

MOLECULAR DYNAMICS STUDIES ON THE STRENGTH PREDICTION OF INTERFACE BETWEEN AL-AL₄C₃ IN METAL MATRIX NANOCOMPOSITES

¹Deni Haryadi, ²Haris Rudianto ³Mohamad Yamin

^{1,2,3} Advanced Materials Laboratory, Department of Mechanical Engineering,
Gunadarma University

Jl. Margonda Raya Number. 100, Depok 16424, West Java

¹deniharyadi97@gmail.com, ²harisrudianto@staff.gunadarma.ac.id

Abstrak

In this study, molecular dynamics simulations (MD) will be applied to modelling the Al₄C₃-aluminum interface in aluminum nanocomposite, Al₄C₃ is an interface that results from the shaker mill process which becomes a bridge that plays an important role in Carbon particles with Aluminium Matrix and Based on observations from the TEM characterization, it is found that the relationship between Al orientation to Al₄C₃ is (111) (002) (220). The characteristics of the interface between Aluminum matrix and Al₄C₃ will be analyzed using uniaxial tension and shear test simulation. The atomic potential used in this simulation is the embedded atom method (EAM) for Al, empirical-order intermolecular potential (AIREBO) for C and Lennard-Jones for the reaction of Al-C atom. The result shows that, the interface orientation is Al matrix (002) || Al₄C₃ (003) has the highest interface strength compared to Al matrix (111) || Al₄C₃ (003) and Al matrix (200) Interface orientation || Al₄C₃ (003). Results from the molecular dynamics simulations are also discussed with analytical results obtained experimentally

Keywords: Molecular dynamics, Interface, Aluminum Nanocomposite

INTRODUCTION

Aluminum matrix nanocomposite is a composite material that combines strength, stiffness and low weight properties with the potential to increase damage tolerance while maintaining certain thermal and electrical properties [1-2]. On Aluminum matrix composite Carbon reinforcement form Interphase Al₄C₃. Al₄C₃ is an interface produced by the shaker mill process which becomes a bridge that plays an important role in Carbon particles with an aluminum matrix [3].

Based on observations of TEM characterization, it was found that the relationship between the orientation of Al to Al₄C₃ was (111) (002) (220) and Plane (002) was coherent [4]. There are major challenges

in the experimental development and characterization of the Al₄C₃-aluminum interface in aluminum nanocomposite due to the difficult and expensive processes involved [5-6].

Therefore, discussing with the computation method which has the advantages of time and low cost will play an important role in analyzing and understanding the characteristics of aluminum-Al₄C₃ in aluminum nano composite materials. [7]

Molecular Dynamics (MD) simulation method is widely used by researchers around the world who are mostly researchers in the field of chemistry and nano metal composites, because the MD method can be used to determine movements, directions and

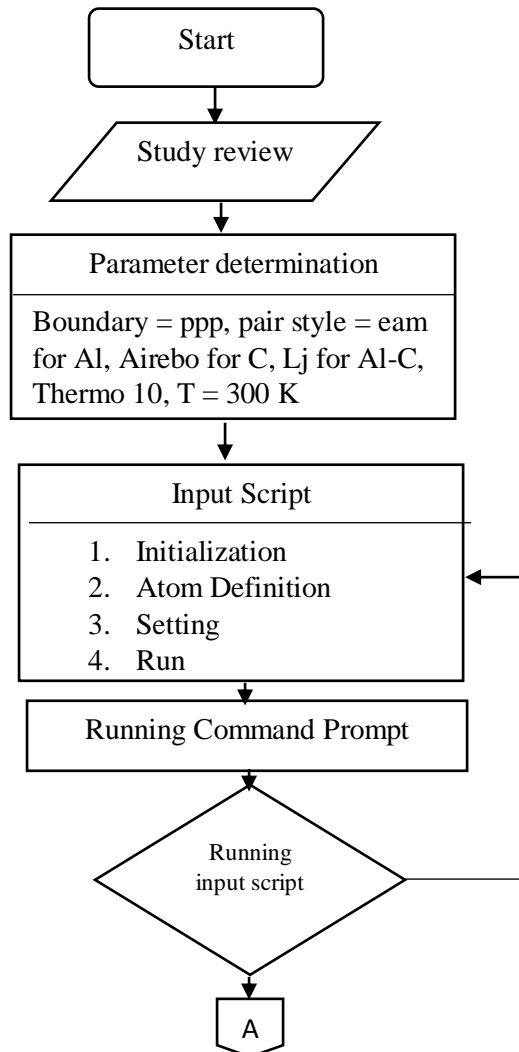
reactions between atoms. In this research, we will study the effect of each interface that is formed on the strength of the interface. The method used to analyze the interface strength of each orientation is using the Molecular Dynamics (MD) method.

