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Research Paper

Comparing Mechanical Properties of AL/Cu Composite Obtained by Mori-Tanaka and Dynamic Molecular Methods

Mostafa Yazdani [1,2], Aazam Ghassemi [1,2*], Mohamad Shahgholi [1,2], Javad Jafari Fesharaki [1,2], Seyed Ali Galehdari[1,2]

1. Department of Mechanical Engineering, Na.C., Islamic Azad University, Najafabad, Iran.

2. Modern Manufacturing Technologies Research Center, Na.C., Islamic Azad University, Najafabad, Iran.

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ABSTRACT

For composites, one of the most important problems is calculating the mechanical properties using properties of the composite contents by a homogenization method. In this paper a macro homogenization method has been compared with dynamic molecular method(MD) for the first time. For this purpose the influence of copper (Cu) content on the mechanical properties of Aluminium (Al) has been studied. For investigation properties of composites in macro scale there are various methods for homogenization. Mori-Tanaka Eshelbi(M-T) is an interesting method for homogenization. On the other hand, MD is an effective and different method for extracting mechanical properties of nanocomposites. In this paper Young modulus of AL/Cu have been calculated by M-T and MD methods and the results have been compared. For this comparison at the first, using MD method, the Al/Cu nanocomposite box's dimensions were set to 80 × 80 × 80 $Å^3$. The Al/Cu nanocomposite was subjected to uniaxial tension using molecular dynamics simulation and LAMMPS package software. For M-T method, Young modulus of AL and Cu, separately, have been extracted by MD using the same box dimension. Then Young modulus of AL/Cu composite has been computed by M-T homogenization method. According the analysis, for low percent of Cu (1% and 2%) the difference between two methods is less than 16% but for higher percent of Cu, the difference is more than 300% . According these results, for higher percent of Cu, M-T as a macro model for simulation of nano scale is not suitable.

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*** Corresponding Author:**
E-Mail: a_ghassemi@iau.ac.ir

1-Introduction

Bimetallic composites show more complex behavior and a greater variety of mechanical properties in comparison with pure metals. Pure Aluminum has lower mechanical properties in comparison with other materials, but in the form of alloys, its mechanical properties are acceptable. Cu has high thermal conductivity and Al/Cu bimetallic composites are widely used in many industries[1-4]. According length and diameter of added nano materials to metals , tensile strength of them can be more than 100 times of high strength steels[5-8]. According experimental results, by adding Cu to Al, Al2Cu will be formed that can improve mechanical properties of Al by hindering the dislocation of Al [9-13]. Wang et. al.[14] investigated the mechanical characteristics of Al-Cu alloy through the wire and arc additive manufacturing technique to achieve enhanced mechanical properties. Muscati et al. using MD, investigated the mechanical behavior of functionally graded Al/Cu alloy reinforced with carbon nano tubes(CNT) [15]. Bian et al investigated the compression and deformation behavior of nano-polycrystalline Cu/Al_2Cu/Al-layered composites, by MD method. According their research, Cu/Al_2Cu/Al materials are sensitive to changes in the interfacial layer due to the asymmetry between tensile and compressive deformations[16]. Haris et. al. researched about influence of Cu content on the mechanical properties of Al using MD. According their research, higher amount of Cu increased the tensile strength of Al, and in this research,10wt% of Cu gave the highest tensile strength[17]. Kumar et. al Studied friction stir welding (FSW) at the atomic level for Cu and Al using MD method. simulation-based tensile and shear deformation tests, revealed that higher tool rotational speeds led to enhanced material interlocking, consequently improving the mechanical strength of the FSW joints[18]. Meng et al.[19] conducted MD simulations of an Al/Cu alloy using a box measuring 162 × 162 × 405 Å^3 containing 640,000 atoms. The simulations incorporated periodic boundary conditions in the XY plane and employed an embedded atom method to model atomic interactions among Cu/Cu, Al/Al, and Al/Cu. The study focused on analyzing the impact of temperature changes on misalignments. Additionally, the research investigated the mechanical properties of Al/Cu alloy, including its elastic modulus and ultimate strength, via molecular dynamics simulation. Furthermore, the study examined how various parameters such as temperature, strain rate, and different volume percentages of Cu influenced the mechanical properties of the Al/Cu alloy. M-T method is one of the most used methods for short fiber composites[20-21]. This method predicts the effective linear elastic properties of composites. Many researchers used this method for homogenization of composites[22-25]. MD method is very interesting for prediction the properties of composites in nano scale but it is considerable that using MD for two phases materials, such as composites, is very time-consuming and expensive. On the other hand, Mori-Tanka is a popular homogenization method that is very simple and cheap for macro scales. in this paper once mechanical properties of Al and Cu, separately, has been obtained by MD and homogenized using Mori-Tanaka and another time the properties of composite has been obtained directly by MD and then the results have been compared. According the mentioned studies comparing macro homogenization methods with MD method has not been done so far. In this paper at the first, young modulus and strength of AL/Cu composite have been extracted by M-T method. For this purpose, using mechanical properties of AL and Cu and volume fraction of them, young modulus and strength of AL/Cu have been computed. This process repeated by MD method and the main purpose is comparing results computed using two methods.

