Molecular Dynamics Simulation of the Metal Particle Formation from Supersaturated Vapors

T. Kraska[C,S] and N. Luemmen
Physical Chemistry, University Cologne, Köln, Germany
t.kraska@uni-koeln.de

The formation of iron and platinum clusters in an inert gas aggregation source is investigated by molecular dynamics simulation [1, 2, 3]. The metal vapor atoms are embedded in the carrier gas, argon, acting as a heat bath. At the beginning of the simulation the metal atoms are in a highly supersaturated vapor state. Once the simulation is started the metastable phase remains for some time, until clusters are formed by homogenous nucleation. The nucleation rates are calculated from the cluster size distribution. The critical cluster size and the excess energy of the critical clusters are estimated from the correlation of the nucleation rates as functions of the supersaturation using the nucleation theorems. In addition, the coalescence of the metal clusters over the course of the growth process is traced in detail [3, 4]. The structure of the metal clusters is investigated by the common neighbor analysis (CNA) [5, 6], which is a simple and powerful method for determining the amount of different crystal structures from molecular simulation configurations. An extension of this method towards binary atomic systems is developed. For four face centered binary structures the new extended signatures are presented. These are the L10 (AuCu), L11 (CuPt), L20 (Cu_3Au), and L60 ($CuTi_3$) structures. The bulk structure as well as the {100}-, {110}-, and {111}-surface structures are included in the analysis.

[1] N. Lümmen and T. Kraska, *Nanotechnology* **15**, 525 (2004).
[2] N. Lümmen and T. Kraska, *J. Aerosol Sci* **36**, 1409 (2005).
[3] N. Lümmen and T. Kraska, *Nanotechnology* **16**, 2870 (2005).
[4] N. Lümmen and T. Kraska, *Phys. Rev. B* **71**, 205403 (2005).
[5] J.D. Honeycutt and A.C. Andersen, *J. Phys. Chem.* **91**, 4950 (1987).
[6] A.S. Clarke and H. Jónsson, *Phys. Rev. E* **47**, 3975 (1993).