MOLECULAR DYNAMICS SIMULATION

In conducting the study, usually preceded by assigning multiple stages or steps

in conducting research. The following will be explained about the research methods from the beginning to end of study, shown through research flow diagram or flowchart as Figure 1.

Molecular dynamics simulation methods will be used in this study to analyze and understand the interface between Al and Al₄C₃ where the software package used is the Large-scale Atomic / Molecular Massively Parallel Simulator (LAMMPS) made by Sandia National Laboratories USA.



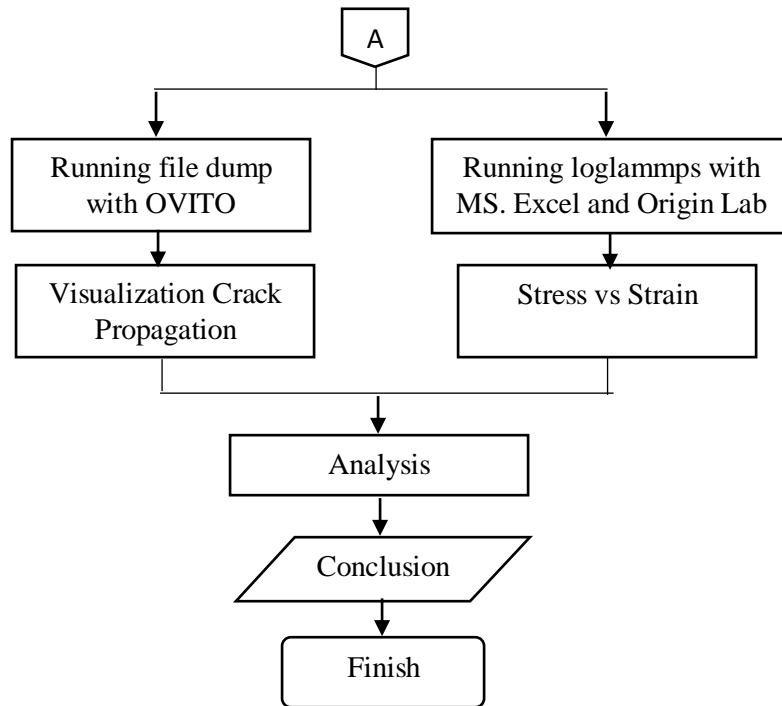


Figure 1. Research Flowchart

Another source code OVITO (Open Visualization Tool) is scientific visualization and analysis software for atomistic and particle simulation data. It helps scientists gain better insights into materials phenomena and physical processes. The program is freely available for all major platforms under an open source license. OVITO is a software that

will be used to make it easier to visualize the results of lammps simulations [7].

1. Potential Function

In this study, the interatomic potential for Al atoms is the Embedded-Atom Method (EAM). Where the total energy E_i of an atom i in EAM is given by,

$$E_i = F_\alpha(\sum_{j \neq i} \rho \beta(r_{ij})) + \frac{1}{2} \sum_{j \neq i} \phi_{\alpha\beta}(r_{ij}) \quad (1)$$

Where F is the embedding energy and is a function of the atomic electron density ρ , and also ϕ is a pair potential interactions and α & β are symbols to distinguish between atoms i and j . The nature of the potential of multi-body EAM (Embedded-Atom Method) is the result of the embedding energy term. The two

sums in this formula include all neighbors j of atom i within the cut off distance [7-9].

In this study the potential used in simulating carbon atoms is the Adaptive Intermolecular Reactive Empirical Bond Order interatomic potential, which is shown as in the equation below.

$$E = \sum_i \sum_{j \neq i} (E_{ij}^{REBO} + E_{ij}^{LJ} + \sum_{k \neq i,j} \sum_{l \neq i,j,k} E_{ijkl}^{TORSION}) \quad (2)$$

Where E^{REBO} corresponds to the shortest distance between bonds which have covalent bonds, E^{LJ} is the Lennard Jones interatomic (LJ) potential is used for interactions that

$$E = 4\epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right], r < r_c \quad (3)$$

Where, r_c is the value of the cut-off radius of the Lennard Jones potential outside of the van der waals interaction will be ignored and will be taken equal to the value of 2.5σ . Parameters ϵ is the coefficients of depth of interatomic potential well and σ is equilibrium distance from potential. Para-

have long distances, for example non-bonded atoms and $E^{TORSION}$ is torsional potential where depends on the angle around the dihedral atom [7-9].

meter ϵ and σ will be used to react between carbon atoms and aluminum atoms and will be calculated using LB rules that are widely used and will be given a value σ 3.1325 Å and $\epsilon = 0.003457$ eV. The values of lennard jones potential parameters for aluminum and carbon atoms are Shown in table 1[7-9].