2- Homogenization using M-T method

According this method, for two phases composite if V^R , V'^f , V'^m are volume of representative element, phase 1 and phase2 respectively then volumetric average stress will be defined as below [26]:

$$\sigma_i = \frac{1}{V^R}\iiint_{V^R}\sigma_i dV = \frac{1}{V^R}\left[\iiint_{V'^f}\sigma_i dV + \iiint_{V'^m}\sigma_i dV\right] \quad (1)$$

$$= \frac{V'^f}{V^R}\left[\frac{1}{V'^f}\iiint_{V'^f}\sigma_i dV\right] + \frac{V'^m}{V^R}\left[\frac{1}{V'^m}\iiint_{V'^m}\sigma_i dV\right] \quad (2)$$

$$\sigma_i = V^f\overline{\sigma}_i^f + V^m\overline{\sigma}_i^m \quad (3)$$

Where $V^f = \frac{V'^f}{V^R}$ and $V^m = \frac{V'^m}{V^R}$ are volume fractions and $\overline{\sigma}_i^f$ and $\overline{\sigma}_i^m$ are internal stresses in phases.
Also, about strains:

$$\varepsilon_i = V^f\overline{\varepsilon}_i^f + V^m\overline{\varepsilon}_i^m \quad (4)$$

According Benveniste formulation, average stress and strain can be computed as relations 5:

$$\varepsilon^f = T \cdot \varepsilon^m \quad (5)$$

$$\sigma^m = A \cdot \sigma^f \quad (6)$$

In this relation A_{ij} is M-T tensor

$$A = C^{-m} \cdot T^{-1} \cdot C^f \quad (7)$$

In this relation C and S are stiffness and compliance matrixes respectively. The tensor T can be computed using Eshelbi matrix, L, as below:

$$T = [(I + L \cdot S^{-m}) \cdot (S^f - S^m)]^{-1} \quad (8)$$

So

$$\sigma = (V^m \cdot I + V^f \cdot A) \cdot A \cdot \sigma^f \quad (9)$$

For two-dimensional formulation

$$\boldsymbol{L} = \begin{bmatrix} L_{1111} & L_{1122} & 0 \\ L_{2211} & L_{2222} & 0 \\ 0 & 0 & 2L_{1212} \end{bmatrix} \quad (10)$$

Where:

$$L_{1111} = L_{1122} = 0, \quad L_{2211} = \frac{\vartheta^m}{2(1-\vartheta^m)}$$

$$L_{2222} = \frac{1}{2(1-\vartheta^m)}[\frac{3}{4} + \frac{(1-2\vartheta^m)}{2}], L_{1212} = \frac{1}{4} \quad (11)$$

Now using M-T method, stiffness matrix of composite becomes as below:

$$S = (V_f \cdot S^f . T + V_m \cdot S^m)(V_f \cdot T + V_m \cdot I)^{-1} \quad (12)$$

It is clear that:

$$V_f + V_m = 1 \quad (13)$$

Therefor using stiffness matrix in relation 12, young modulus of composite can be calculated.

3- Extracting mechanical properties of AL/C by MD method

Using LAMMPS package software, the Al/Cu nanocomposite was subjected to uniaxial tension. The Airebo [30,31], embedded atom method (EAM) [32], and Lennard-Jonse [33] potentials were utilized to describe the interactions between Cu/Cu, Al/Al, and Al/Cu atoms, respectively. The Al/Cu nanocomposite box's dimensions were set to 80 × 80 × 80 Å^3. An isolated system with a fixed number of atoms (N),fixed pressure (P), and a fixed temperature (T) (NPT) ensemble was used to balance the system, with variables representing the number of atoms, ambient pressure, and temperature. The system was found to be in perfect equilibrium with a relaxation time of 1000 pico second (ps) and a time step of 1 femto second (fs).

4- Results

For homogenization method , M-T, uniaxial test of Al and Cu, separately, has been obtained by MD and output graphs are illustrated in figures 1 and 2.

