



Molecular Dynamics Studies of The Effects of Copper on The Mechanical Properties of Aluminum

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ABSTRACT– In this research, molecular dynamics (MD) simulations were performed to model the effects of copper content on aluminum properties. Copper has a low solubility in aluminum. Therefore, the main purpose of this research is to study the influence of copper content (Cu) on the mechanical properties of aluminum. Modeling and simulation of nano indentation and uniaxial tension tests were carried out to observe the mechanical properties under the conditions of copper content starting from 0.5 up to 10wt% at 300°K. The interactions between the atoms of aluminum and copper were modeled using Embedded Atom Method (EAM) potentials. The calculation showed that a higher amount of copper increased the tensile strength of aluminum, and in this research, 10wt% copper gave the highest tensile strength. But when it comes to the nano indentation test to determine hardness value, it showed that 1wt% copper gave the highest hardness, it assumes that this is related to localization of nano indentation test position optimum formation of intermetallic aluminum-copper, Al₂Cu on a certain area.

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Introduction

Aluminum is a material that is widely used in the automotive industry, specifically used as a material for pistons and engine blocks because aluminum has several suitable properties such as lightweight, machinability, and low expansive thermal coefficient when combined with silicon. However, aluminum is a material that has lower mechanical properties than other materials that are often used in industry, such as steel [1]. Aluminum is a material that can improve its mechanical properties, and there are several methods to improve the mechanical properties, such as alloying, coating, and heat treatment [2-3].

The alloying elements method is the most widely used in improving the mechanical properties of aluminum. In this process, aluminum is combined with other alloying elements such as Mg, Si, Cu, etc. These alloying elements can also possibly form precipitates or intermetallic phases due to the reaction between aluminum and alloying elements. Based on experimental results, copper (Cu) is the most widely added to aluminum because aluminum and copper alloys will be able to form a precipitate, namely, Al₂Cu. Al₂Cu is a precipitate that can improve its mechanical properties by hindering the dislocation of the aluminum matrix [4-8].

Because copper and aluminum have a limit of solubility, repeated experiments are needed to obtain the optimal Cu composition of aluminum and obtain the desired results. The repeated experimental method has several drawbacks in terms

of the high cost and the time required. Therefore, we need a method that can overcome this [9].

Molecular dynamics (MD) has been widely used to predict the properties of materials using atomic scale calculation. For the last couple of years, some researchers have been starting to simulate metals using molecular dynamics especially on aluminum.

Computational materials research in the field of aluminum alloys, especially at the atomic level, is pretty limited when using molecular dynamics methods. Therefore, this research will study and simulate alloying elements between aluminum and copper using molecular dynamics methods. Molecular dynamics is a computer simulation where atoms will interact with each other over a certain period based on the laws of physics. Molecular dynamics simulations provide static and dynamic information at the atomic scale, static and dynamic information at the atomic scale can then be processed into property information on the macroscopic scale [10].

Materials and Methods

In this study, the analysis was carried out at the molecular level using the Large-Scale Atomic / Molecular Massively Parallel Simulator (LAMMPS) program developed by Sandia National Laboratories under the United States Department of Energy, USA. Distributed in open source code under the GNU General Public License [4].

A. Potential Functions

In this research, the potential of the Embedded-Atom Method (EAM) method was used to define the interatomic interactions of Al and Cu atoms. The embedded atom method is an approximation that describes the energy between two atoms. The energy is a function of a sum of separation functions between an atom and its neighbors. It was first developed by Daw and Baskes (1984) to study the defects in metals. EAM is widely used in MD simulations. In the EAM, the system's total energy as two additive terms is the pairwise sum of interactions between atoms and a term representing the electron density of each atomic site, as shown in the equation below [3].

$$E = \sum_{i=1}^N F_i \left(\rho_{h,i}(r_i) \right) + \frac{1}{2} \sum_{i,j}^N \phi_{ij}(r_{ij}) \quad (1)$$

where F_i is embedding function and $\phi_{ij}(r_{ij})$ is repulsive pair potential. Embedding function F_i on Equation 1 obtained empirically and local electron density $\rho_{h,i}$ on position r_i Calculated based on distribution from electron $\rho_{h,i}$ in all atoms, including interactions in the range as follows [3].

