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EFFECT OF PARTICLE SIZE ON IGNITION AND OXIDATION OF SINGLE ALUMINUM: MOLECULAR DYNAMICS STUDY

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Abstract

Alumina nanoparticle is one of the attractive nanoparticles synthesized by the plasma method. The oxidation step in this method is challenging to explain experimentally. This work was to perform a molecular dynamics simulation to determine the oxidation mechanism of aluminum nanoparticles with different sizes and oxidation levels in the oxide layer. This work was to perform a molecular dynamics simulation to determine the oxidation mechanism of aluminum nanoparticles with different sizes and oxidation levels in the oxide layer. The simulation method employed the ReaxFF potential. The material used is aluminum nanoparticles in three different sizes (8, 12, and 16 nm) with an oxide layer thickness of 0.5 nm. Aluminum nanoparticles were given a relaxation treatment of 300 K for 1 ps and then heated to a temperature of 3250 K with a heating rate of 5×10^{13} K/s and cooled to 300 K. The ensemble used is a canonical ensemble with the Nose/Hoover thermostat method. The result shows that the higher the temperature applied to the system, the more oxygen molecules adsorption occurs on the surface of the oxide layer and the diffusion of oxygen to the particle core. The higher temperature applied also causes gaps, or void spaces, between the core and the shell. The reaction barrier for diffusion of oxygen also decreased significantly due to void space, and the surface of the aluminum core dissociates to the surface (alumina shell). Particles with a smaller size have a shorter ignition delay time. In addition, the smaller the particle size, the more oxygen molecules' reacted with aluminum particles in the particle core.

Keywords: aluminum nanoparticles, oxidation of aluminum, molecular dynamic simulation, reaxFF.

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1. Introduction

Aluminum (Al) is a reactive and easily oxidized material frequently used to synthesize aluminum oxide or alumina [1]. Aluminum also has energetic properties that increase reaction energy and catalytic activity. Thus, it is often used for propulsion applications [2, 3]. Some report that producing 1–100 nm nanoparticles improves alumina properties [4]. Compared to micro size, nano size has better properties such as reaction speed, increased surface area/volume ratio, increased melting process speed, and smaller characteristic mass and energy [5–8]. Due to its benefit, improving the performance of nanomaterials is highly considered. Some research has widely developed and applied nanoparticle products using various materials and sizes [9, 10]. Aluminum nanoparticles (ANP) can be synthesized into aluminum oxide using various methods, including plasma. Plasma is the fourth phase after solid, liquid, and gas [11]. Powder synthesis, including thermal plasma, applies various types of plasma. Plasma formation is also inseparable from the presence of plasma-forming gas, in this case, oxygen which is also a component of alumina synthesis [12]. Thermal plasma has a high temperature reaching 10,000 K at the closest point [13]. At each point, the arc plasma has a different temperature and energy level; the farther away, the temperature gets lower. The injection of aluminum particles into plasma at a high temperature will cause a melting process, and the particles break

down into tiny sizes up to nanoparticles [1]. Furthermore, if the environment uses oxygen, aluminum will be oxidized to metal oxide particles called alumina [14].

There have been many advances in the efficient, low-cost production of nanoparticles. Therefore, several researchers have conducted studies on nanoparticles to explore the possibility of systematic control of oxidation reactions. However, it is still tricky to experimentally distinguish atomistic mechanisms in single nanoparticles with different particle sizes because the space scale and reaction time are minimal [15]. Research on Al oxidation has been carried out using various methods, ranging from experiments to simulations. One of the most widely used simulation methods is molecular dynamics (MD) [16–18]. Molecular dynamics refers to computer simulation method to analyze the physical movements of atoms and molecules. The atoms and molecules are allowed to interact for a fixed period of time, giving a view of the dynamic «evolution» of the system. Research conducted experimentally shows the behavior of particle size on the ignition process on aluminum also indicates that the smaller the particle size, the faster the ignition process, which also accelerates the burning time [6, 19, 20]. In addition, the reaction process of the particle surface to different amounts of oxygen significantly influences the oxidation behavior of Aluminum [21]. The combustion process in aluminum at other particle size conditions also affects the optimal energy output, which is the optimal system for maximum energy release. Energy release in the combustion reaction in aluminum will be more robust when the particle size is below 10 nm [22]. The results of the combustion of aluminum also show that as the initial diameter of the aluminum particles increases, the content of Al atoms also increases. In contrast, the range of O atoms decreases, indicating that the combustion process in aluminum does not occur properly [23]. Some literature reported various researches related to aluminum oxidation. These stated MD simulation with Streitz-Mintmire electrostatic plus (ES+) potential [24], the response of Al/Al_2O_3 core during heating process [17], the effect of ionization on aluminum oxidation [25], and study of atomistic mechanisms on laser flash heating of Al/Al_2O_3 nanoparticle cores [26]. Despite these experimental and simulation research efforts, several key questions remain unanswered. Thus, this work performed a molecular dynamics simulation to determine the oxidation mechanism of aluminum nanoparticles.

