

Use of foundation model for defects in BCC metals

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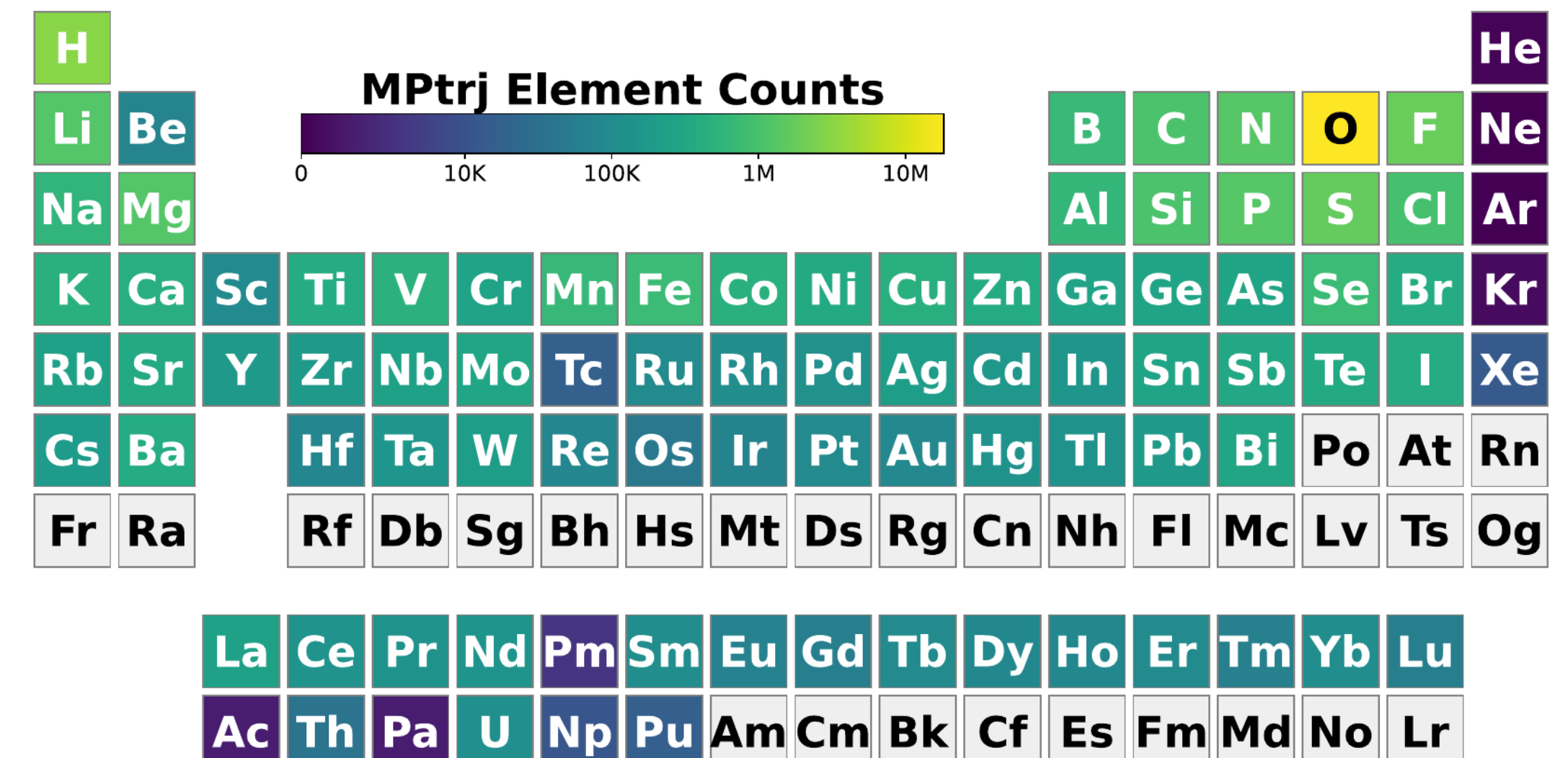
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Introduction

