Prediction for prismatic slip behavior in Mg based on multiple neural network potentials

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Prismatic slip behavior in Magnesium at high temperature is governed by a thermally activated double-cross-slip process of the stable basal <a> dislocations. However, at low temperatures, the prismatic flow stress is athermal and exhibits an instability and observed “jerky” flow; the origins of this behavior are not understood. Here, we use a range of neural network potentials (NNPs) for Mg along with Molecular Statics and the Nudged Elastic Band (NEB) method to examine the prismatic glide processes. All NNPs are very similar in predictions of the prismatic transition states and other typical Mg properties, and all exhibit an athermal instability for prismatic glide but at widely differing critical stresses. DFT calculations of the basal-prism-basal transition path reveal excellent agreement for one particular NNP (NNP77), which shows the athermal instability at a stress comparable to experiments. Full 3D simulations of prismatic loop expansion using NNP77 further verify this non-thermally activated activation mechanism in a realistic geometry, and show behavior similar to that observed in TEM studies. This new insight into the athermal instability of prism slip in Mg demonstrates the power of using machine-learning potentials for discovery of new mechanisms and phenomena.

Keywords: Magnesium, Prismatic slip, Neural network potential

References:

[1] Markus Stricker and W. A. Curtin, “Prismatic Slip in Magnesium”, The Journal of Physical Chemistry C, 124, 2020, 27230–272.
[2] Markus Stricker et al, Machine learning for metallurgy II. A neural-network potential for magnesium, Phys. Rev. Materials, 4, 2020, 10360.
[3] A. Couret and D. Caillard, An in-situ study of prismatic glide in magnesium—II. Microscopic activation parameters, Acta Metallurgica, 33, 1985, 1455–146.
[4] A. Akhtar and E. Teghtsoonian, Solid solution strengthening of magnesium single crystals—II. The effect of solute on the ease of prismatic slip, Acta Metallurgica, 17, 1969, 1351–1356.