Abstract Submitted
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Embedded-atom method potential for niobium[1] MICHAEL FELLINGER, HYOUNGKI PARK, JOHN WILKINS, The Ohio State University — Large-scale simulations of plastic deformation and phase transformations require classical interatomic potentials. We construct a force-matched [1] embedded-atom method potential [2] for niobium as the first step in alloy potential development. The program *potfit* [3] produces a reliable and transferable potential by optimizing the model parameters to DFT forces, energies, and stresses. The model accurately describes properties related to the fitting data, and also produces excellent results for quantities outside the fitting range. Structural, elastic, defect, and thermal properties compare well with DFT and experiment, e.g., surface energies are within 4% of DFT values, generalized stacking-fault energies are within 10% of DFT values, and the melting temperature is within 2% of the experimental value.

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