Hybrid *ab initio*-machine learning simulation of dislocation-defect interactions

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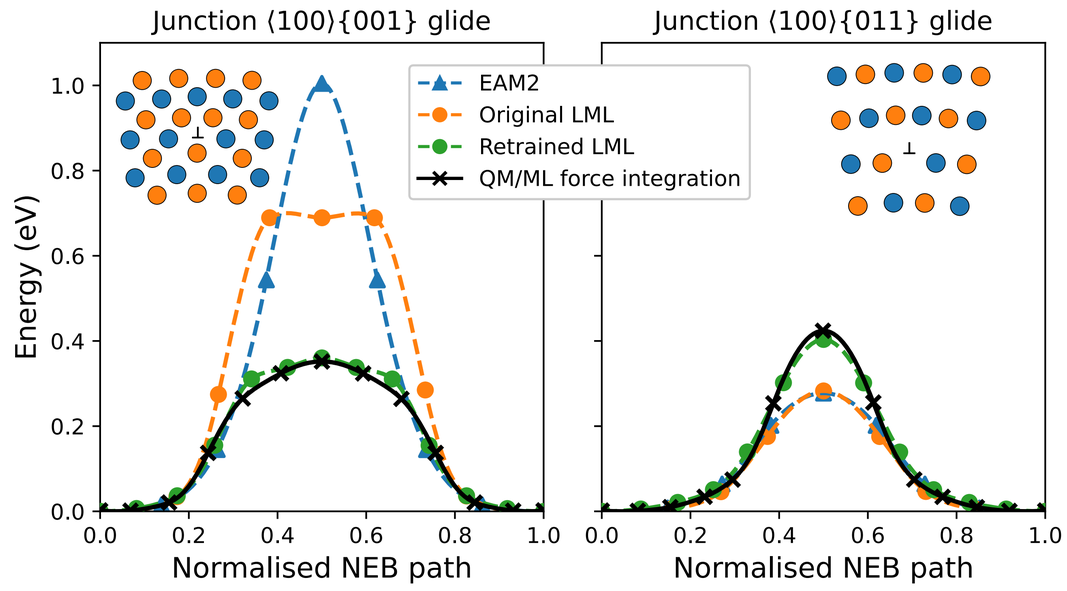
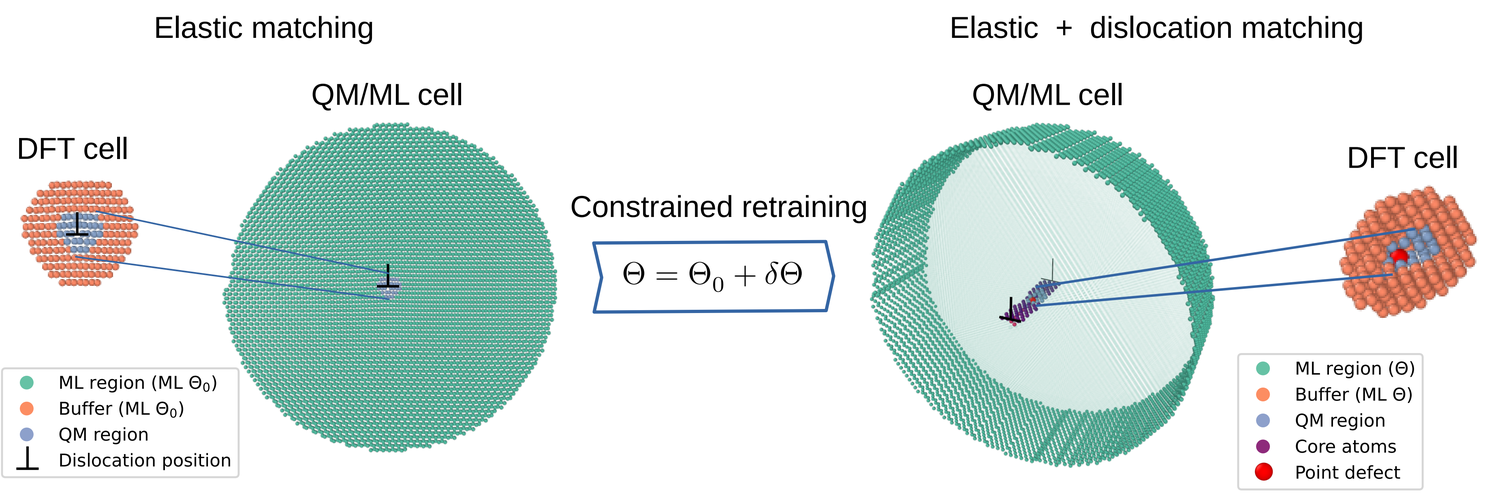
Abstract

The *ab initio* simulations of dislocations are essential to build quantitative models of material strength, but the required system sizes are often at or beyond the limit of existing methods. Many important structures are thus missing int he training or validation of interatomic potentials, whilst studies of dislocation-defect interactions must mitigate the effect of strong periodic image interactions along the line direction. We show how these restrictions can be lifted through the use of linear machine learning potentials in hybrid simulations, where only a subset of atoms are governed by *ab initio* forces. The linear form is exploited in a constrained retraining procedure, qualitatively expanding the range of training structures for learning and giving precise matching of dislocation core structures, such that lines can cross the quantum/classical boundary. We apply our method to fully three dimensional studies of impurity segregation to screw dislocations in tungsten. Our retrained potentials give systematically improved accuracy to QM/ML reference data and the three dimensional geometry allows for long-range relaxations that qualitatively change impurity-induced core reconstructions compared to simulations using short periodic supercells. More generally, the ability to treat arbitrary sub-regions of large scale simulations with *ab initio* accuracy opens a vast range of previously inaccessible extended defects to quantitative investigation.

