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Atomic-scale investigation of the formation of Al nano-cluster in the Pulsed Laser Ablation Technique

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Abstract

The researcher's described the formation of metallic nano-cluster in the PLAL technique using a qualitative approach. The size, shape, and surface reactance of the produced nano-particles/colloids are characterized by the experimentally obtained results. In this work, we have introduced the Molecular Dynamics approach to simulate the formation of the Aluminum-nano cluster in the aqua environment by the PLAL technique. We have also characterized the produced nano-cluster by its size and shape. We choose to use the Reactive Force Field (ReaxFF) as the interaction potential among the atoms and molecules of the considered system.

Keywords: REAXFF potential, Aluminum, LAMMPS, High intense laser pulse, Cluster analysis, Cluster structure, OVITO.

1. Introduction

Laser ablation is a very well known method for the modification of metal surface and the fabrication of nano-colloids [1]. The laser bombardment on the metal surface produces the plasma of the metal at a very high temperature. The nano-cluster is formed in the system when the temperature reduces to room temperature. The designed system is described as:

- Plasma states at 5000K and the room temperature 300K.
- Temperature steps: 10K/ps and Total runtime: 1ns
- System molecules: Al (32), O (48), Water (160)
- ReaxFF potential for bond analysis [2].

2. Methods

- **Molecular Dynamics (MD) simulation** For many-body system, the MD evaluate the atoms position using Newton's second law of motion as:

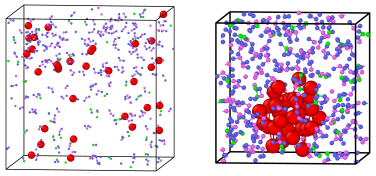
$$F_i(t) = m_i \frac{d^2 r_i(t)}{dt^2}, i = 1, 2, ..., n \quad (1)$$

- **Reactive force field (ReaxFF)** It is given by:

$$E_{system} = E_{over} + E_{under} + E_{bond} + E_{val} + E_{lp} + E_{vdwaals} + E_{tors} + E_{Coulomb} \quad (2)$$

3. Results and Discussion

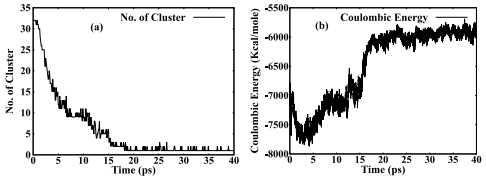
- Formation of Nano-cluster



(a) (b)

Figure 1:The (a) initial (t=1ps) and (b) final state of the system (t=1ns) show the formation of Al-cluster. The atoms in red color represent the Al atoms in the aqua environment.

- Growth rate of the Al-cluster



(a) (b)

Figure 2:The effect of Al cluster formation on Coulomb's energy of the system. (a) The number of Al clusters in the system as a function of time. This graph also represents the formation rate of the Al cluster in the system, and (b) The Coulomb's energy of the system as a function of time.

- Crystallization of the Al-cluster

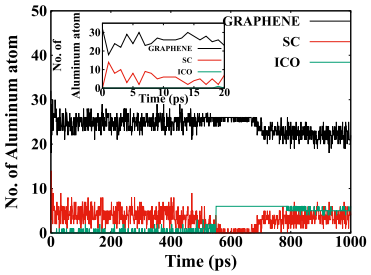


Figure 3:Distribution of the number of aluminum atoms corresponds to the three crystal structures GRAPHENE, SC, and ICO throughout the simulation as a function of time represented in black, red, and green color, respectively.

Table 1:The number and proportion of the Al atoms corresponds to the crystal types observed by the PTM at the end of the simulation (t = 1ns).

Crystal structure type	Number of atoms	Proportion (in %)
GRAPHENE	22	68.8
ICO	6	18.8
SC	4	12.5

- System equilibration

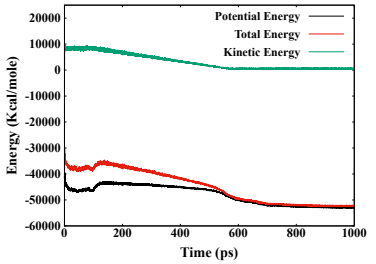


Figure 4:The dynamics of the energies confirm that the system approached the equilibrium state after 800ps of simulation time.

4. Conclusion

- We have shown the formation of the metallic nano-cluster from the Plasma state considering the PLAL technique.
- After completing the simulation, we found one Al nano-clusters.
- The crystallization of the atoms confirm the dominance of the Graphene Structure.
- The considered system is found to be in the equilibrium state after 800ps.

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