

NEW MODEL FOR TRACER-DIFFUSION IN AMORPHOUS SOLID

P.K. Hung and P.H. Kien

TÓM TẮT:

The N-simplexes have been investigated in amorphous iron model containing 2×10^5 atoms. The simulation reveals that the concentration of 4-simplex increases and of N-simplex with $N > 4$ decreases upon relaxation. We found a large number of vacancy-simplexes which could play a role of diffusion vehicle for iron atom and varies with relaxation degree. New diffusion mechanism for tracer diffusivity is proposed of which the elemental atomic movement includes a jump of neighboring atom into the vacancy-simplexes and then collective displacement of a large number of atoms.