Nanoscale Physics

Effect of nickel atom position on the carbon's atom drift: the case of BCC isolated Fe-Ni-C nanocluster

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A small isolated body-centred cubic (BCC) Fe-Ni-C nanocluster containing 15 atoms was choosen, where a carbon atom was located inside of it. The formation of such cluster could be a result of the fast nonequilibrium processes during the phase transition.

The nanocluster energy was calculated by molecular mechanics method using Lennard-Jones potential [1,2].

Various nickel atom positions relative to the carbon atom position were taken into account for determine of the most energetically advantageous configuration of atoms in the system. It is found that potential barrier may exist or be absent in depending on the drift direction of carbon atom to the surface.

The simulation showed that nanocluster energy was different when a carbon atom was located in the octahedral or tetrahedral interstices. In addition the nanocluster energy and its stability are severely depended on the distance between atoms. Such a nanocluster energy changes exceed 50%.

The calculations indicate the possibility of manipulating the movement of carbon atom by changing the position of nickel atom in the iron nanocluster. That opens additional opportunities in nanotechnology.

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. *Halicioğlu T., Pound G.M.*. Calculation of potential energy parameters form crystalline state properties// Physica Status Solidi A.-1975.-**30** (2), P. 619-623.