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Efficient gradient-based Monte Carlo simulation of materials: Applications to amorphous Si and Fe and Ni clusters[1] DIL LIMBU, PARTHAPRATIM BISWAS, The University of Southern Mississippi — We present a simple and efficient Monte-Carlo (MC) simulation of Iron (Fe) and Nickel (Ni) clusters with N=5-100 and amorphous Silicon (a-Si) starting from a random configuration. Using Sutton-Chen and Finnis-Sinclair potentials for Ni (in fcc lattice) and Fe (in bcc lattice), and Stillinger-Weber potential for a-Si, respectively, the total energy of the system is optimized by employing MC moves that include both the stochastic nature of MC simulations and the gradient of the potential function. For both iron and nickel clusters, the energy of the configurations is found to be very close to the values listed in the Cambridge Cluster Database, whereas the maximum force on each cluster is found to be much lower than the corresponding value obtained from the optimized structural configurations reported in the database. An extension of the method to model the amorphous state of Si is presented and the results are compared with experimental data and those obtained from other simulation methods.

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