

Structural change of aluminum thin film in the temperature range from 300 K to 1000 K

Riser Fahdiran^{1,*}, Erfan Handoko¹, Iwan Sugihartono¹, Anggara Budi Susila¹, Esmar Budi¹, and Setia Budi²

¹State University of Jakarta, Physics Department, Jalan Rawamangun Muka 13220 Jakarta Timur, Indonesia

²State University of Jakarta, Chemistry Department, Jalan Rawamangun Muka 13220 Jakarta Timur, Indonesia

Abstract. We study the structural change of Aluminum thin film due to heat treatment. The film is heated up from room temperature of 300 K to 1000 K where it is already above melting temperature of Aluminum. Molecular dynamics simulation is employed to observe the behavior of the system since it provides atomistic detail. The structural transformation is investigated based on the structure factor and pair distribution function which indicated the broadening of the peak of crystal structure due to phase transition of the material. Atomistic information revealed the local lattice structure change based on Common Neighbor Analysis (CNA) methods.

1 Introduction

The properties of a material will be altered due to heat treatment. The main properties that will change always related to the structure of the material itself.

In experimental point of view, it will be difficult to see the structural change of a material due to heat treatment. When we heated a material, usually it is a separated experiment with the measurement using X-ray or neutron diffractometer. In the case of laser induced structural change of a materials perform by Nicoul *et.al.* [1], they investigated the structural response of a material by means of time-resolved diffuse X-ray scattering.

For the case of melting due to laser irradiation, Zhigilei and his co-workers investigated the structural change of materials by means of molecular dynamics (MD) simulation [2,3]. MD simulation could provide atomistic point of view of structural change since it follows the trajectory of the atoms within the simulation. In the general case where Lennard-Jones material is considered to shows the evolution of laser induced structural change of nanoparticle and thin film, Fahdiran and Urbassek [4,5] used MD simulation to show the small-angle scattering structural change due to heat absorbed from the laser. The results show that MD simulation could give insight into the material, especially the structure of the system.

In this article, we investigate the structural change of Aluminum thin film due to general heat treatment. The methods will be performed using MD simulation from room temperature and increased gradually up to slightly above melting temperature. The structural changes of the material are provided base on the structure factor, pair distribution function as well as Common Neighbor Analysis (CNA).

2 Simulation Method

Molecular dynamics (MD) simulation is used to follow the evolution of the system in the temperature range from 300 K to 1000 K. Large-scale atomic/molecular massively parallel simulator (LAMMPS) is employed to conduct the simulation [6]. The Aluminum thin film is consists of 55296 atoms with thickness 9.7 nm in free condition with FCC(100) orientation on z direction and lateral size 9.7 nm x 9.7 nm which are set in periodic. The interaction potential between atoms are based on Liu with cut-off radius 6.06 Å [7]. The system is relaxed at 300 K for 20 ps before the heat treatment is started.

To observe the evolution from atomistic point of view, we use OVITO for atomistic point of view and also Common Neighbor Analysis (CNA) which are provided by the software [8–10]. Atomistic point of view for temperature are also calculated including the virial theorem [11,12]. To show the structural change due to heat treatment we also calculate the structure factor and pair distribution function with definition from Egami and Billinge [13] using Debyer [14].

3 Results and Discussion

The sequence of the heated Aluminum thin film are shown in Figure 1. At the beginning (a), all the local atoms indicated that the system is relaxed in the temperature range of 300 K. Continuing to part (b) where the system temperature is increased to 400 K, the inner part of the film is heated up and continue to spread until 500 K (c). In part (d), (e) and (f), the temperatures are 600 K, 700 K and 800 K respectively, all the local atoms already suffered for high temperature. Figure 1 (g) shows the condition of the system reaching the melting point of Aluminum, $T_m = 933$ K [15], where the system

* Corresponding author: riser-fahdiran@unj.ac.id

is in the temperature of 900 K. At temperature 1000 K (h) where it is already above the melting point, the local atoms are already homogenized with high temperature throughout the system. This indicated that the phase of the system already transformed from solid to liquid state.

