Dynamical and structural properties of Au$_6$ cluster

H. Arslan · M. H. Güven

Abstract The dynamical and structural properties of the Au$_6$ cluster are studied using microcanonical molecular dynamics simulations. The interaction between the atoms in the cluster is modeled by an empirical model potential. The cluster is heated up to 2000 K and during the melting-like transition an isomer of the cluster in C$_{5v}$ (flat pentagonal pyramid) geometry is observed. The cluster’s melting temperature is determined as $\sim 665$ K.

1 Introduction

Investigation of the phases and phase change dynamics and chemical reactivity of atomic and molecular clusters or, more generally, interactions of clusters with individual atoms and molecules, and the evaporation of charged and neutral Van der Waals clusters, have been and remain in the focus of theoretical and experimental studies. Clusters play a central role in a variety of natural phenomena (e.g., in the upper atmosphere and in the soil) and in processes of environmental concern, as well as in technologies related to heterogeneous catalysis, microelectronics, materials design and fabrication, etc., as documented in Allen and Tildesley (1987), Haberland (1994), and Haile (1992).

Small clusters can be described and understood in purely dynamical terms. A melting-like transition in a cluster can be viewed as a transition from a highly restricted and correlated motion of the constituent particles, characteristic of a solid, to their uncorrelated large amplitude or even diffusive motion, characteristic of a liquid.

We do not have truly adequate potentials for metal clusters at present and semiempirical and empirical potentials are being used in theoretical studies to understand the melting behavior of these clusters.

In this study, the constant energy, solid-to-liquid phase transition in isolated Au$_6$ microclusters was studied by using microcanonical molecular dynamics (MD) simulations. In the simulation, an empirical model potential, which contains two and three body atomic interactions, was used and the melting behavior of the cluster was presented.

The potential and the computational procedure are given in Sect. 2. The results and discussion are presented in (Sect. 3). The conclusions are summarized in (Sect. 4).

2 Theoretical background and computational procedure

The potential energy of the cluster as a function of its configuration is modeled by Erköç (1989) and has the following form

$$\Phi = \Phi_2 + B\Phi_3$$

where $\Phi_2$ is the two-body (pair potential) interaction term, more explicitly

$$\Phi_2 = \sum_{i<j} U(r_i, r_j) = \sum_{i<j} U(r_{ij}) = \sum_{i<j} U_{ij}$$

$$U_{ij} = A \left[ \left( \frac{r_o}{r_{ij}} \right)^{2n} e^{-2\alpha(r_i/r_j)^{1/2}} - \left( \frac{r_o}{r_{ij}} \right)^n e^{-\alpha(r_i/r_j)^{1/2}} \right]$$

with $r_{ij} = |r_i - r_j|$, $A = 9.16$ eV, $\alpha = \ln 2$, $r_o = 2.47 \times 10^{-1}$ nm and $n = 2.806960$ for gold. The $\Phi_3$ is the three-body interaction potential expressed as the linear combination of the pair energies formed by the three particles. It is given by

$$\Phi_3 = \sum_{i<j<k} W(r_i, r_j, r_k) = \sum_{i<j<k} W(r_{ij}, r_{ik}, r_{jk}) = \sum_{i<j<k} W_{ijk},$$

where $W(r_{ij}, r_{ik}, r_{jk})$ is the three-body interaction energy of the cluster.


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The total energy in the individual atom) large enough to observe the solid to liquidlike transition in cluster. The total energy in the individual runs was conserved within 0.003%.

We extracted the structural and dynamical properties of cluster from microcanonical molecular dynamics simulations. Hamilton’s equations of motion were solved by Erkoç model potential (1989) for all the atoms in a cluster on a grid of total energies using Hamming’s modified fourth-order predictor-corrector propagator with a step size $5 \times 10^{-18}$ s. The cluster was prepared with zero initial total linear and angular momenta. Trajectories of length of 2.5 $\times$ $10^6$ steps generated on a grid of total energies (per atom) large enough to observe the solid to liquidlike transition in cluster. The total energy in the individual runs was conserved within 0.003%.

The minimum energy geometry of the Au$_6$ cluster is obtained by thermal quenching and found to be $O_h$ which is shown in Fig. 1. The binding energy per atom calculated from the model empirical potential is compared with the other reported values in Table 1. Since the minimum energy geometry is obtained correctly and the calculated binding energy per atom using the model’s empirical potential is comparable with that given in the literature, the melting behavior of the cluster is simulated using this model potential.

Static quantities of the cluster can be calculated from the averages taken along the trajectory.

The calculated static quantities are described in Jellinek et al. as

$$W_{ik} = B(U_{ij}f_{ik} + U_{jk}f_{ki} + U_{jk}f_{ji})$$

with

$$f_{ij} = e^{-r_{ij}^2 / r_i^2}$$

$$f_{ik} = e^{-r_{ik}^2 / r_i^2}$$

and

$$f_{jk} = e^{-r_{jk}^2 / r_j^2}$$

with $B = -1.290433$ for gold. Since B has a negative value, the three-body potential has a positive contribution to the total interaction energy.

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