Use of foundation model for defects in BCC metals

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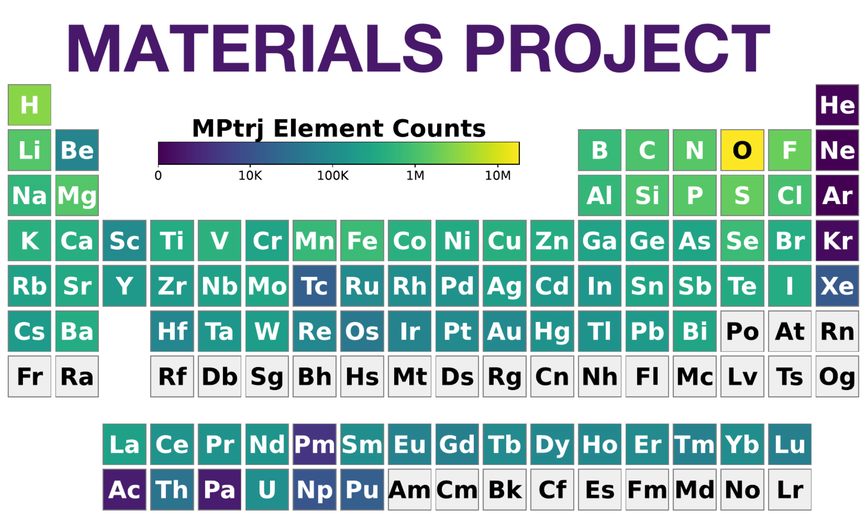
Introduction

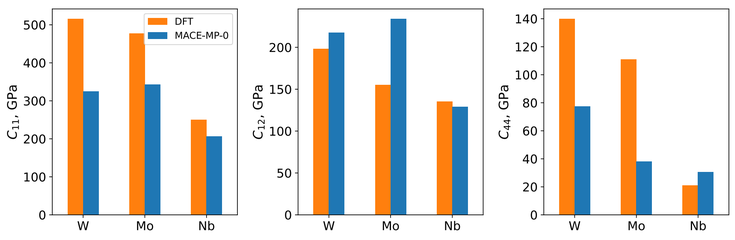
Recent advancement of machine learning force fields allowed the development of universal models capable of describing large number of elements and chemical environments. Here we test a novel model MACE-MP0 [1] which is based on MACE architecture [2] and is trained on a public database of 150k inorganic structure types (1.5M configurations in total) composed of 89 elements [3]. We look at properties of point and extended defects in three BCC metals: W, Mo, Nb. For the case of W we demonstrated how the model can be used as a "foundation model" allowing for further fine *tuning for a given application.*

The MP dataset includes 3 elemental tungsten, 2 elemental molybdenum, and 2 elemental niobium structures. They are all crystalline without any defects.

