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Atomistic investigation on the effect of temperature on mechanical properties of diffusion-welded Aluminium-Nickel

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Abstract: Atomistic investigation of diffusion welding between Aluminium and Nickel has been investigated, by means of Molecular Dynamics (MD) simulation. This study focuses on examining the effect of temperature on diffusion welding between Al-Ni for which it is still lacking. Employing several different temperatures, this study aims to examines the influence of temperature on the mechanical properties of diffusion-welded Al-Ni. The results have shown that the structural evolution significantly affected by the temperature. Better bonding structure is achieved as the temperature is increased which indicated by the wider interfacial region thickness on concentration profiles. However, as the temperature is increased lower ultimate tensile strength is obtained. Therefore, precisely estimates the temperature for particular materials in diffusion welding is a critical point. In this study, the optimum condition that fit on the diffusion welding process is when the temperature set on 500 K.

Keywords: Molecular Dynamics Simulation, diffusion welding, effect of temperature, Aluminium-Nickel, Mechanical Properties

1. Introduction

Joining two or more parts one of the industrial manufacturing processes required to satisfy the shape that either for functionality and appearance [1]. Several joining techniques have been proposed to satisfy these needs, and have shown very good performance for several applications, such as joining both similar and dissimilar metals [2]. By tracing the history of joining processes, at the first place, joining processes requires sort of fusion between the two, which in some cases will either reduce the performance of the material and sometimes also introducing several crack growth and embrittlement because it involves rapid solidification processes, thus heat treatment is necessary [3]. Furthermore, these techniques require other complex techniques to achieve an optimum parameter makes it economically not applicable [4]. Nowadays, solid-state welding in which the fusion of the materials during joining processes could be avoided is introduced. One of the methods of solid-state welding that is now widely used is diffusion-welding. Instead of only could be used for joining pure materials that are less complex, these techniques could also deal with the more complex materials ranging from alloys, compounds, several polymers, and so forth.

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Even though diffusion welding introduces many advantages compared to the conventional fusion welding, however, several parameters involved in this process have to be determined carefully. Therefore, finding the best parameters that fit with diffusion-welding is necessary to achieve the desired joint properties. The complexity of the joining process in the manufacturing industry has led to many investigations, especially to achieve the optimum condition that fit for joining particular material. The difference of material properties like physical and mechanical properties means different applied parameters to join those kinds of materials, including temperature and holding time. In diffusion welding, the temperature has shown very importantly, whether on the result of the structure or on the mechanical properties [5–8]. The outstanding properties of Ni and Al has been made it used in many applications such as for turbine airfoils [4], batteries [9–11], interlayers for some joining of dissimilar Ti-alloys [12, 13], coating of tungsten layer [14], and extreme ultraviolet (EUV) mask absorber [15], in which in some applications joining process is obviously necessary to satisfy both shape and appearance. However, the experimental works on the investigation of the joining process are known as the very costly as stated by the American Welding Society and thus the numerical method is expected to shorten those sorts of investigations [12].

The method of MD simulation is mainly built by the solution of the Newtonian equation of motion numerically which runs under a particular ensemble of atoms where can be used to investigate the material behaviors [16-29]. In the application of diffusion welding, there are several investigations using MD simulation like, Chen et al. when perform an investigation of diffusion bonding between Cu-Ag [5] and Cu-Al [6] which revealing the mechanism of diffusion bonding and shed light on the importance of pressure, temperature, and surface roughness on the process. On the mechanical properties, the tensile behavior of Ni-Al, Hu et al., [7] and current authors' previous study [26] have demonstrated the effect of temperature during a tensile test, that as the temperature increase the tensile strength is decreased. Even though the tensile test usually runs under room temperature (i.e. around 300 K), that study suggests to applied temperature properly, especially when the specific mechanical properties are expected. Zhang and Jiang [30] have demonstrated the effect of temperature on the final result of the diffusion-bonded structure and how the temperature and surface roughness affect the mean square displacement (MSD) which shows the diffusion ability of both stainless steel and pure Ni. The aim of the present research is to study the effect of temperature on the mechanical properties of diffusion-welded Aluminium-Nickel at atomic-level using Molecular Dynamics (MD) simulation

2. Simulation Modelling and Method

The interatomic potential embedded atom method (EAM) developed by Mishin in 2002 [31-32] and optimized in 2009 is adopted in this simulation. The total energy of a binary system A-B is represented as:

$$E_{tot} = \frac{1}{2}\sum_{ij}\Phi_{ai-aj}\left(r_{ij}\right)+\sum_{i}F_{ai}(\bar{\rho}_i) \quad (1)$$

Here Φ_{ai-aj} is a pair interaction potential as a function of the distance r_{ij} between atoms *i* and *j* that have chemical sorts $_{ai}$ and $_{aj}$ (= *A* or *B*) and F_{ai} is the embedding energy of an atom of a chemical sort $_{ai}$ as a function of the host electron density $\bar{\rho}_i$ induced at site *i* by all other atoms in the system.