$$\rho_{h,i}(r_i) = \sum_{j \neq i}^N \rho_j^{at}(r_{ij}) \quad (2)$$

B. Molecular Modeling

To understand the effects of copper content on aluminum, we will develop two testing models: one is uniaxial tension testing and nanoindentation. The initial geometry configuration for the alloy model is shown in Figure 1. in the simulation box, the positions of the copper atoms are represented randomly. Atomic model for nanoindentation and box-shaped uniaxial tension with dimensions $\alpha 12 \times \alpha 12 \times \alpha 12$ for nanoindentation and $\alpha 12 \times \alpha 12 \times \alpha 12$ for uniaxial tension. Where α is the equilibrium lattice parameter for aluminum with a value of 4.05 Å.

In uniaxial tension simulation, there are three parts: first, fix, middle, and upper zone. The fix zone is the static mode position part, then the middle zone is an area to observe crack propagation from atomic and fracture, and the upper zone is a tension area with the direction of Y.

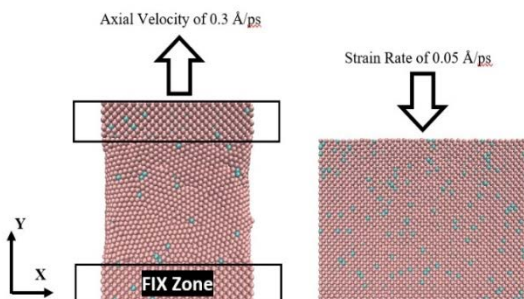


Figure 1. Modeling of tensile test and nano indentation test.

Results and Discussions

A. Nano Indentation Simulation

Nano indentation is an experimental technique for measuring the hardness of materials on the nanoscale. As such, it can measure the properties of thin films and nanoparticulate materials. Nano indentation simulation represents the hardness value from a material when given a static load until it deforms, as investigated by several researchers [3-6].

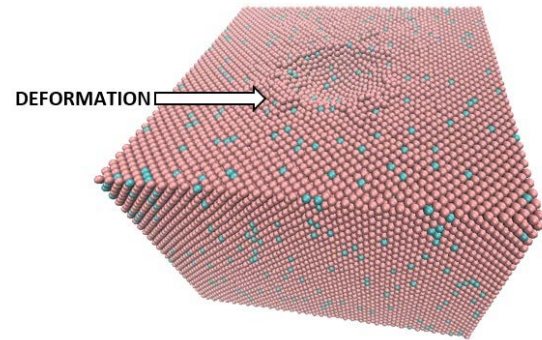


Figure 2. Deformation caused by nano indentation

In Figure 2, deformation caused by indentation occurs, for the indentation speed in this simulation is set at 0.5 Å/ps where the initial position of the indenter is at 15 Å from the surface of the simulation box.

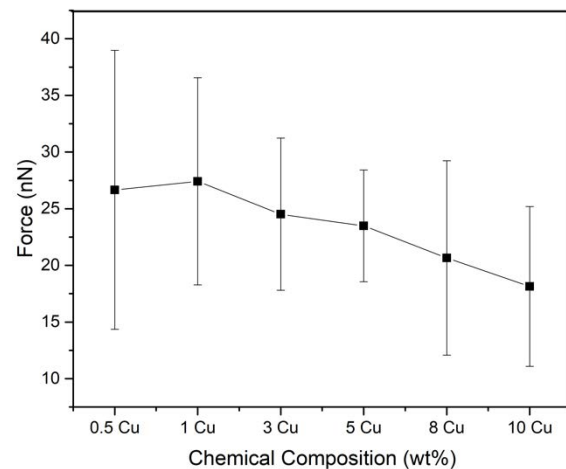


Figure 3. Effects of Cu content on nano indentation force.