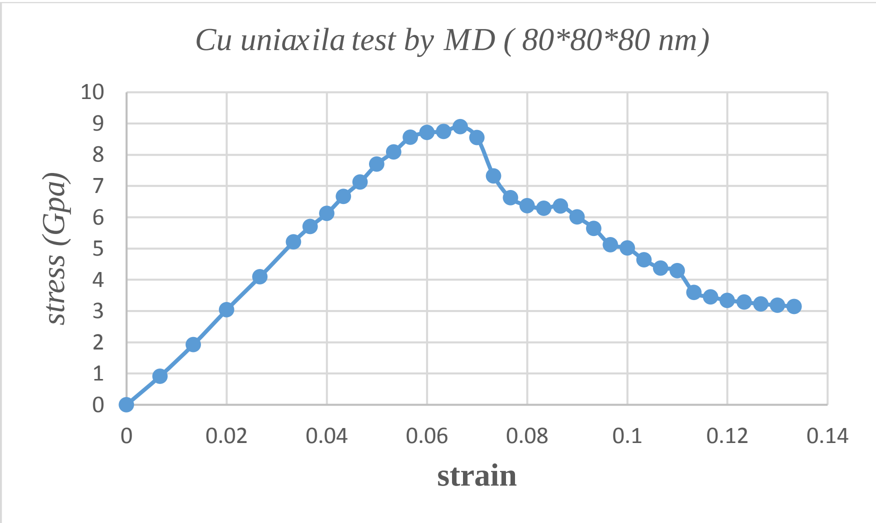

Fig. 1. Uniaxial test of Cu by MD method

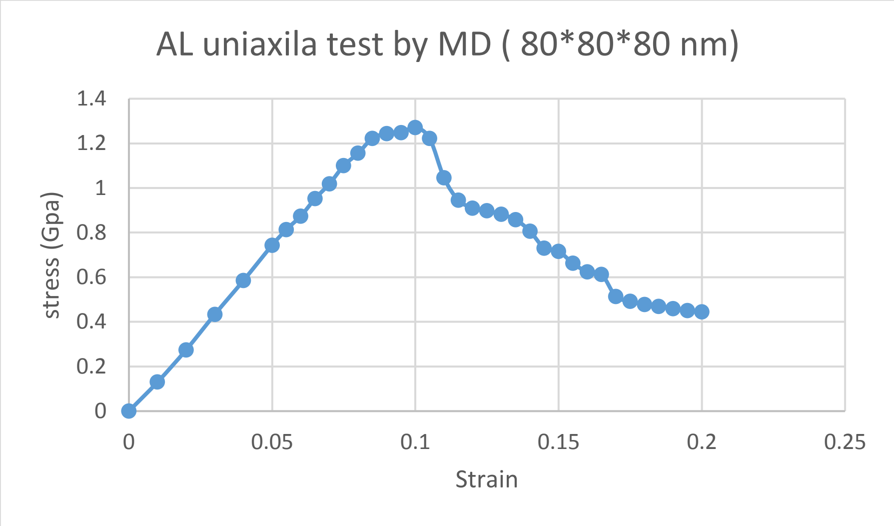

Fig. 2. Uniaxial test of Al by MD method

According uniaxial tests:
Young modulus of Al is 14.4Gpa and ultimate tensile strength is 1.24Gpa
Also, Young modulus of Cu is 151Gpa and ultimate tensile strength is 8.55Gpa

According equation (12) for AL/Cu composite with different carbon content, according M-T method properties of AL/Cu composite with different percentage of Cu is as below:

Table 1. Properties of AL/Cu alloy with a variety of percentages of Cu (MD and M-T methods).

Cu content (%)	1 %	2 %	6 %	8 %	10 %	15 %	20 %
Elastic modulus (GPa) (MD method)	17.101	17.504	57.98	58.73	60.098	61.983	65.207
Elastic modulus (GPa) M-T method)	14.51	14.63	15.11	15.36	15.62	16.33	17.13

According table1, elastic modulus of AL/Cu computed by two methods, up to 2% of Cu are very close to each other, but for higher percent of Cu, difference of two methods is more than 300%.

5- Conclusion

In this paper elastic modulus of AL/Cu has been compared using MD and M-T methods. Elastic modulus of AL and Cu has been obtained by MD method. According the results, elastic modulus obtained by two methods are very different specially for higher percentage of Cu. Since in M-t method intermolecular forces are not modeled, different results show that the effect of these forces are considerable. So, homogenization methods in macro scale such as M-T, is not suitable for nano scales.

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