Typically, classical MD simulation consists of three steps. They are initialization, production, and relaxation. In this study, first, the system is initialized with the NPT ensemble with room temperature and atmospheric pressure. This step is performed for a quite short time only to obtain an equilibrium condition; thus, the system is ready for the next production step. After the system is reaching an equilibrium state, constant pressure and temperature were applied. This stage is performed for 200 ps under the NPT ensemble. After diffusion welding is performed, the system then cooled down to 300 K to perform a tensile test. The data regarding the relationship between stress and strain which corresponds to the tensile test is generated along with the simulation during the tensile test. It has to be noted here that, during the initialization step, how long the simulation takes to prepare the equilibrated system is depending on the complexity of the system. It could be monitored in LAMMPS by the energy associated with the system, typically potential and kinetic energy. If the system is running for diffusion welding and subsequently tensile test whilst it is not equilibrated properly, it may be resulting in the inaccuracy of the output generated.

The system consists of Al (red) and Ni (blue) slab with a dimension of approximately 7.2 nm x 9.2 nm x 9.2 nm for both Ni and Al slabs and followed by fix slab in each edge of the material (cream white and white) as shown in Figure 1. Lattice constant applied to the mono-crystal Al and Ni is 4.05 and 3.52, respectively as investigated by the references [32, 33]. The boundary condition of the simulation is set to periodic in all three directions that are, x, y, and z of the models. This setting allows an atom to passes through one side of the cell and enters the cell from the opposite side with the same velocity, which allows the simulation cell to maintain a constant atom number during the process of deformation. Also, each atom in the simulation cell interacts with the closet image of the remaining atoms, thus the boundary effect on the simulation can be avoided. Meanwhile, to perform a simulation, a statistical ensemble is required to be defined to represent the state of the modeling system. This project will use Isobaric-Isothermal (NPT) with constant particle number, pressure, and temperature. Furthermore, since the algorithm used by LAMMPS is Verlet, which implements MD

simulation through the calculation and solution of the equation of motion, this algorithm is adopted in this project.

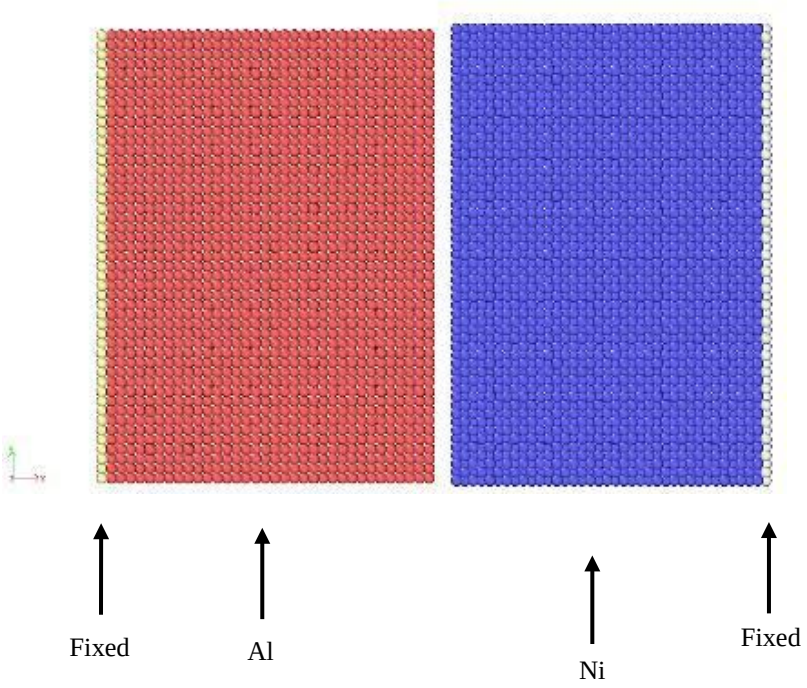

Fig. 1 – Initial condition of diffusion welding between Aluminium (red) and Nickel (blue) slabs with a fixed layer of atoms at the edge of each slab

