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Thermal stability of undercooled amorphous silver nanoparticles

J. Rojas[(1,2)*], C. V. Landauro[(1)], I. Lobato[(2)], Ch. Rojas[(1)]

(1) GIMC, Universidad Nacional Mayor de San Marcos, Av. Venezuela Cdra 34, P.O. box 14-0149, Lima 14, Perú, e-mail: jrojas@unmsm.edu.pe
(2) División de materiales, Instituto Peruano de Energía Nuclear, Avenida Canadá 1470, Lima 41, Perú.
* Corresponding author.

Abstract – The structural evolution and dynamical properties of amorphous silver nanoparticles during isothermal annealing have been studied by means of molecular dynamics simulation. The amorphous nanoparticles were obtained after rapid cooling from liquid state to 300 K with cooling rate of $2.5x10^{13}$ K/s It is shown that the amorphous nanoparticles are highly unstable; several structural changes were observed during the annealing process. Crystallization begins, depending on the annealing temperature, after 100-140 ps. The local symmetry corresponding to an icosahedral order decreases with the annealing time whereas the fcc local symmetry increases. It is also found that higher annealing temperatures allow faster and complete crystallization.

The thermal stability of undercooled silver nanoparticles is interesting due to increasing applications of these nanoparticles in nanotechnology[1,2]. In this work the molecular dynamic simulation has been used to study the thermal stability of silver nanoparticles of 561 atoms, i.e. corresponding to an icosahedral magic number. The interaction of silver atoms is modelled by a semiempirical Tight-binding interatomic potential. Simulations were carried out in a cubic box without applying periodic boundary conditions. Initially, the nanoparticle was equilibrated at two temperatures, 1100 K and 1300 K, both above the melting temperature of the given nanoparticle (~780 K), during 10^5 steps (250 ps). Then, the nanoparticle was cooled from 1100 K, or correspondingly 1300 K, to 300 K with an equal cooling rate of $2.5x10^{13}$ K/s. These conditions allow us to obtain amorphous structures at room temperature. Finally, the amorphous nanoparticle was relaxed at room temperature for 2 x 10^5 steps. Ten independent runs were carried out recording the data every 25 ps. Pair correlation function (PCF) and common neighbour analysis technique (CNAT) were performed to study the global and local structural changes produced during the cooling process.

Fig. 1 shows the typical behavior of the potential energy during the annealing process where sharp variations indicate structural transformations. In fact, The PCF shows a gradual transformation from amorphous to crystalline phase (see Fig. 2). The CNAT analysis indicates that the icosahedral local symmetry decreases to zero with time, while the fcc and hcp local structures (indices 1421 and 1422, respectively) increase, as shown in Fig. 3. It is also found that the degree of crystallization depends strongly of the initial cooling temperature.

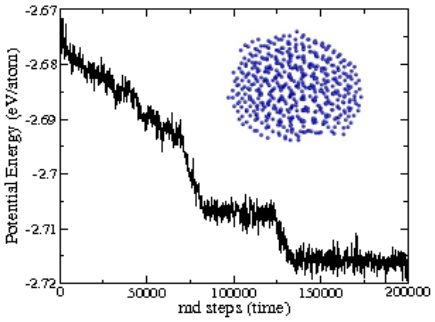

Figure 1: Energy change of silver nanoparticle during the annealing at 400 K, cooled from 1100 K. The snapshot show the atomic arrangement after 250 ps.

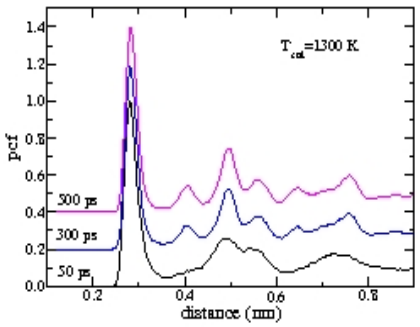

Figure 2: Pair correlation during the relaxation at 300 K. Before annealing the nanoparticle was cooled from 1300 K.

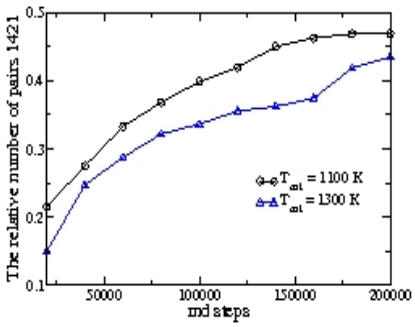

Figure 2: Time evolution of pairs 1421 during the annealing at 400 K. Before annealing the nanoparticle was cooled from 1300 K.

References

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