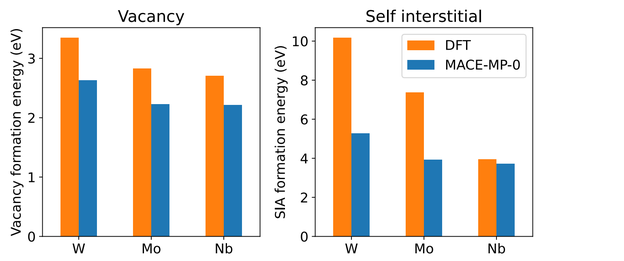


Out of the box performance

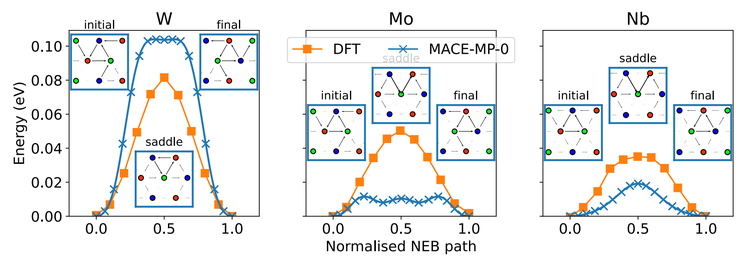
Elastic constants



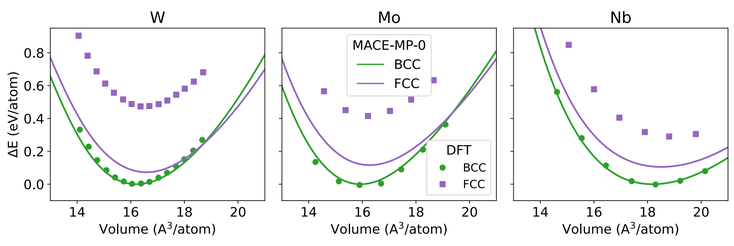
Point defects



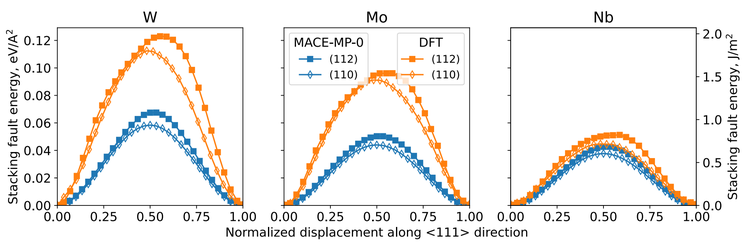
Screw 1/2<111>{110}dislocation



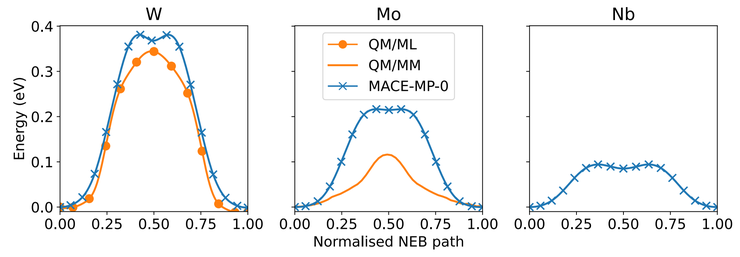
BCC/FCC energy vs volume



Stacking faults



Edge <100>{001} dislocation



*Details of the calculation methods and sources of reference ab initio data can be found in [1], section A.13: Point and extended defects in BCC metals.

Fine-tuning for W

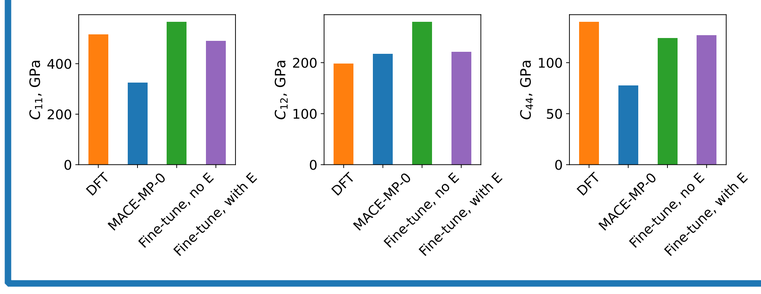
Training data

MACE-MP-0 medium model fine tuned on W DFT data:

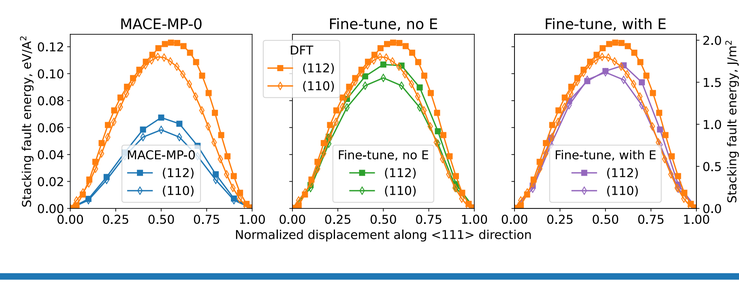
- 100 BCC and FCC cubic cells (close to equil. volume)
- 60 surface cells
- 122 stacking fault configurations
- 4 x 135-atom screw dislocation quadrupoles
- 3 x 53-atom vacancy cells

100 epochs of fine-tuning on 90% of data (10% validation)
Fits with and without DFT energies (to check E0 effects)

Elastic constants

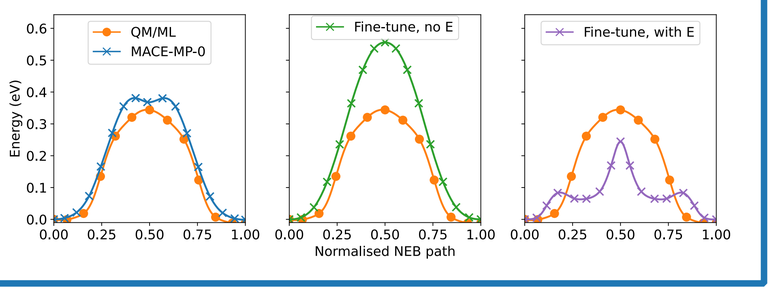


Point defects



Stacking faults

Screw 1/2<111>{110}dislocation



Edge <100>{001} dislocation

Conclusions

Testing original MACE-MP-0 for model for W, Nb, Mo revealed:

- Softer elastic properties for all three metals
- Point defect formation energies are well reproduced with underestimation of interstitial formation energy for W and Mo
- Stacking fault profiles are underestimated for W and Mo
- Screw dislocation easy core stability is reproduced only for Nb

Fine-tuning on the selected database improves elastic properties, interstitial and stacking fault energies as well as screw dislocation properties.

Future work will include:

- Start from improved MP-0b model and updated fine-tuning method
- Does fine-tuning of W data improve properties of other metals?
- Iterative fine-tuning on one DB class at a time

References:

[1] I. Batatia et al, A foundation model for atomistic materials chemistry, arXiv:2401.00096
[2] I. Batatia et al, MACE: Higher Order Equivariant Message Passing Neural Networks for Fast and Accurate Force Fields. In S. Koyejo, S. Mohamed, A. Agarwal, D. Belgrave, K. Cho, & A. Oh (Eds.), Advances in Neural Information Processing Systems (Vol. 35, pp. 11423–11436).
[3] Jain, A. et al. The Materials Project: a materials genome approach to accelerating materials innovation. APL Mater. 1, 011002 (2013).

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