Table 1. Lennard-jones pair potential parameters for C and Al atoms

Lennard jones Potential parameters	Carbon	Aluminum
$\sigma(\text{Å})$	3.41500	2.8500
$\epsilon[\text{eV}]$	0.00239	0.0050

Before conducting a simulation to analyze the interface characteristics between Al4C3 with aluminum, the equilibrium simulation is carried out for 10000 times and each time the timestep is equal to 1 fs and carried out at room temperature that is 300 K. In equilibrium simulations, NVT and NPT conditions will be applied, where NVT stands for number or number of atoms, volume and tempratur while NPT stands for number, pressure and tempratur. after the equilibrium simulation process, Molecular dynamics simulation process is carried out in NVT conditions or ensemble by fixing at each end of the RVE and when in unaxial tension simulation will be given a stran rate at a speed of $0.05 \text{ Å} / \text{fs}$. Molecular dynamics

simulations will run for 250000 steps with each step equal to 1 fs.

2. Material Design

Interface orientation Al matrix – Al4C3

To know the interface orientation of the Al matrix - Al4C3 interface. So in this study refers to experimental research that has been done. Al matrix orientation interface - Al4C3 was successfully identified by X-ray Diffraction testing where, the Oversea interface was identified with Al4C3 003 orientation with Aluminum orientation fields 002, 111 and 220. to verify the simulation methods and procedures to determine the mechanical properties of Al4C3-Aluminum matrix, the results of the simulation of the

mechanical properties of Interface Al_4C_3 – Aluminum with dimensions $13\text{\AA} \times 60\text{\AA}$ will be used as a material for consideration and reference to predict the mechanical properties of the AMC material. First, Supercell simulation will be divided into two parts,

namely the top and the bottom. the upper part is the aluminum matrix while the lower part is the Al_4C_3 interface. The stress-strain curves of a Al_4C_3 -Aluminum matrix along axis y directions obtained from the simulation are shown.

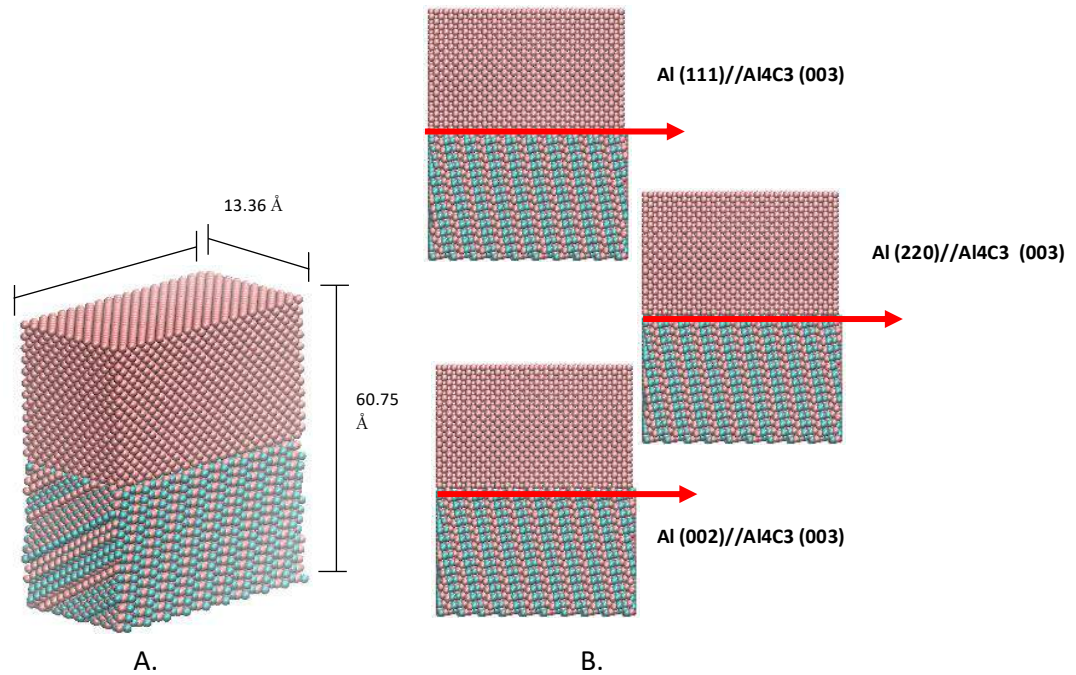


Figure 2. A. Crystal structure: Interfaces Al_4C_3 . B. The simulation variable simulation

RESULTS AND DISCUSSION

Supercell from of interface between Al- Al_4C_3 as shown in Figure 2 is is a subject that will be given a process of equilibrium simulation, uniaxial tension and shear tension to study the nature and characteristics of the Al matrix interface with Al_4C_3 . Obtained comparative results between the tensile behaviour of interface between Al- Al_4C_3 nanocomposite in Axis Y directions are plotted in Fig. 3 and 4.

