Atomistic modeling of mechanical properties of base-centered cubic multi-component alloys

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Refractory multi-component alloys (MCA) have base-centered cubic (BCC) structure and form an important class of materials with high potential for use in severe conditions. It is well known that the static and dynamic properties of dislocations have a crucial effect on the mechanical properties of metals and alloys. The low energy of nucleation and movement of the screw dislocations in ZrNbTaTiHf is the reason for ductility at room temperature [1], so the properties of dislocations define the brittle-to-ductile transition temperature (BDTT). In the present study, to achieve high accuracy in classical molecular dynamics simulations of dislocation motion, we apply the technique of machine learning for interatomic potential development. The influence of datasets on the reliability of machine-learning potentials (MLPs) is discussed. Results of modeling movement of dislocation with MLPs in MoNbTa and ZrNbTa are shown in Fig. 1. The unusual (112) slip plane, which is different from the usual 110 slip plane in single BCC metals, can be seen.

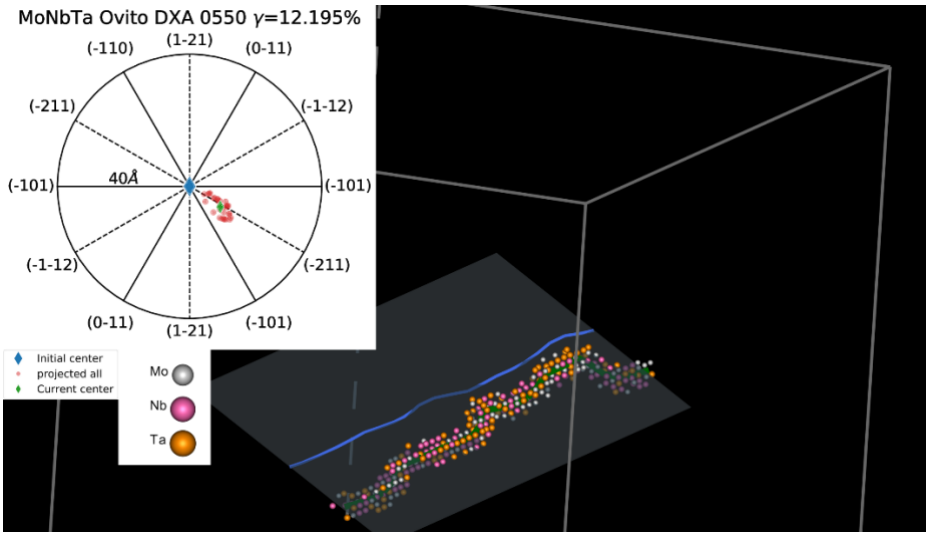

Fig.1: Screw dislocation kink-type glide on a (112) plane in MoNbTa MCA.

[1] T. Tsuru, S. Han, S. Matsuura, Z. Chen, K. Kishida, I. Lobzenko, S. Rao, C. Woodward, E. George, H. Inui “Intrinsic factors responsible for brittle versus ductile nature of refractory high-entropy alloys” // Nature Communications, **15**, 1706 (2024).