"Nanoscale physics"

On the possibility to control an interstitial atom's motion using substitutional atom in cubic iron nanocluster

N.V. Bondarenko[1], A.V. Nedolya[1]

[1] *Applied Physics and Nanomaterials Department, Zaporizhzhya National University, 66 Zhukovsky str., 69600 Zaporizhzhya, Ukraine.*
E-mail: avnedolya@hotmail.com

The energy of the isolated cubic iron nanocluster was calculated by the molecular mechanics method using Lennard-Jones potential depending on the position of interstitial and substitutional atoms [1, 2].

It is shown that there were positions of substitutional atom that significantly affected on nanoclusters' energy. In addition the calculation results indicated that position of the interstitial atom in the octahedral and tetrahedral interstices were depended on substitutional atoms position. The different adjacent interstitial atoms configurations in cubic nanocluster were investigated with relation to an energy minimum.

The substitutional atom positions were identified, which significantly affected the height of potential barriers of the octahedral and tetrahedral interstices and its determined the possible direction of interstitial atoms' drift. This allows manipulating atoms at the surface of the nanoclusters and controls the growth of nanocluster.

1. *Halicioglu T., Pound G.M. Calculation of potential energy parameters form crystalline state properties* // *Phys Status Solidi A*.-1975.-**30.-**P. 619-623.

2. *Yang Q., To A.C.* Multiresolution molecular mechanics: A unified and consistent framework for general finite element shape functions // Comput Methods Appl Mech Engrg.-2015.-**283**.-P. 384-418.