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Growth of Cu-Ni Nanostructures on Cu(111): A Molecular Dynamic Study BERK ONAT, Informatics Institute, Istanbul Technical University, Istanbul, Turkey, SONDAN DURUKANOGLU, Faculty of Engineering and Natural Sciences, Nanotechnology Research and Application Center, Sabanci University, Istanbul, Turkey — We have studied energetics and growth mechanisms on nanostructures both using molecular dynamic simulations and total energy calculations to understand the nature of Ni and Cu growth on Cu(111) surface. The interactions between the atoms in the systems are defined using a many-body type potential developed for Cu-Ni alloys within the EAM formalism. Our simulations on Cu-Ni systems with mono/double-layer Ni islands on Cu(111) show that Cu atoms could migrate to Ni islands and decorate the bottom and even the upper layer of Ni islands. Furthermore, we find that the formation of the islands is governed by the nature of the decoration process. From total energy calculations we also discuss the governing diffusion mechanisms for the formation of Cu-Ni islands on Cu(111).

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