2. Materials and Methods

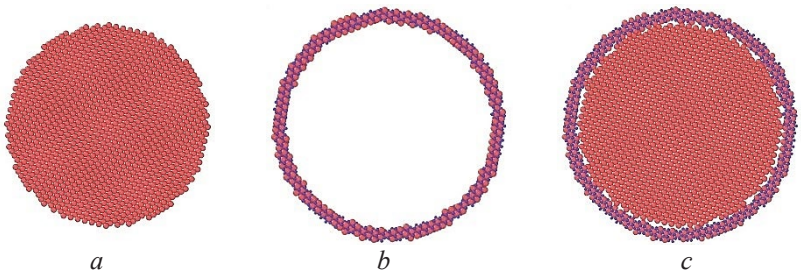
2. 1. Simulation system

This simulation system consists of an Al atom as the core surrounded by an alumina shell with an oxygen environment. The particle diameter sizes were 8, 12, and 16 nm. Let's denote the system as ANP with ANP8 for 8 nm, ANP12 for 12 nm, and ANP16 for 16 nm. The layer thickness of all ANPs used is 0.5 nm representing the initial conditions of the aluminum particles [27]. All ANPs were given the same treatment model. The distance between the core and the alumina layer is 1 Å. Therefore, it reduces contact tightness after fusion [25]. The simulation process was carried out as follows:

1) ANP was given a relaxation treatment for 1 ps with a temperature of 300 K, after that;

2) the heating process was carried out from 300 K to 3250 K with a heating rate of 5×10^{13} K/s. In this stage, to evaluate the melting temperature of ANP usage, the current ReaxFF description was found;

3) cooling to 300 K at a two times slower cooling rate. **Fig. 1** shows the start of the ANP model. The blue atom is oxygen, and the red atom is Aluminum.