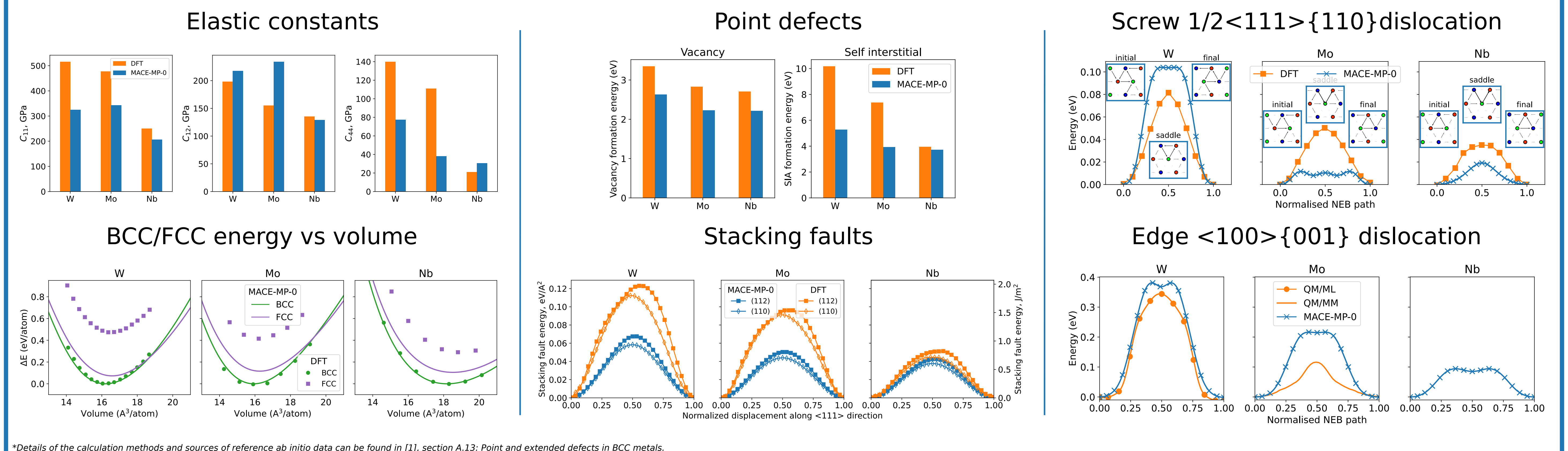
Recent advancement of machine learning force fields allowed the development of universal models capable of describing large number of elements and chemical environments. Here we test a novel model MACE-MP0 [1] which is based on MACE architecture [2] and is trained on a public database of 150k inorganic 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.

MATERIALS PROJECT

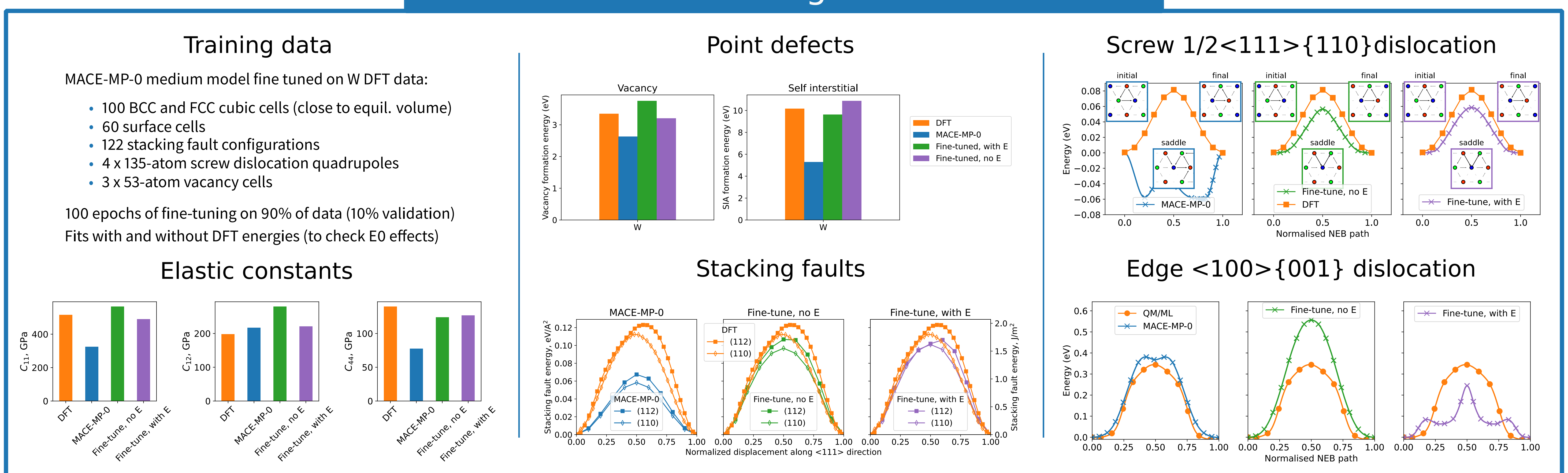


Out of the box performance



*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



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).

For updates visit [grigorev.github.io](https://github.com/grigorev) and [tomswinburne.github.io](https://github.com/tomswinburne)

