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Concentration-dependent embedded atom method potential for Al-Cu system SULEIMAN OLORIEGBE, SEWELL THOMAS, THOMPSON DONALD, ZHEN CHEN, SHAN JIANG, University of Missouri-Columbia, YONG GAN, Zhejiang University, Zhejiang, China — A concentration-dependent interatomic potential for Al-Cu alloys has been carefully constructed in the framework of embedded atom method (EAM) refer to here as CDEAM potential. The interatomic interaction terms for the pure components Al and Cu were adapted from a previously published EAM work. The new potential incorporate interactions between Cu and Al using a pair potential function that is augmented with a fourth order polynomial function to account for concentration dependence. The potential was optimized using experimental heat of mixing for liquid Al-Cu alloys at 1467 K, second-order elastic constants and zero Kelvin formation energies from DFT for various alloy configurations and compositions. The resulting potential is able to reasonably reproduce the heat of formation across the entire composition. The heat of formation at zero Kelvin and mixing enthalpy at 1467 K as well as the second-order elastic constants are compared with existing Al-Cu potentials in the literature. Our potential reasonably reproduces the alloy mixing enthalpies at 1467 K. As a further test, we computed properties not included in the fit, such as liquid structures, self-diffusion coefficient, liquid densities, enthalpies and heat capacities as a function of temperature. The results of these properties computed using CDEAM potential are in good agreement with experimental data.

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