At the ***initialization*** process, the pressure is maintained at atmospheric pressure using isobaric-isothermal (NPT) ensemble and the temperature is maintained at room temperature that is about 300 K for 10 ps. ***At the equilibrium*** state, the temperature is designed to vary from 300 K, 500 K, and 700 K. Meanwhile, the pressure is set at 100 MPa in the x-direction in each simulation for 200 ps. ***At the end*** of the simulation, the structure is cooled down from the highest temperature, for instance from the temperature of 700 K to 300 K, to perform a tensile test at a temperature of 300 K with a strain rate of 2.64e9/s while the timestep is set to 1 fs.

3. Results and Discussions

Displacement vector analysis is employed to the structural evolution during diffusion welding and tensile examination. This technique enables us to determine the displacement of each atom consists of the system, thus giving an insightful idea of whether or not a single atom experiencing long displacement and eventually to the bulk material for which the deformation occurs. The time evolution of diffusion configuration during diffusion-welding between Al- Ni is presented in Figure 2 at the time of 50 ps, 100 ps, 150 ps, and 200 ps and its corresponding diffusion interface is presented next to them. By examining the atomic view, it indicates that the temperature showing significant influence. The mechanism of bonding between the two slabs is promoted by the high diffusion energy affected by temperature, whilst the applied pressure introduces defects at the interface and thus promoting a wider area of deformation which eventually the greater number of atomic exchanges occur. Defects that promoted by the applied pressure at low temperatures (S1) which is 300 K has not shown a good bonding structure as indicated in the corresponding diffusion interface that the atomic exchange between two slabs (Al-Ni) is low. Rising the temperature to 500 K, the good bonding structure is greatly achieved, while at a temperature of 700 K the bonding structure is also good but it causing some unusual structural and defects. Point defects [34] that are promoted by both high temperature and pressure during diffusion welding have shown to make the interface of the two slabs way stronger than the base metal, and the reader will see that it affects to the deformation during the tensile tests never happen at the interface but instead at the Al base metal, which has the lowest strength compared to the Ni-base metal and the interstitial interface of the two materials. Furthermore, defects that occur during the diffusion welding of Al-Ni in every condition showing similar phenomena that it is not only affected by a single parameter but both temperature and pressure. This point defects that are promoted by those parameters could lead us to an insightful idea on how to improve the mechanical properties of materials more than what can be obtained by only the base pure metal. At this step, at the temperature of 500 K (Figure 2(b)), the best bonding structure is indicated by good atomic exchange and its behavior on the diffusion welding process is achieved compared to other temperatures. This study shows similar behavior with our previous study on the Cu-Al materials [35] and from Chen *et al*. with Cu-Ag in ref. [5].