Al_4C_3 has a unique crystal structure, where Al_4C_3 crystal structure consists of intermittent Al_2C and Al_2C_3 layers. and an Al atom will be coordinated with 4 carbon atoms to form a tetrahedral crystal structure. A carbon atom can form different bonds, one of which is an octahedron of 6 Atom Al with a bond distance of 217 pm. to get the Al_4C_3 interface to pass through the reaction as shown below.[10].



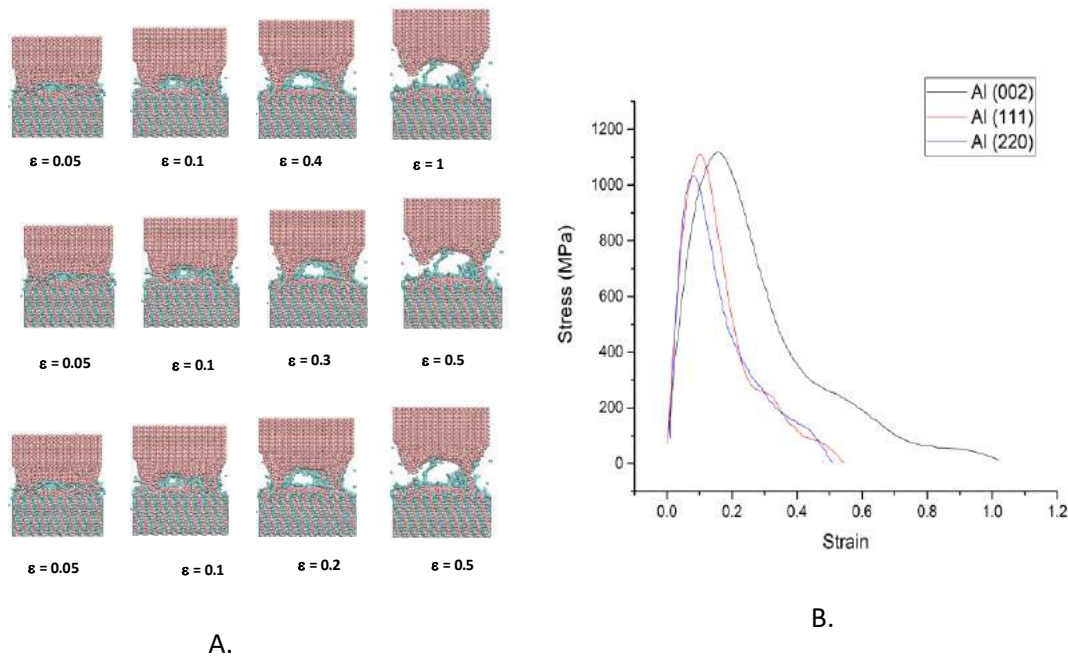


Figure 3.A. Atomic snapshot at different strains of the model B. Stress vs Strain curves of Interface Al Matrix- Al_4C_3 of uniaxial load test

The orientation of interfacial plays a crucial role in the Aluminum nanocomposite mechanical behavior. One reason for increasing modulus can be understood by considering the effect of interface orientation. Uniaxial strain results on MD simulations that depend on the quality of potential functions are not as reliable as the first principle calculation, but MD simulations can provide important insights into the atomic mechanism of the kinetic processes that occur during deformation [11].

Effect of Interface Orientation Al matrix and Al_4C_3 on Tensile Test

Tensile simulation aims to determine the properties of the Interface orientation Al matrix and Al_4C_3 when getting the force in the direction of the y axis. From the three variables, it can be analyzed that the interface

orientation of Al matrix (002) \parallel Al_4C_3 (003) has a higher inter-face strength compared Al matrix to interface orientation (111) \parallel Al_4C_3 (003) and interface orientation Al matrix (220) \parallel Al_4C_3 (003).