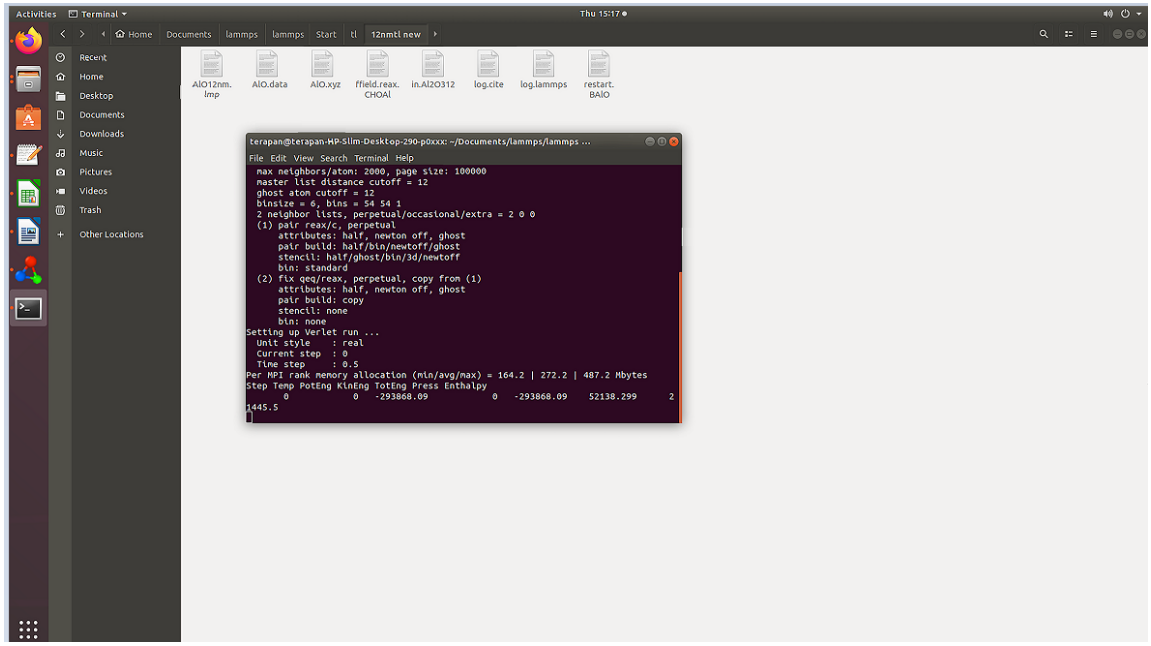


a *b* *c*

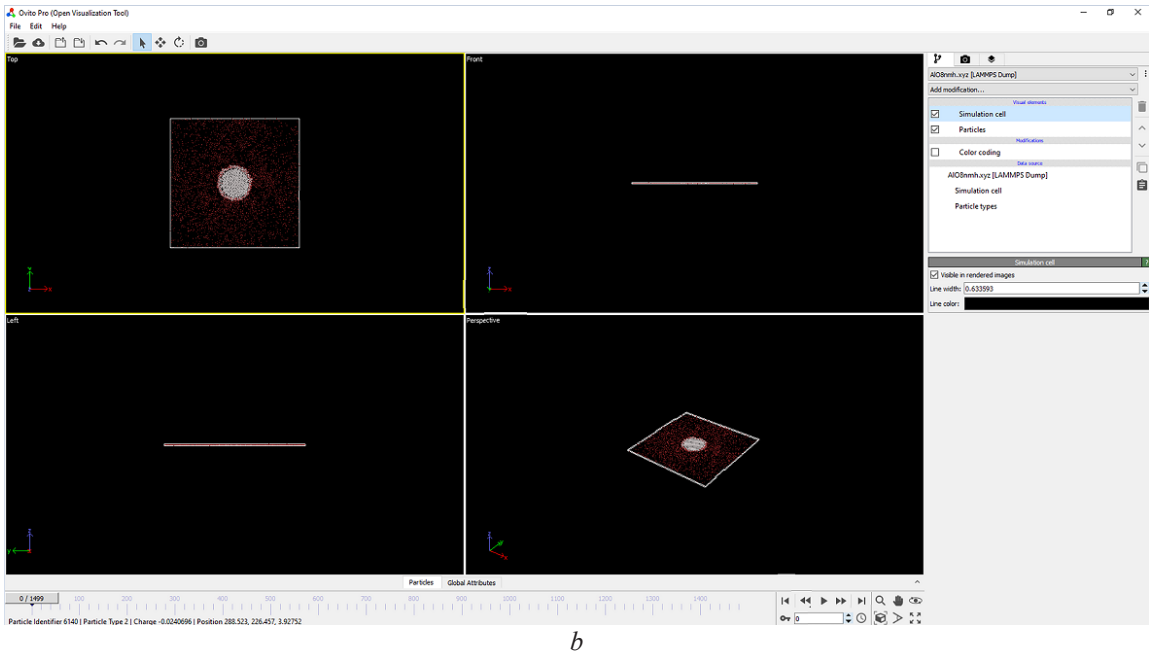
Fig. 1. Views of the ANP8 in different modelling periods: *a* – an alumina shell model; *b* – initial Al core with a diameter of 8 nm; *c* – fusion of an alumina shell with Al core

2. 2. Simulation setup

The simulation box is organized as a cubic box with periodic boundaries. The box dimensions used are 320×320×7 Å which applies to all ANPs. Molecular oxygen is distributed randomly with an atomic number of 5455. Since this study focused mainly on ANP oxidation as a function of system temperature, it was essential to control the system temperature during the MD simulation. For this reason, the canonical ensemble is used: a constant number of atoms, volume, and temperature. The Nose/Hoover thermostat method was used because it has been suggested for canonical ensembles [17]. All Molecular Dynamics simulations were implemented on the LAMMPS code version 29 March 2019 (http://lammps.sandia.gov) with the REAX-C package. OVITO is used as post-processing software and as a visualization tool for simulation results [28]. Screenshots of LAMPPS and OVITO software can be shown in **Fig. 2**.



