МІНІСТЕРСТВО ОСВІТИ І НАУКИ УКРАЇНИ
СУМСЬКИЙ ДЕРЖАВНИЙ УНІВЕРСИТЕТ

ФІЗИКА, ЕЛЕКТРОНІКА, ЕЛЕКТРОТЕХНІКА

ФЕЕ: 2016

МАТЕРІАЛИ
та програма

НАУКОВО-ТЕХНІЧНОЇ КОНФЕРЕНЦІЇ

(Суми, 18–22 квітня 2016 року)

Суми
Сумський державний університет
2016

MD simulation of AlCoCuFeNi high-entropy alloy nanoparticle

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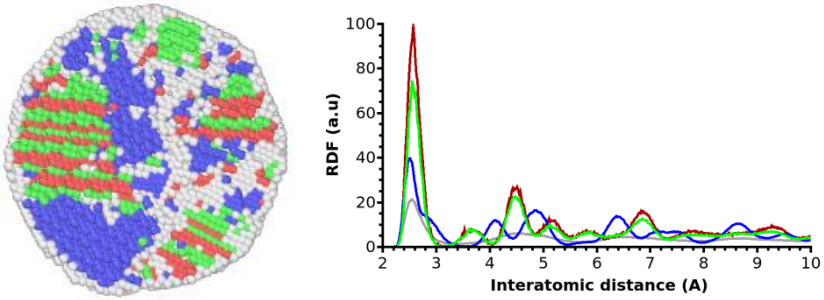
High entropy alloys (HEA) are metallic compounds containing from 5 to 13 metallic elements in equiatomic ratios. In HEAs, because of the high mixing entropy, formation of brittle intermetallic phases is usually avoided and simple solid solutions are rather stabilized (BCC and/or FCC). This study used molecular dynamics (MD) package LAMMPS to simulate the AlCoCuFeNi nanoparticle (NP) crystallization.

The MD simulation was performed using an EAM potential and NVT ensemble. The simulated NP was composed of 50000 atoms (Al, Co, Cu, Fe, Ni in equiatomic ratio) and the average size of NP was ~ 10 nm. System was heated up to 2300 K and subsequently annealed at this temperature for 200 ps. After this, the NP was quenched from a molted state at a rate of 1×10^{11} K/s to 300 K. After quenching the radial distribution function (RDF) was calculated for determining the average structure. Also the adaptive common neighbor analysis (CNA) was performed to get a precise understanding of which atoms are associated with which phases.

By the CNA analysis it has been established, that the simulated NP contains the FCC phase (15,1 %), BCC phase (31,5 %), HCP phase (9,5 %) and the unrecognized phase (43,9 %), which, in accordance with RDF, had an amorphous structure. The estimated BCC lattice parameter from the present MD simulations is 0,290 nm and the FCC one is 0,365 nm.



a b

Figure 1 – Cross section of AlCoCuFeNi nanoparticle (a), calculated RDF patterns (b): ● – FCC, ● – BCC, ● – HCP, ● – other.