Effect of Interface Orientation Al matrix and Al_4C_3 on Shear Test

In the tensile and shear simulation results as shown in Figures 2 and 3. Where Interface orientation is Al matrix (002) \parallel Al_4C_3 (003) has the highest interface strength. Where Interface orientation is Al matrix (002) \parallel Al_4C_3 (003) have UTS 1100 MPa and 1 for tensile test and 305.6 and 3.5 strain for Shear test. On Aluminum matrix nanocomposites reinforced with Graphite, in a reaction between carbon and liquid aluminum it will produce a layer of aluminum carbide, which can reduce the strength of the material,

although it can improve the wetting properties of Al_4C_3 particles.

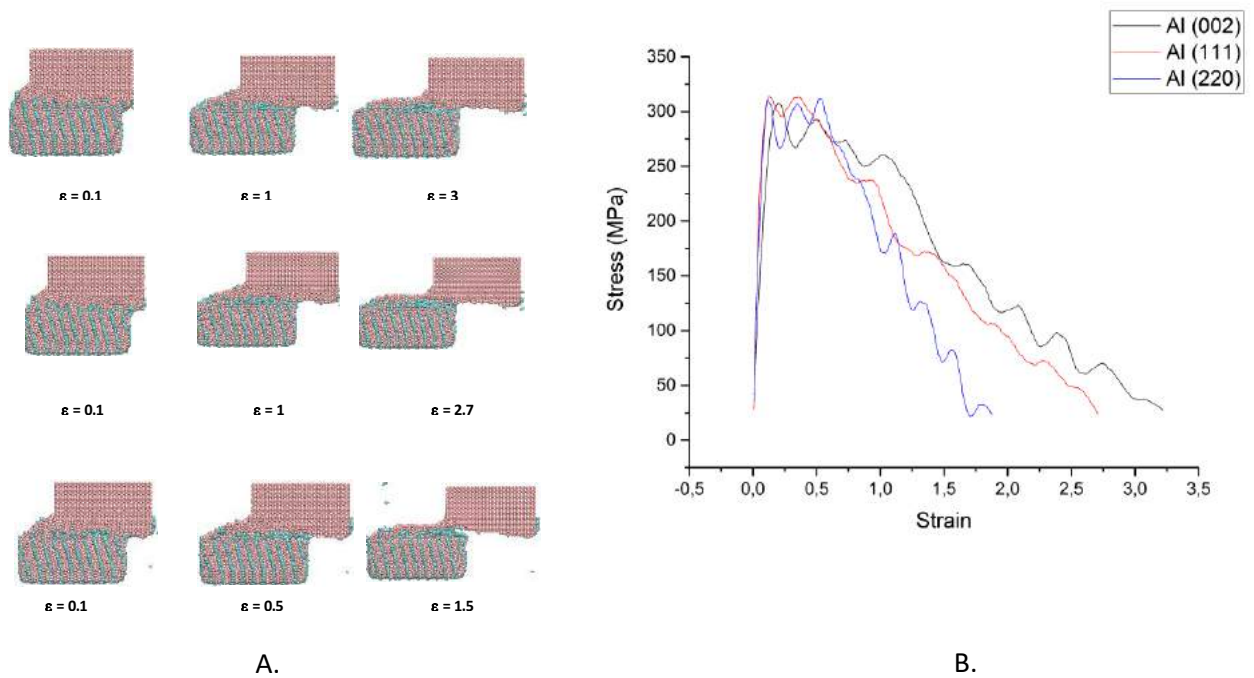


Figure 4.A. Atomic snapshot at different strains of the model B. Stress vs Strain curves of Interface Al Matrix- Al_4C_3 of Shear test

To increase the load transfer at the interface between Graphite and Aluminum matrix in Aluminum material with graphite reinforcement, then the formation of Al_4C_3 with a small amount will have an impact on the increase. With the formation of Al_4C_3 , it can increase shear resistance in the interface between Aluminum and Al_4C_3 so that, it will improve mechanical properties.

CONCLUSIONS

On the three interface orientation Al matrix $\parallel \text{Al}_4\text{C}_3$ is known that, Interface orientation is Al matrix (002) $\parallel \text{Al}_4\text{C}_3$ (003) has the highest interface strength compared to Al matrix (111) $\parallel \text{Al}_4\text{C}_3$ (003) and Al matrix

(200) Interface orientation $\parallel \text{Al}_4\text{C}_3$ (003). This can be verified by experimental data that interface orientation of Al matrix (002) $\parallel \text{Al}_4\text{C}_3$ (003) is a coherent interface, so it can be concluded. Interface orientation of Al matrix (002) $\parallel \text{Al}_4\text{C}_3$ (003) is the best interface.

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