a



b

Fig. 2. Screenshot of running simulation software: *a* – LAMMPS; *b* – OVITO

2. 3. ReaxFF reactive force field

ReaxFF is a program for modeling chemical reactions with atomic potential based on a reactive force field approach. After nearly two decades of development, ReaxFF has been successfully applied in many fields: heterogeneous catalysis, vanadium catalyst, atomic layer deposition, and other reaction systems on the nanoscale [29–32]. The reaction process of Al and O atoms occurs in a Bond-order (BO) mechanism, which can be explained by the ReaxFF potential [16]. The total energy in the ReaxFF force field is described in equation (1) by:

$$E_{system} = E_{bond} + E_{over} + E_{under} + E_{lp} + E_{val} + E_{tors} + E_{vdWaals} + E_{Coulomb}, \quad (1)$$

where E_{system} is total energy, E_{bond} is bond energy, E_{over} is over-coordinated, E_{under} is uncoordinated, E_{lp} is lone-pair, E_{val} is valence angle energy, $E_{vdWaals}$ is van der Waals, and $E_{Coulomb}$ is Coulomb energy. Unbound interactions are calculated independently of bonding interactions, so there are no contradictory data [16]. At the core of ReaxFF is bond order, which is determined by the distance between two atoms. The bond order will be updated during the simulation process, and after a certain number of iterations, all atoms are considered bonded.

3. Results and Discussion

Through the observations in **Fig. 3**, all O atoms interacting with ANP become negatively charged. **Fig. 3** shows a typical process of oxygen adsorption on the surface of an alumina shell in the case of ANP8. Initially, the oxygen molecules are in a floating environment outside the shell. Then the O atoms are attracted by the positively charged Al atoms on the surface. The oxygen molecules move towards the surface and produce an unbalanced charge distribution, as shown in **Fig. 3, *b***. Later, the oxygen molecule binds to the Al atoms on the surface and the charge distribution on oxygen molecules into equilibrium.

Fig. 4 is a graph of changes in the number of atomic lattices to change the time. Before the heating process, the structure on the aluminum core is FCC lattice. When Aluminum is heated, the structure of the aluminum atoms moves and shifts in a specific direction, resulting in changes in the structure. Changes in the FCC lattice structure in the Al core indicate information about the melting process. ANP8, ANP12, and ANP16 had a similar trend, but the FCC number decreased drastically in ANP8 at 75 ps and reached 0 at 150 ps. While the ANP12 experienced a drastic decrease at 225 ps, then slowed down at 225 ps and 0 at 300 ps. In ANP16, the decrease in the number of FCC was slighter than the other measures. At 0 ps to 175 ps, there was a prolonged decrease in the number of FCC. Then at 200 ps, it decreased drastically to 450 ps and the number of FCC 0 at 475 ps. The decreased number of FCC lattices means that the Al atoms have entered a solid-liquid coexistence state. The decrease in the number of FCC lattices means that the Al atoms have entered a solid-liquid coexistence state which is considered a crucial stage before the aluminum particles are completely melted [33–35]. The difference in the speed of time in decreasing the number of FCC in each size shows that the size can affect the speed of the melting process [16]. This indicates that the smaller the particle size, the faster the melting process occurs.

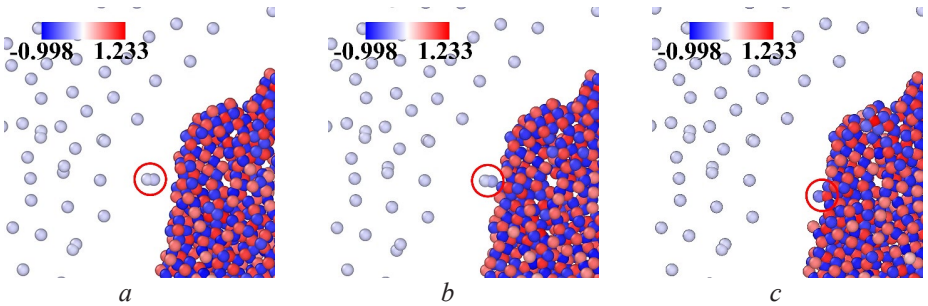


Fig. 3. Mechanism of oxidation: *a* – molecular oxygen in the environment; *b* – molecular oxygen is attracted by Al on the surface of the shell; *c* – adsorbed oxygen molecule and turns into an equilibrium charge distribution

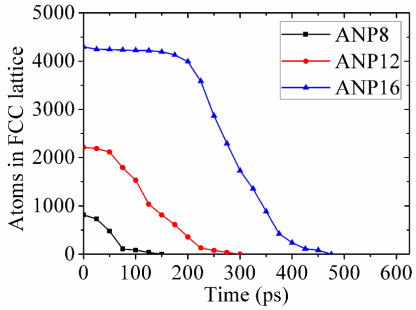


Fig. 4. Face centered cubic atomic lattice resistance against time in the process of heating

