MOLECULAR DYNAMICS SIMULATION OF NANOSINTERING PROCESSES

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ABSTRACT

In this thesis, two scenarios of nanosintering simulations are studied by molecular dynamics (MD) method. The first one will investigate the neck growth in the laser sintering of different-size gold (100) nanoparticles under different heating rates. The numerical simulations are carried out for four pairs of two spherical nanoparticles where one particle has the same diameter of 4 nm and the other one varied from 4 nm to 20 nm. The results show that the stable neck width increases as the size of the other nanoparticle increases. Once the limit stable neck width is reached, it no longer is affected by the nanoparticle size. For the subsequent laser heating to the same final temperature, a lower heating rate results in a larger stable neck width due to the longer sintering process. The other one will study the deposition of Ni(100) nanocluster with zero initial kinetic energy on Cu(100, 110) surface. It's found that the burrowing process goes extremely slow as temperature is equal or less than 900K. There is no burrowing below 500 K. The completeness of burrowing Ni on Cu(110) is earlier than Cu(100) due to the lower surface energy of Cu(110). Vacancy migration is found to be the main cause of the site-exchange of atoms between Ni cluster and Cu substrate.