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Embedded Atom Method (EAM) interatomic potential for Zinc (Zn) AMITAVA MOITRA, SUNGHO KIM, JEFFRY HOUZE, BOHUMIR JELINEK, LAALITHA LIYANAGE, Dept. of Physics and Astronomy; Center for Advanced Vehicular System, Mississippi State University, MARK F. HORSTEMEYER, Dept. of Mechanical Engineering; Center for Advanced Vehicular System, Mississippi State University, SEONG-GON KIM, Dept. of Physics and Astronomy; Center for Advanced Vehicular System, Mississippi State University — We developed a new spline-based embedded-atom method (EAM) interatomic potential for Zinc by matching forces to those of ab-initio calculations. The material parameters such as cohesive energy, equilibrium atomic volume, and bulk modulus were used to optimize the potential. The applicability of the new potential was demonstrated by performing atomistic simulations for different surfaces. The formation energies, and various point defects were also calculated. The applicability of this EAM potential to the stability analysis of small clusters was also tested.

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