The oxide growth process during the heating process is shown in **Fig. 5**. It was seen that the oxide growth on ANP8 increased significantly from 0 ps to 50 ps. Then it slows down at 50 ps to 100 ps and increases again drastically to 150 ps. Furthermore, the increase was almost complete at 500 ps. ANP12 has a similar trend to ANP8, where from 0 ps to 50 ps significantly increases. However, from 50 ps to 80 ps, the increase in oxide growth rose slowly, and then there was a drastic increase from 80 ps to 500. The ANP16 also has a similar trend with the size of 8 nm, only the increase in lower oxidation growth, and the Al core is not oxidized as a whole. This is affected by the reaction temperature and the kinetic reaction slowdown [36].

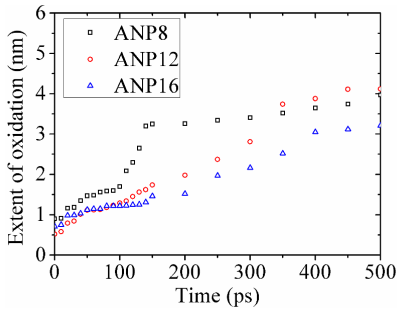


Fig. 5. Rate of oxidation growth on the heating process of aluminum nanoparticles

Fig. 6 is a change in the radius of aluminum nanoparticles without Al_2O_3 coating in the heating and cooling process. All ANPs showed expansion followed by contraction. The particles' expansion rate (percentage increase in radius) from the initial value to the maximum value of the ANP8, ANP12, and ANP16 systems were 19 %, 12 %, and 6 %, respectively. The particle radius is calculated by averaging the distance from the system's center to all the atoms in the largest oxide fragment. However, all ANPs during the heating process will experience an expansion process and will experience contraction or shrinkage during the cooling process. The expansion process is caused by stretching the atomic positions and the diffusion of O atoms towards the Al core so that the final radius is increased from the initial radius of the system [37].

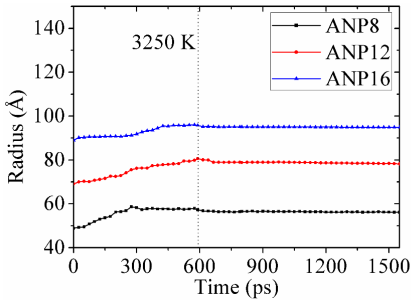


Fig. 6. The radius of aluminum nanoparticles as a function of time

The potential energy curve against time is shown in **Fig. 7**. Oxygen atoms in the environment diffuse to the shell region of the ANP. Therefore, the thickness of the oxide increases. This phenomenon shows that ANP8 has undergone surface combustion of the aluminum process before 150 ps. In the early stages, the core Al atoms maintain their position in the alumina shell or near the alumina shell region without diffusing to the surface. The O atoms have diffused into the core region in the next stage. And the dissociation of Al atoms on the surface area of the Al core towards the shell. In the self-sustain combustion stage, almost all the Al atoms in the ANP8 atom are bonded to the O atom, and the potential energy curve slope is close to 0. ANP12 at 150 ps also indicates the diffusion of O atoms into the Al core region. A gap between the Al core and the shell results in the dissociation of Al atoms towards the shell. Therefore, the oxidation reaction is indicated by the thickening of the oxide.

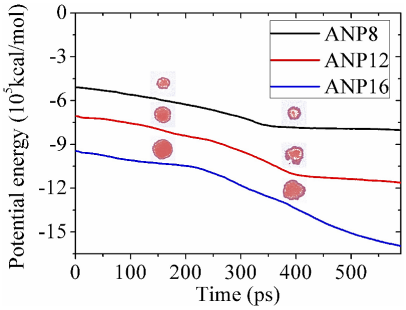


Fig. 7. Curve of potential energy with time and relevance snapshot ANP8, ANP12 and ANP16 at 150 ps and 400 ps

Meanwhile, at ANP16, before 150 ps, it is clear that Al atoms and O atoms still occupy the core region and are only adsorbed on the surface of the oxide shell. The oxide shell strongly inhibits the diffusion of O atoms into the core region during the first 150 ps. At 400 ps, some Al and O atoms have bonded, but the O atoms do not diffuse to the core region consistently. Many Al atoms dissociate towards the surface. A boundary gap between the Al core and the oxide shell also exists.

