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CRYSTALLIZATION KINETICS EFFECT ON THE NANOPARTICLES SHAPE BY MOLECULAR DYNAMICS SIMULATION

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In recent years, Metal nanoparticles have attracted large attention due to their extraordinary properties. For example, gold (Au) nanoparticles are promising in optical, electronic, catalytic and biomedical applications such as single electron tunneling devices, nanolithography, CO/CO2 catalyst, DNA or antibody sensors and so on.
Molecular dynamics simulation of the crystallization behavior of a liquid gold (Au) nanoparticle, on cooling was performed based on the modified embedded-atom-method potential. In this work, it has been found that the final structure of a gold nanoparticle strongly depends on cooling rate during crystallization from liquid. As cooling rate decreases, the final structure of the particle changes from amorphous to crystalline via icosahedron-like structure. While the outer shell of the icosahedron-like particle shows crystalline feature with {1 1 1}-like facets, the inner core remains amorphous. It is found that the structure of the fully crystallized particle is polycrystalline face-centered cubic (fcc). The fcc structure of the gold nanoparticle is proved energetically the most stable form. the final structure of nanoparticles is affected by cooling time and size of nanoparticles.