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Atomic and electronic properties of copper nano-particles: theoretical and experimental results

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Abstract – The atomic and electronic properties of the copper nanoparticles, from 19 atoms up to ~8000 atoms, were studies employing molecular dynamics and a tight-binding Hamiltonian. The results show that copper nanoparticles have a spherical-like shape with the atoms ordered in an icosahedral or fcc-like arrangement for small, respectively, large clusters. Furthermore, from the electronic point of view, clusters with diameters larger than 3 nm behave like solid copper.

The research in the field of nanoparticles is the basis for the development of nanotechnology [1]. Metallic clusters, specially those in the nanometer-scale, possess unique physical properties [2]. In particular, Cu-nanoclusters have potential applications in optics, magneto-electronics and catalyst systems [2,3]. An interesting open question in this research area is the following: how many atoms are required for a cluster to show the properties of the bulk material? In this work, regarding the electronic properties of these systems, we address this question employing a tight-binding Hamiltonian where first- and second- neighbor inteactions are allowed. For this purpose, the most stable geometrical structures of Cu-clusters containing from 19 atoms up to more than 8000 atoms were obtained by means of molecular dynamics (based on the semi-empirical embedded-atom method [4]), and thermal quenching simulations.
The results show that the Cu clusters have a spherical shape changing from an icosahedral structure (for small clusters) to an FCC-like structure after increasing the system size (number of atoms). These results are compared with nanoparticles synthesized by means of ultrasound and microwave irradiation which allow us to obtain small nanoparticles.
Moreover, after comparing the electronic density of states (DOS) of these clusters with the corresponding solid system (modeled as a cluster with ~500000 atoms in an FCC arrangement) we can conclude that clusters with more than 2000 atoms (~2 nm diameter) behave like solid Cu, where the inner part of the cluster contributes more significantly to the DOS than the surface (outer part), as expected in macroscopic solid samples. We also study the influence of on-site disorder on the electronic spectrum employing the energy level statistic method.

References

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[4] The MD calculations were performed using the XMD program developed by the group of Rifkin, at the Center for Simulation, University of Connecticut.