

Abstract Submitted
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Ab initio-based interatomic potentials for body-centered cubic refractory metals¹ MICHAEL FELLINGER, HYOUNGKI PARK, JEREMY NICKLAS, JOHN WILKINS, The Ohio State University — A fundamental understanding of transformation and deformation processes in the bcc refractory metals (V, Nb, Ta, Mo, and W) is vital for designing new bcc-based commercial alloys with desired properties. Such an understanding is aided by computational methods capable of reaching length and time scales needed for meaningful simulations of phase transformations and extended defects responsible for plastic deformation. Classical interatomic potentials are indispensable for simulating such phenomena inaccessible to first-principles methods. We develop accurate and robust embedded-atom method (EAM) [1] and modified-EAM (MEAM) [2] potentials for the bcc metals by fitting the model parameters to accurate first-principles data. The potentials are applicable for studying mechanical and thermodynamic properties, yielding excellent agreement with both experiments and first-principles calculations.

[1] M. S. Daw and M. I. Baskes, Phys. Rev. Lett. 50, 1285 (1983).

[2] M. I. Baskes, Phys. Rev. Lett. 59, 2666 (1987).

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