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Production of Metal Cluster and Study of their Properties Using the Lammps Software

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Abstract: Metal clusters are small groups formed by the assembly of metal atoms in a certain order. They usually consist of several atoms and play an important role in the fields of nanotechnology and materials science. This cluster is important in the design of nanomaterials and the development of new technologies. is important .

Key words: Metal atoms, cluster structure, nanotechnology, reactivity, channels, physical properties, electrical conductivity.

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Metal clusters, structures consisting of a few atoms and usually at the nanoscale, are important in modern materials science and nanotechnology. They have different properties and are used to create new materials and improve the properties of existing materials. In this article, the process of generating metal clusters and studying their properties using LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) program is considered.

Lampps program.

LAMMPS is an atomic and molecular dynamics simulation program that supports very large systems and various types of potential energy models. Using LAMMPS, several parameters can be changed to study metal clusters, their structure and properties.

Formation of metal clusters.

To generate metal clusters using LAMMPS, first of all, the desired potential energy model is selected. For example, Sutton-Chen, Lennard-Jones or EAM (Embedded Atom Method) models can be used.

1. Define the system: determine the size, number and location of the system using the LAMMPS script.

1. Bash
2. Copy the code
3. units metal
4. atom_style atomic
5. lattice fcc 3.61
6. region box block 0 10 0 10 0 10
7. create_box 1 box
8. create_atoms 1 random 100 12345 box

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2.Applying potential energy models: Choosing an appropriate potential for metal clusters and entering it in the script.

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pair_style eam

pair_coeff * * Cu_u3.eam

3. Specifying the simulation parameters: Set the necessary parameters to determine the movement and heat transfer.

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fix 1 all nve

timestep 0.01

run 10000

Study of properties of metal clusters.

Several methods can be used to study the properties of metal clusters:

1. **Energy Calculation:** Calculate the potential energy of a cluster and relate it to its structure.

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compute 1 all pe/atom

dump 1 all custom 100 dump.energy id c_1

2. **Structure analysis:** Obtaining cluster structure data and analyzing it.

Bash

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compute 2 all coordinates/atom

fix 2 all ave/time 100 100 100 c_2 file coord.txt

3. **Dynamics and movement**: Study of cluster movements and analysis of heat transfer.

Bash

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compute 3 all temperature

fix 3 all ave/time 100 100 100 c_3 file temp.txt

Results.

When analyzing the results, information about energy, temperature, and coordinates is collected. Based on these data, it is possible to draw conclusions about the physical and chemical properties of the cluster. Determining the relationships between the analysis results and the cluster structure is important for further research.

Summary.

The process of creating metal clusters and studying their properties using the LAMMPS program is important not only from a theoretical point of view, but also from a practical one. These studies help in

developing new materials and improving the properties of existing materials. The results obtained using LAMMPS serve as a basis for further research on nanoscale materials.

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