Assessing entropic and quantum contributions to dislocation glide using *ab initio* calculations and machine learning potentials

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Résumé pour poster

Predicting the plastic response of metals from first principles requires accurate descriptions of dislocation behavior across the full temperature spectrum, from cryogenic conditions to elevated temperatures. Both limits are potentially influenced by crystal vibrations, respectively through zero-point effects and entropy, and pose stringent challenges to atomistic modeling, particularly regarding the reliability of interatomic potentials. This contribution reports on an effort to apply machine learning interatomic potentials (MLIPs), trained on extensive density functional theory calculations of dislocation configurations, to quantify vibrational effects on screw dislocation glide in body-centered cubic iron and tungsten.

At finite temperature, we compute the activation Gibbs free energy for kink-pair nucleation and find that the activation entropy is essentially constant with respect to both temperature and applied stress, consistent with a harmonic transition-state description [1]. This result supports yields stress predictions in agreement with experiments, and contrasts with recent reports based on empirical embedded-atom method (EAM) potentials attributing large and strongly varying entropic contributions to dislocation glide. We identify this discrepancy as an artifact of EAM potentials, which systematically fail to reproduce the topology of the potential energy surface in the vicinity of dislocation cores.

At low temperature, we provide the first quantitative evaluation of quantum zero-point energy (ZPE) corrections to the Peierls stress, combining *ab initio* calculations with MLIP-based simulations. While ZPE corrections reduce the well-documented overestimation of the Peierls stress relative to cryogenic experiments [2], we show that they appear insufficient to fully resolve it — even with highly accurate underlying potential energy surfaces. EAM potentials again strongly overestimate vibrational effects, but the residual discrepancy observed with MLIPs points to limitations that transcend the choice of potential, possibly reflecting fundamental gaps in current theoretical and computational models.

Collectively, these results illustrate both the promise and the current boundaries of MLIP-based modeling of dislocation properties: well-calibrated MLIPs resolve artifacts present in classical potentials and enable improved predictions, yet quantitative discrepancies remain, defining open questions for crystal defect modeling.

[1] Allera, A., Swinburne, T.D., Goryaeva, A.M., Bienvenu, B., Ribeiro, F., Perez, M., Marinica, M.C. and Rodney, D., 2025. Activation entropy of dislocation glide in body-centered cubic metals from atomistic simulations. Nature Communications, 16(1), p.8367.

[2] Proville, L., Rodney, D. and Marinica, M.C., 2012. Quantum effect on thermally activated glide of dislocations. Nature materials, 11(10), pp.845-849.

[3] A. Allera, L. Ventelon, D. Rodney, L. Proville, M.-C. Marinica, in prep.