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Development of the EAM Potential for Fe-C Alloy Systems BOHUMIR JELINEK, JEFF HOUZE, SUNGHO KIM, AMITAVA MOITRA, LAALITHA LIYAGNE, MARK HORSTEMEYER, SEONG-GON KIM, Mississippi State University — The ab-initio calculations based on density functional theory (DFT) are performed for Fe and C in their ground state crystal structures. Heats of formation are then calculated for different Fe-C alloy compounds. The lattice constant (volume), bulk modulus and shear moduli for cementite are determined from the total energy calculations. These material parameters are then used to construct the Spline-based Embedded-Atom Method (Spline EAM) potentials for Fe-C alloy systems. The results of the new potential are compared with the results of ab-initio calculations.

Prefer Oral Session
 Prefer Poster Session

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