Hardness is one of the most important properties, and it is commonly used to give a general indication of the strength and resistance to plastic deformation. It can be defined as the ability of a material to resist permanent indentation or deformation [11]. The results of the nano indentation simulation tests show that the highest hardness value is 1wt% Cu content with the average force required in the indentation for 26.3 nN. However, at the higher content of Cu, the hardness decreased due to lower nano indentation force. This is assumed to be the position where the nano indentation test occurred. Higher results are expected in nano-scale mechanical testing than in macro- or micro-scaled mechanical testing.

In the aluminum-copper alloy, intermetallic phases will be formed, especially Al-Cu binary phases such as Al₂Cu. The reaction for Al₂Cu formation is shown below;



Al₂Cu is commonly found on aluminum-copper alloys, especially after strengthening precipitation hardening or T6 heat treatment. Intermetallic Al₂Cu has high mechanical properties [12-15].

B. Uniaxial Tension Simulation

The simulation used molecular dynamics after constructing and stabilizing the model for the uniaxial tensile test. This model allowed us to predict the mode of deformation as well as the results of deformation at the atomic scale. The uniaxial tension test is a tensile testing simulation where the alloying model will be given y-axis force until the alloying model fractures with the speed of 14 Å/ps. This simulation's results will represent the alloying model's mechanical properties.

The results from the simulation of the uniaxial tension test will contain data loggers for pressure and elongation. As shown in Figure 4, the atomic movement appears visually supported by OVITO.

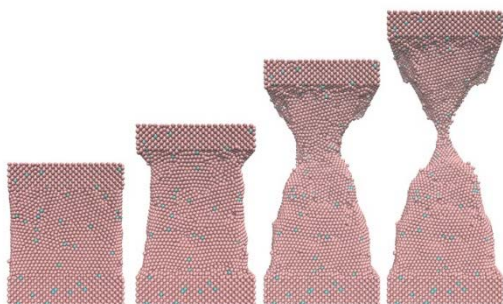


Figure 4. Modeling of uniaxial tensile test

Figure 5 is the ultimate tensile strength data from the simulation results of the uniaxial tension test, where the highest value of ultimate tensile strength is aluminum with a copper mixture of 10%wt. There is a tendency for the ultimate tensile strength of the alloy model to increase with increasing copper content. This is because the increase in copper means more Al₂Cu precipitate will be formed [6]. The distance between the precipitate particles is getting closer for precipitates that increase in number. This tight precipitate acts as a barrier, which causes dislocation shifts to become more difficult when deformation occurs in the alloy model.

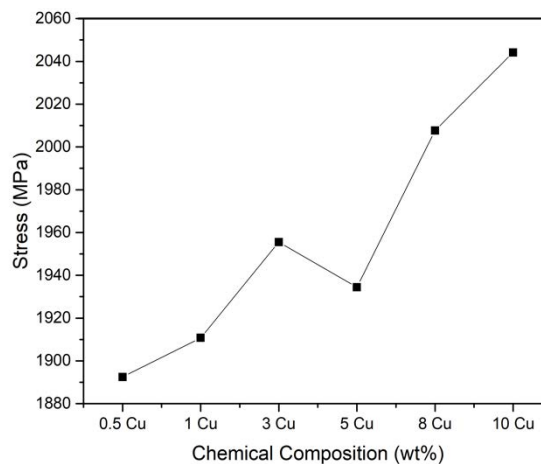


Figure 5. Effects of Cu content on ultimate tensile strength

Based on experimental research in the past, adding copper as the primary alloying addition into aluminum will possess higher strength properties but with limited corrosion resistance properties than other aluminum alloys. Many aluminum alloys also have relatively good elevated-temperature strength properties. Magnesium is also added to the 2xxx series alloys for crack sensitivity and the possibility of forming another intermetallic phase, such as the Al-Cu-Mg system. AA2024 is one of the highest strengths in the aluminum alloy series [15].

Conclusion

In this research, it showed that copper has significant effects on the mechanical properties of aluminum. Hardness and ultimate tensile strength increased with increasing amounts of copper. Formation of intermetallic phase Al₂Cu and test position have important effects on nano-scale indentation test. It has the optimum result for hardness with 1wt% copper and decreases afterward. In the case of the uniaxial tensile test, the highest ultimate tensile strength was obtained with the highest amount of copper in this research for 10wt%.

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