<100> dislocation glide

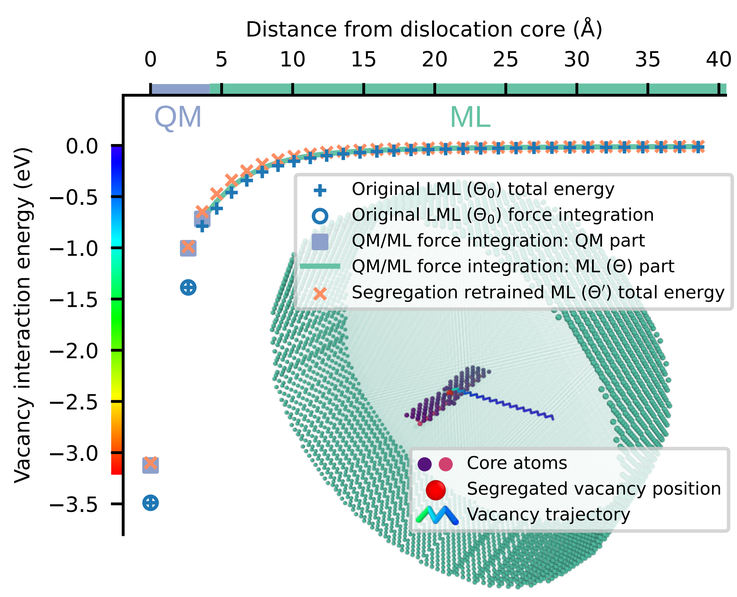


Constrained retraining

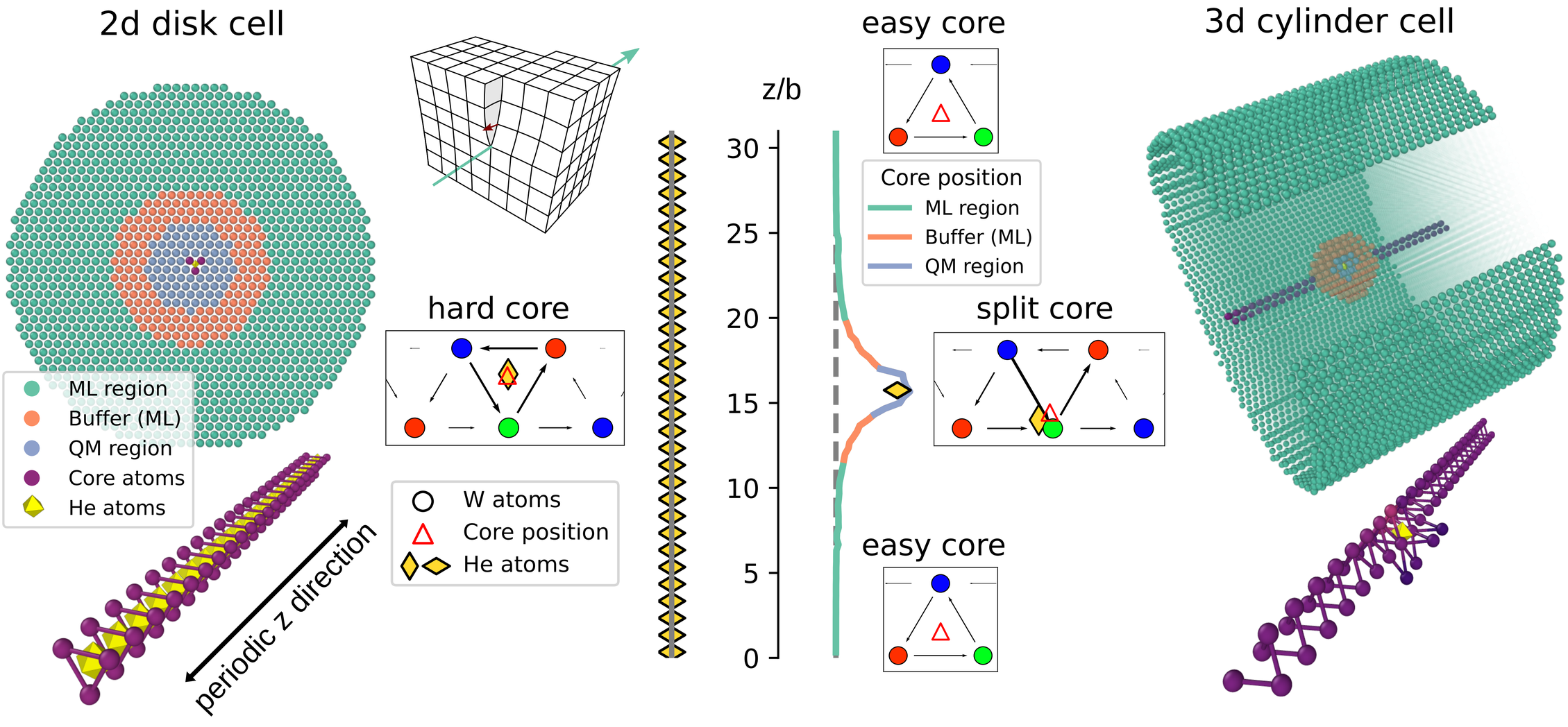


- ✓ Dislocation core structure and glide barrier
- ✗ Periodic along straight dislocation line
- ✓ Point defect segregation energies
- ✓ Long range core effects along the line

Vacancy segregation



Spherical QM region/retrained ML coupling: He induced screw dislocation core reconstruction



More details: *Calculation of dislocation binding to helium-vacancy defects in tungsten using hybrid ab initio-machine learning methods* Acta Materialia 247 p. 118734 (2023)

News and updates: pgrigorev.github.io and tomswinburne.github.io