Melting dynamics of Gold thin film: A Molecular Dynamics study

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Abstract. We studied the melting dynamics of Gold in the form of thin film. The thin film thickness is 9.756 nm. The systems are heated from room temperature up to slightly above melting point, T_m = 1338 K. The evolution of the atoms in each system is followed using Molecular Dynamics (MD) scheme up to 20 ps. Thermodynamics analysis indicated that thin film is suppressed by the uniform heat while the temperature is increasing. Structural analysis compared with Common Neighbor Analysis (CNA) expressed the condition that melting conduction occurred at the end of simulation.

1. Introduction
Properties of material due to heat treatment is important to understand. The change of material phase is significant to be understood in order to characterize the material for specific applications. During heat treatment where the temperature exceeded melting point, the dynamics of melting is interesting to be analyzed from structural point of view [1].

The experiment to observe melting dynamics is limited to the instrument that are used during heating process. Difficulties comes when observation of structural change could not be easily performed during material processing. In order to mimics the processes, MD simulation was done for the case of Aluminum thin film [1] and Gold nanoparticle [2,3].

In current paper the MD simulation is carried out to follow the temperature properties and structural change of Gold thin film. The thin film is heated until slightly above melting point from room temperature. Some explanation on structural change reported in this article will be the main focused of the analysis.

2. Simulation methods
The trajectories of the atoms is followed using MD scheme employing Large-scale atomic/molecular massively parallel simulator (LAMMPS) [4]. The system is heated to temperature 1400 K which already above melting point of Gold (T_m = 1338 K,) [5] from room temperature. The thin film is filled with 55296 atoms in FCC (100) direction which set periodic in lateral directions (9.756 nm x 9.756 nm) and free at thickness (9.756 nm) surface. Interatomic potential by Foiles et al are used with cut-off radius 5.55 Å [6]. The system is relaxed at 300 K and zero pressure for 20 ps before the simulation begin.
OVITO package is employed for visualizing the system along with the analysis of local crystal structure based on Common Neighbor Analysis (CNA) [7-9]. Virial theorem is included in the thermodynamics analysis [10,11]. The structure function is calculated using package of Debyer [12] with some theoretical aspect related to the crystal structure analysis [13-15].

3. Results and discussion

The thin film visualization during heat treatment is shown in Figure 1. The system is heated gradually from room temperature (a) until it melts at $T = 1400$ K (g). During the increasing of temperature, the uniform heat is built up deeper into the system and expand the system. As can be seen from the figure, at $T = 900$ K (d), the system is dominantly homogeneous while it still suffered from uniform heating in the inside part. At the end of simulation, $T= 1400$ K (g), the system is completely melted. It is comparable with the case of nanoparticle [2].

![Figure 1. Gold thin film at temperature: (a) 300 K, (b) 500 K, (c) 700 K, (d) 900 K, (e) 1100 K, (f) 1300 K, (g) 1400 K. Atoms are visualized using color scale of temperature in K.](image)

The structural analysis based on structure factor is shown in Figure 2. At the beginning of simulation, the pattern of perfect crystal structure is indicated by $T = 300$ K. During the increasing of temperature, several peaks are merged which indicate the breaks of symmetry within the crystal. To perform better calculation of structure factor, larger size of system is needed to indicate sharp peak at each point of scattering vector [15]. At $T = 700$ K, the peaks at large scattering vector already merged and vanished at the end of simulation. The peak between scattering vector of $4 – 6 \, \text{Å}^{-1}$ is also merged and survived until $T = 1100$ K. At the end of simulation when temperature reach 1400 K, the structure factor indicated melting profile where the value of $S(Q)$ is approaching unity.

The thickness of the thin film is expanding as the temperature increases shown in Figure 3 (left). The dynamics of the thickness depends on the interaction between atoms which oscillates due to heat dynamics. It was shown that the increasing of thickness is correlated with the distance of the atoms which already move faraway from original distance in crystalline state.
Figure 2. Structure factor at several temperature points, T = 300 K, 700 K, 1100 K and 1400 K. Shifted S(Q) in order to clarify the transformation of the structure.

Figure 3. Left: The thickness of thin film during temperature evolution. Right: Local FCC percentage as a function of temperature.

Analysis on local crystal structure in CNA, indicated the decrement of crystallinity percentage as can be seen from Figure 3 (right). At crystalline state where the system is at room temperature, it consists of 85.6% of FCC structure. The surfaces are at free condition, hence the local crystallinity does not show perfect percentage of FCC structure. By increasing the temperature, the structure is broken and collapsed. It confirms the results of structure factor where the distance of the atoms is playing significant role in forming local crystal structure and breaks due to increasing temperature. At T = 1400 K, where the system is completely melted, no FCC structure is detected [1,2].

4. Conclusion
We studied the melting dynamics of Gold thin film by means of MD simulation from room temperature up to above melting point. The transformation of the system from crystalline state to melting state is
strongly indicated by the analysis of structure factor and CNA. The evolution of the system suggesting that melting processes occurred due to increased temperature.

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