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MULTI-SCALE MODELLING OF CLUSTER FORMATION

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ABSTRACT

Numerical modeling is performed to study cluster formation both from solid targets and in a gas phase. The developed model allows us to compare the relative contribution of the two channels of the cluster production by laser ablation: (i) direct cluster ejection from a target under rapid heating, expansion or impact, such as laser interaction, and (ii) condensation, evaporation and coalescence in a gas phase. These mechanisms are used in many immerging techniques of nanoparticle synthesis, such as laser ablation, sputtering, collisional plasma sources, etc. To study these processes, we develop multi-scale models based on combinations of atomistic (Molecular Dynamics, Direct Simulation Monte Carlo) and continuous (hydro dynamical) approaches.

First, we present the results of both hydrodynamic and molecular dynamics simulations of a rapid target decomposition that leads to cluster formation [1,2]. The results of the calculations demonstrate that cluster precursors are formed during material expansion through both thermal and mechanical processes. Molecular dynamics is used to obtain new insights into rapid expansion of a heated material and its decomposition into fragments. In particular, these atomistic calculations provide information about the minimum achievable mean pressure as a function of expansion rate and temperature. A simple estimation of the required mean pressure can then be used in larger scale calculations [3].

Then, we study cluster evaporation and growth in collisions with a background gas. Rapid gas flow expansion and cooling lead to cluster condensation. In the presence of a background gas, additional collisions with background gas species affect the cluster size distribution. Growth of larger clusters can be observed at this stage.

Evaporation and condensation rates are investigated for a molecular cluster (Figure 1) surrounded by a molecular background gas by using molecular dynamics simulation. The influences of the parameters, such as initial cluster temperature and size, background gas temperature and density, on the cluster evolution are analyzed. Calculation results demonstrate that the evaporation rate of a cluster depends essentially

on the gas characteristics and on the initial size of the cluster. A series of the separate molecular dynamics calculations are performed to obtain the required thermodynamical parameters for theoretical analysis of the obtained results based on the available theories (Rice Ramsperger and Kassel, or RRK model [4] and the Classical Nucleation Theory).

The developed models are used to study cluster formation in such experiments as laser ablation, plasma reactors and liquid fragmentation. Calculation results explain many recent experimental observations obtained in these experiments.

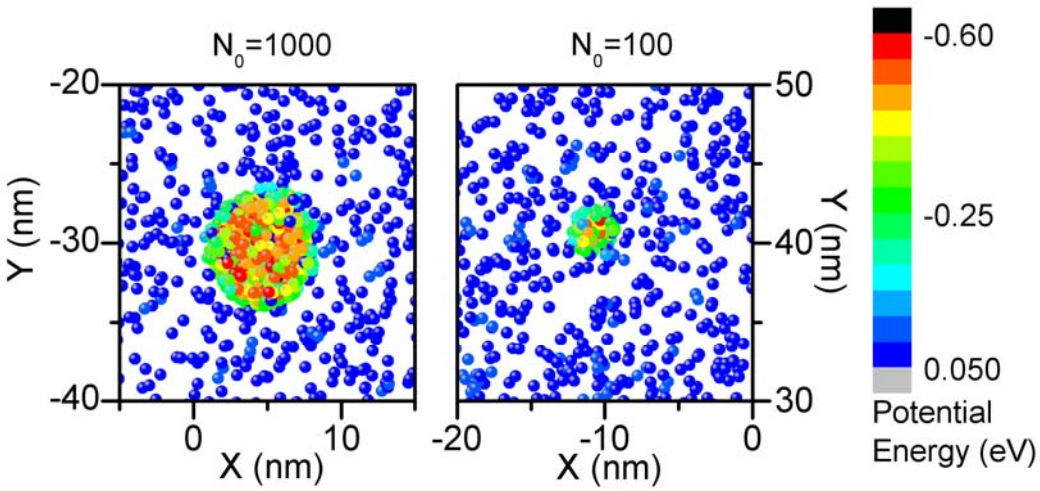

Figure 1. Snapshots obtained in molecular dynamics study of evaporation and condensation processes for two clusters composed of 1000 particles (left) and 100 particles (right) in a background gas. These results are obtained at 3 ns after the end of slow cluster heating to the initial temperature of 1000 K. The colors correspond to the potential energy of the particle.

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