To study in more detail, radial distribution function (RDF) is used to analyze the evolution process of the relative position of each component. Diffusion of Al atoms is essential in the early stages of combustion. The relationship between Al and O atoms in the early combustion stage (before 400 ps) is shown in **Fig. 8**.

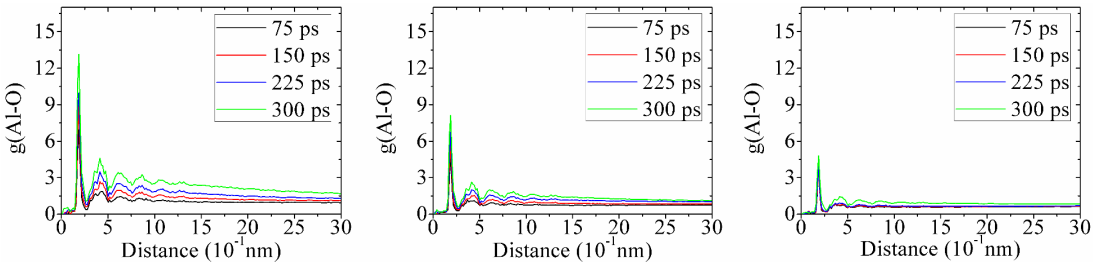


Fig. 8. Radial distribution function result of Al-O pair in the oxidation process before 300 ps: *a* – ANP8; *b* – ANP12; *c* – ANP16

In **Fig. 8, *a***, the ANP8 RDF plot is characterized as a graph of fluctuations with peaks. The first peak appears at 1.875 A°, which is the bond distance between Al and O atoms. As the temperature increases, the peak height becomes sharper at 300 ps. The peak at 1.875 A° also marks the start of the combustion process. The reason is that Al atoms in the core region have been exposed to an external oxygen environment. The oxidation reaction will be more intense as the temperature increases. The RDF plot in ANP8 does not shift horizontally. These characteristics indicate that the relative structure between Al and O atoms does not change. While **Fig. 8, *b*** RDF ANP12 plot and **Fig. 8, *c*** RDF ANP16 plot shows the first peak that also appears at 1.875 A°. The subsequent peaks

also did not experience a horizontal shift as in ANP8. These characteristics show that the relative structure between Al and O atoms does not change much.

To show a comparison of several parameters that are affected by differences in particle size during the heating process are shown in **Table 1**.

Table 1
Parameters of the difference in particle size

Particle size	Total time of decreasing number of FCC (ps)	Max. expansion (%)	Extend of oxidation on 150 ps (nm)	first peak appears of RDF (A°)
8 nm	150	19	3.25	1.875
12 nm	300	12	1.74	1.875
16 nm	475	6	1.46	1.875

This work is inherently limited by some factors such as:

– the NPS containing alumina in diameter size of 8, 12, and 16 nm and the layer thickness of 0.5 nm;

– the treatment temperature of 300 K and the heating temperature in range of 300 K to 3250 K with a heating rate of 5×10^{13} K/s;

– the simulation box is assumed as a cubic box with periodic boundaries in dimensions of 320×320×7 Å;

– molecular oxygen is distributed randomly with an atomic number of 5455.

4. Conclusions

As the temperature increases during the heating process on aluminum particles in an oxygen environment, the oxidation process on aluminum will increase. Oxidation mechanisms occur when oxygen particles in the environment attach to surfaces due to differences in charge. The oxygen particles move toward the particle nucleus until the charge distribution is equilibrium. However, the presence of an oxide layer on ANP provides an obstacle in the diffusion of oxygen molecules to the Al core in ANP. As the particle size increases in this case at 16 nm (ANP16), the rate of oxidation is getting slower. where at 150 ps, the addition of oxide thickness in ANP16 is only 1.46 nm, which is smaller than that of ANP8 which is 3.25 nm. Thus, the smaller the particle size, the faster the overall oxidation reaction to the particle core. The result of this work is an empirical study to determine the oxidation mechanism of aluminum nanoparticles. However, it requires experimental approach to gain insight of oxidation mechanism.

Conflict of interest

The authors declare that they have no conflict of interest in relation to this research, whether financial, personal, authorship or otherwise, that could affect the research and its results presented in this paper.

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Data availability

Manuscript has no associated data.

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