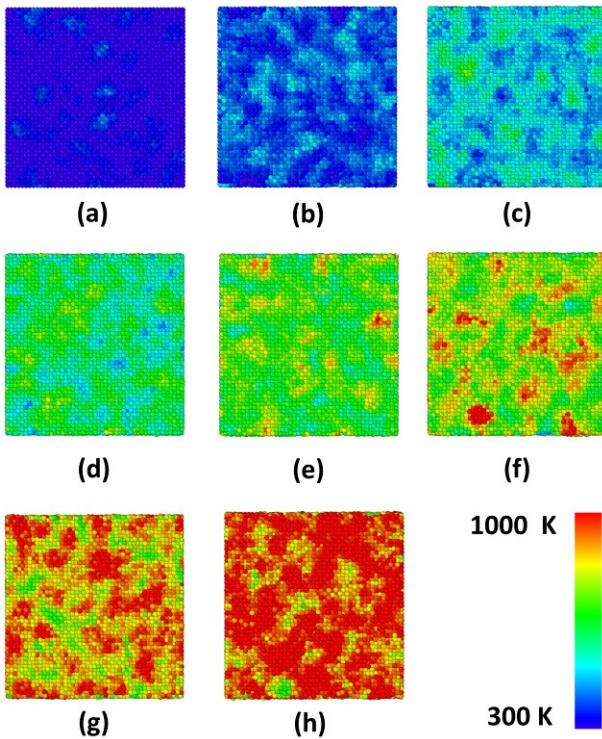


Fig. 1. Evolution of thin film. Atoms are colored based on local temperature in K (temperature color scale are given). (a) 300 K. (b) $t = 400$ K. (c) 500 K. (d) 600 K. (e) 700 K. (f) 800 K. (g) 900 K. (h) 1000 K.

In Figure 2, the structure factor $S(Q)$ of several conditions of temperature are given. At the beginning of the simulation, where the system is in equilibrium at room temperature ($T = 300$ K), all the peaks are still sharp indicating that the system is still in its crystalline state. Noted that the merged of several peaks, especially at $Q > 5 \text{ \AA}^{-1}$, comes from the fact that we built the system in small size. Referring to Lin and Zhigilei [3], system size is responsible to construct the peak width of the $S(Q)$ from the simulation point of view.

When we increased the temperature to $T = 500$ K, the $S(Q)$ value is decreased. This indicated the fact that the coordination between local structure is interrupted. Following the system to $T = 700$ K, we can see at $Q > 5 \text{ \AA}^{-1}$, some peaks are merged or loosing its condition. By the end of the simulation, $T = 1000$ K, the system already above melting temperature. The $S(Q)$, shows this condition from the fact that all peaks at $Q > 5 \text{ \AA}^{-1}$, are vanished and some of it merged with the closest one.

The pair distribution function, $g(r)$, is presented in the same temperature correspond to the $S(Q)$ results. As $g(r)$ is the Fourier transform of $S(Q)$, it gives insight on the positions of the atoms in a material or the possibility to find atoms in the range of cut-off radius [3,13,16].

At room temperature, $T = 300$ K, the strong peak of $g(r)$ shows the possibility to find atom up to radius 10 \AA .

It was clearly shown by Figure 3 that at maximum distance the peak is still sharp. Noted that if we follow the calculation up to the size of the system (thickness, $d = 9.7 \text{ nm}$) several peaks will still exist since it is in crystalline state. The lattice constant of Aluminum is 4.032 \AA in the form of FCC structure. The distance between each monolayer is approximately 2 \AA , this was confirmed in the $g(r)$ profile where the first peak is around 2.5 \AA indicating the possibility to find an atom within this distance is quite high.

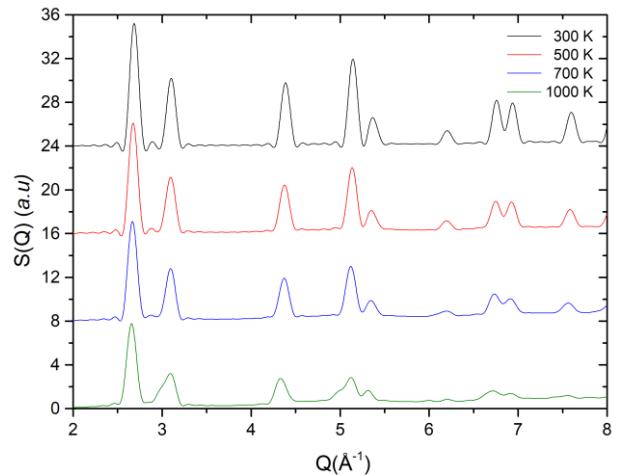


Fig. 2. Structure factor [$S(Q)$] profile.

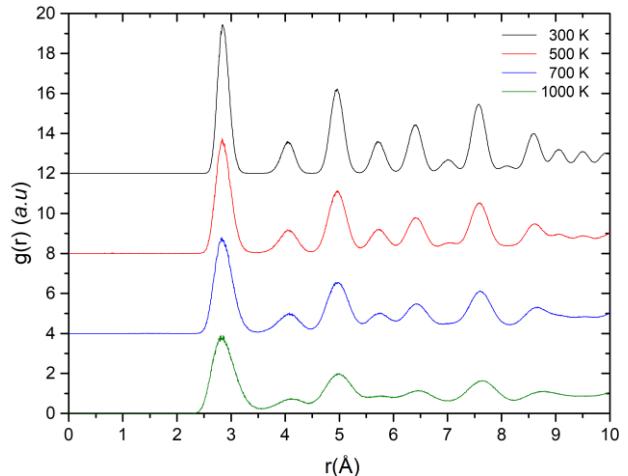


Fig. 3. Pair distribution function [$g(r)$] profile.