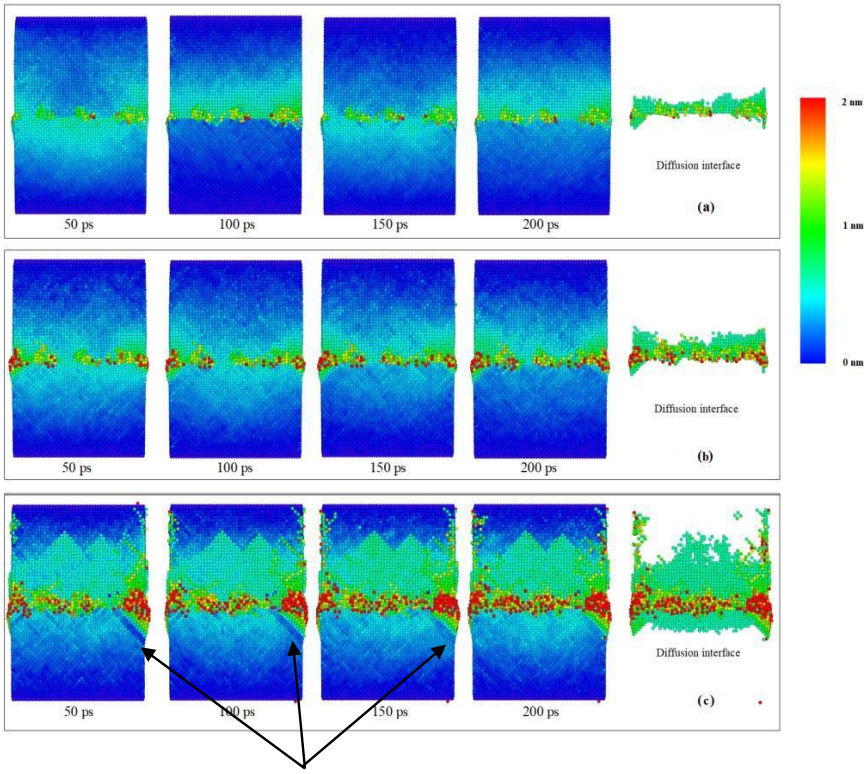

Fig. 2 - Displacement vector analysis of structural evolution during diffusion welding between Al and Ni at pressure of 100 MPa and hold for 200 ps with temperature at (a) 300 K, (b) 500 K, (c) 700 K, referred as S1, S2, and S3 and its corresponding diffusion interfaces

Figure 3 shows the comparison of concentration distribution between those mentioned conditions while Table 1 shows its corresponding approximated interfacial region thickness. As the temperature is increased, the diffusion zone is increased. On the temperature of 300 K, the thickness of the interfacial region reaches up to 3.94 Angstrom. However, on the temperature of 300 K, there is no significant difference in the concentration distribution profiles and the structural evolution as discussed previously. Since the thickness of the interfacial region is small, it should be considered that at this temperature is not fit for the application of diffusion welding between Al and Ni, because the small interfacial region thickness may promote the dissolving of the material. Meanwhile, for the welding on the temperature of 500 K and 700 K, excellent interfacial region thickness is obtained which are around 4.47 Angstrom and 8 Angstrom, respectively. To some level, a small diffusion zone means that the deformation due to temperature and pressure that induced to the system is less likely severe, thus reduce the strength of the interface. Meanwhile, a wider diffusion zone means the opposite, that it introduces more defects to the crystalline structure which in some cases makes the interface stronger that both base metal Al and Ni. Even though the temperature of 700 K shows outstanding results compared to the welding at 500 K, but as observed in the structural evolution, it causes some unusual initial deformation which may cause some other bigger deformation.

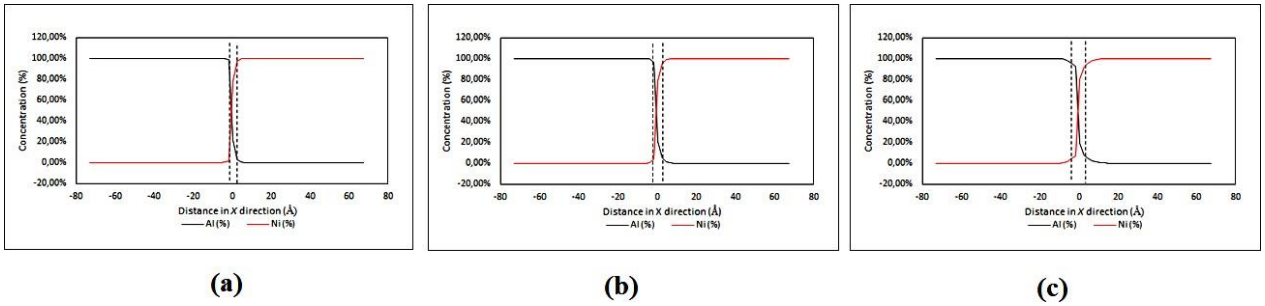

Fig. 3 - Concentration distribution of diffusion-welded Al-Ni at a pressure of 100 MPa and holding time of 200 ps with a variation on temperatures: (a) 300 K, (b) 500 K, and (c) 700 K

Table 1 - Interfacial region thickness of diffusion-welded at a pressure of 100 MPa and holding time of 200 ps with a variation on temperatures at 300 K, 500 K, and 700 K referred to as condition S1, S2, and S3, respectively

Condition	Interfacial region thickness (Å)
S1	3.937
S2	4.474
S3	7.996

During the tensile examination, the increase of temperature shows that the deformation becomes more random. Deformation at low temperature i.e. 300 K occurs around the interface, while as the temperature increases the deformation cannot be estimated where it will occur. However, the randomness of deformation during the tensile tests may happen due to the relatively high applied pressure, i.e. on 100 MPa. Since the applied pressure has a huge influence on the diffusion welding process [5], and thus the deformation and defects during the welding process may lead to the deformation during the tensile test. In this case, the sample of S3, with temperature of 700 K shows unusual deformation during diffusion welding processes (Figure 2(c)), it has shown that it has the worst behavior during tensile test (Figure 4(c)) while the best one is obtained on sample of S1 (Figure 2(a) & 4(a)). Even though the best and the worst behavior can be observed, however, the estimation of the behavior of diffusion-bonded Ni-Al cannot be performed, since it has shown no pattern that can be used for that. Furthermore, it is clear that the diffusion welding of Al-Ni is significantly influenced by temperature.

