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PAIR DISTRIBUTION FUNCTION ANALYSIS FOR PT-PD-CO ATOMIC MOBILITY IN NANOPARTICLES

Through in situ monitoring of fuel cells in oxidation-reduction processes with high-energy X-ray diffraction for ternary systems (Pt-Pd-Co), the PDF is created through the Fourier transform of the diffraction pattern of a sample. It has been seen that the lattice strains in nanostructures are reflected in the oscillation of the peaks of the atomic pair distribution function (PDF). The analyses have revealed that there is atomic mobility within the ternary nanoparticles. Thus, it is sought that atomic structural models reproduce the oscillation of the PDF peaks at a certain moment, to have the average atomic distribution of the nanoparticles in the fuel cell. Different atomic structural models were created and these were applied molecular dynamics simulations using LAMMPS with second neighbor MEAM potentials. And the pair distribution function of the models was calculated trying to reproduce the experimental PDF. It is shown that a non-uniform distribution of the elements of the ternary system within the structures is the cause of the lattice strain oscillations for the nanostructures, mainly the radial distribution of Co turns out to have a greater effect on the peaks of interest in the PDF altering the general structure of the nanoparticles.

Keywords

Nanoparticles, Pair-Distribution-Function, Strains, Ternary, Diffusion, Simulation, MEAM.

Reference

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