At temperatures of 500 K and 700 K, we can see that the $g(r)$ value at higher distance already vanished. This indicated the reason that the crystal structure already interrupted and confirm the $S(Q)$ results. By the end of the simulation, $T = 1000$ K, the crystal structure already lost the FCC configuration as it can be seen in Figure 4 while the $g(r)$ converge to value of 1. Indicating that even at higher distance the probability to find atom is definite.

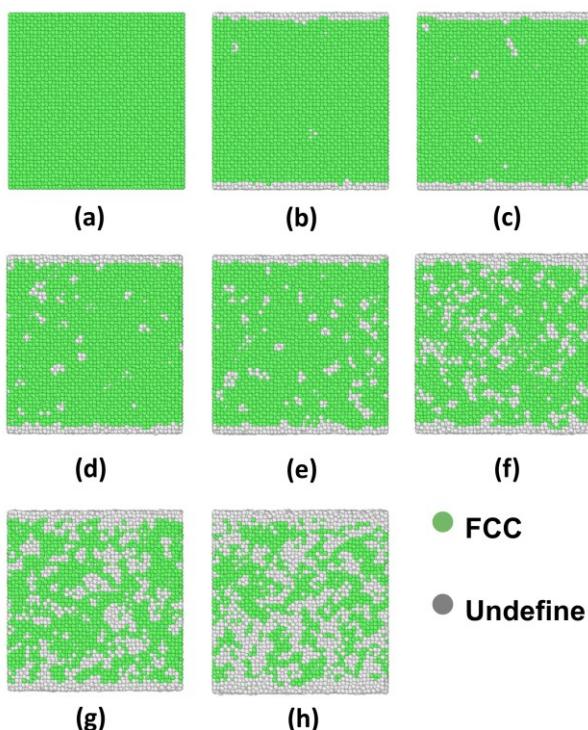


Fig. 4. Local structure based on Common Neighbor Analysis (CNA). (a) 300 K. (b) t = 400 K. (c) 500 K. (d) 600 K. (e) 700 K. (f) 800 K. (g) 900 K. (h) 1000 K.

By using Common Neighbor Analysis (CNA) we investigated the local structure of the system. As it was confirmed by S(Q) and g(r), the crystalline structure of the system is FCC at room temperature, T = 300 K. By increasing the temperature up to 900 K we can see that the local structure is damaged. And at the temperature of 1000 K the local structure consists of FCC only fulfilled 43.5 % of the system. CNA results confirm the fact from S(Q) and g(r) that the system already undefined at the end of the simulation.

In summary, we studied the structural change of Aluminum thin film due to heat treatment. The thermodynamics point of view indicated that the system melts at T = 1000 K. The structure factor and pair distribution function results indicating the change of the system structure as a function of temperature and confirmed by CNA analysis where the system is suffered by temperature due to heat treatment.

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References

1. M. Nicoul, F. Quirin, a. M. Lindenberg, a. Barty, D. M. Fritz, D. Zhu, H. Lemke, M. Chollet, D. a. Reis, J. Chen, S. Ghimire, M. Trigo, M. Fuchs, K. J. Gaffney, J. Larsson, T. Becker, S. Meyer, T. Payer, F. Meyer zu Heringdorf, M. Horn von Hoegen, M. Jerman, and K. Sokolowski-Tinten, EPJ Web Conf. **41**, 04013 (2013)
2. Z. Lin, E. Leveugle, E. M. Bringa, and L. V. Zhigilei, J. Phys. Chem. C **114**, 5686 (2010)
3. Z. Lin and L. V. Zhigilei, Phys. Rev. B **73**, 1 (2006)
4. R. Fahdiran and H. M. Urbassek, Adv. Mater. Res. **1112**, 120 (2015)
5. R. Fahdiran and H. M. Urbassek, Eur. Phys. J. D **69**, 35 (2015)
6. S. Plimpton, J. Comput. Phys. **117**, 1 (1995)
7. X. Y. Liu, F. Ercolessi, and J. B. Adams, Model. Simul. Mater. Sci. Eng. **12**, 665 (2004)
8. A. Stukowski, Model. Simul. Mater. Sci. Eng. **18**, 015012 (2010)
9. D. Faken and H. Jónsson, Comput. Mater. Sci. **2**, 279 (1994)
10. J. D. Honeycutt and H. C. Andersen, J. Phys. Chem. **91**, 4950 (1987)
11. T. J. Colla and H. M. Urbassek, Radiat. Eff. Defects Solids **142**, 439 (1997)
12. A. K. Upadhyay and H. M. Urbassek, J. Phys. D: Appl. Phys. **40**, 3518 (2007)
13. E. Takeshi and S. J. L. Billinge, *Underneath The Bragg Peaks: Structural Analysis of Complex Materials* (Pergamon Materials Series, Oxford, 2003)
14. M. Wojdyr, <https://github.com/wojdyr/debyer> (2016)
15. C. Kittel, *Introduction to Solid State Physics* (John Wiley & Sons, Inc., New York, 1996)
16. C. L. Farrow and S. J. L. Billinge, Acta Crystallogr. Sect. A Found. Crystallogr. **65**, 232 (2009)