Nanoscale physics

Evaluation of energy of the isolated metastable FCC iron nanocluster with carbon atom in the tetragonal interstice

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The energy of isolated Fe nanocluster was calculated by molecular mechanics method using Lennard-Jones potential [1]. The cluster included a carbon atom, which drifted from an inside octahedral interstice to a terahedral interstace in <111> direction. In addition one of 14 iron atom was replaced by a nickel atom, the position of which was changed during simulation.

Energy of nanocluster was estimated at the different interatomic distances [2]. As a result of simulation, was determinated optimal interatomic distances of Fe-Ni-C nanocluster in which height of a potential barrier was a maximum and FCC nanocluster was a most stable. It is shown that there were of three main position of a nickel atom that significantly affected to nanocluster's energy.

The calculation results indicate that the position of carbon atom in the octahedral interstice was more energetically favorable than tetrahedral interstice in case of FCC nanocluster. From the other side, the potetntial barrier was less in the direction of <111> than in the direction <110>.

This indicates that there are two ways for carbon atom to drift to the surface of the nanocluster.

1. *Riech M.* Nano-engineering in science and technology: an introduction to the world nano-design/ Singapore: World Scientific Publishing Co Pte Ltd, 2003, 151 p.
2. *Ridley N, Stuart H, Zwell L.* Lattice parameters of Fe-C austenites at room temperature // Trans IAME.- 1969, N 245.-P. 1834–1840