Nanoscale physics

The change of energy of the cubic subnanocluster of iron under influence of interstitial and substitutional atoms

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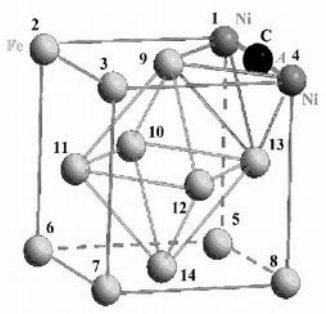
The energy changes of subnanocluster of iron atoms of face-centered cubic type depending on the position of interstitial carbon atom and substitutional nickel atoms was evaluated using molecular mechanics method [1]. Calculations of all possible positions of impurity atoms show that the energy changes of the system are discrete and at certain positions of the atoms are close to continuous.

The position, when all impurity atoms consolidated on the one edge of atomic group, is more energetically profitable for carbon atom than other positions. The presence of the nickel atoms at the edge of cubic cluster resulted to decrease of potential barrier for carbon atom and decrease of energy in all cluster. The similar drift of carbon atom from central octahedral interstitial site to the surface in the direction <011> occurred under the influence of surface factors.



Energetically favorable configuration of pair of nickel atoms with the carbon atom on the surface

Such configuration corresponds to decreasing symmetry of subnanocluster and it corresponds to the condition of spontaneous crystallization process in isolated system.

Taking into account the accidental positions of nickel atom in the iron cluster, the behavior of carbon atom can explain the mechanism of growth of a new phase and the formation of new clusters [2] in the presence of atoms of other sort as a result of influence of surface factors.

1. *Ramachandran K. I., Deepa G., Namboori K.* Computational chemistry and molecular modelling. Principles and applications/ Berlin Heidelberg: Springer-Verlag, 2008, 406 p.

2. *Baumgartner J., Dey A., Bomans P.H.H., Coadou C.L., Fratzl P., Sommerdijk N.A.J.M. and Faivre D.* Nucleation and growth of magnetite from solution// Nature Materials.-2013.-**12**, P. 310-314.