reducing friction in machinery to enhancing wear resistance in extreme environments.

References

[1] Eder, S. J., Rodríguez Ripoll, M., Cihak-Bayr, U., Dini, D., & Gachot, C. (2020). Unraveling and mapping the mechanisms for near-surface microstructure evolution in CuNi alloys under sliding. ACS Applied Materials & Interfaces, 12(28), 32197-32208.

[2] Eder, S. J., Grützmacher, P. G., Ripoll, M. R., Gachot, C., & Dini, D. (2022). Does speed kill or make friction better? — Designing materials for high velocity sliding. Applied Materials Today 29, 101588.

[3] Ehrich, H. J., Dollmann, A., Grützmacher, P. G., Gachot, C., & Eder, S. J. (2024). Automated identification and tracking of deformation twin structures in molecular dynamics simulations. Computational Materials Science, 236, 112878.

[4] Ehrich, H. J., Gachot, C., & Eder, S. J. (2025). ML pre-processing and model optimization for MD data: Insights from CuNi and Fe systems. Journal tbd, in preparation.