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Embedded Atom Method Potential for Ni-Cu Alloys and Its Applications for Ni, Cu growth on Cu(111)[1] BERK ONAT, Informatics Institute, Istanbul Technical University, Istanbul, Turkey, SONDAN DURUKANOGLU, Nanotechnology Research and Application Center, Faculty of Engineering and Natural Sciences, Sabanci University, Istanbul, Turkey — We developed a semi-empirical, many-body type model potential to investigate static and dynamic properties of Ni-Cu alloys. The formalism is based on the embedded atom method with improved optimization techniques. The Ni-Cu alloy potential was determined by fitting to data on lattice parameters, cohesive energies for $L1_0$, $L1_1$, $L1_2$, and $L1_3$ phases, together with vacancy formation energies, bulk modulus and elastic properties for $L1_2$, $L1_3$ phases. Our preliminary calculations for energy barriers for the diffusing Ni and Cu atoms on Cu(111) based on the nudged elastic band method are found to be consistent with the available experimental and other theoretical results. Our ultimate goal is to describe the varying characteristics in growing islands of pure Cu, Ni atoms and mixed Ni-Cu combinations on Cu(111) [S. Pons et al., Surf. Sci., **511**, 449, (2002)].

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