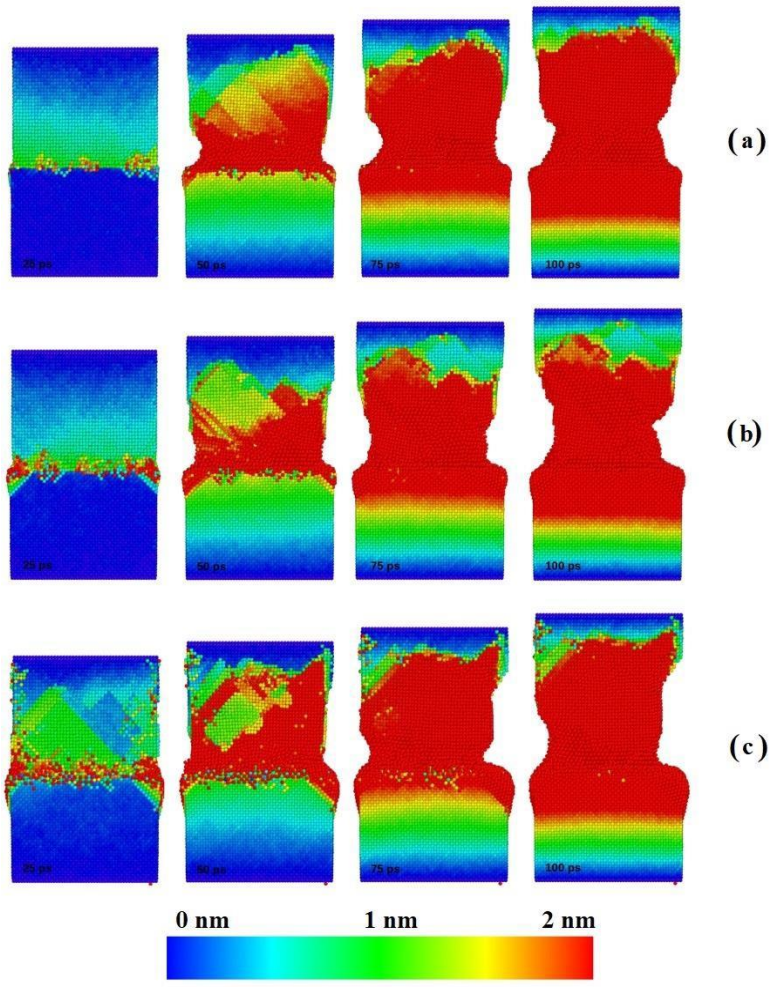

Fig. 4 - Structural evolution on the tensile test of diffusion-bonded of Al-Ni at various temperature of welding (a) 300 K, (b) 500 K, and (c) 700 K at a pressure of 100 MPa with a holding time of 200 ps referred as S1, S2, and S3 respectively

In an effort to find the best condition and figuring out other possible phenomena that occur, the simulation results of the condition of S1-S3 have been presented in Figure 5 as the stress-strain curve and in Table 2 as the ultimate tensile strength value. Welding on the temperature of 300 K shows great strength, since it has less defect compared to those with higher temperature, with ultimate tensile strength value of 4.4 GPa, respectively. However, the rising phase of the stress-strain curve on these two conditions (black and orange line) very fluctuates and thus this kind of condition should be avoided. Additionally, it confirmed that on the temperature of 300 K, there are no significant differences whether on the bonding structure, concentration profiles, or tensile examination. Meanwhile, on the temperature of 500 K shows far better ultimate tensile strength compared to the welding temperature on 700 K with 4.085 GPa and 3.2 GPa, respectively, with a difference up to 0.8 GPa. Also, the rising-phase shows good behavior that it is rises linearly, instead of fluctuating.

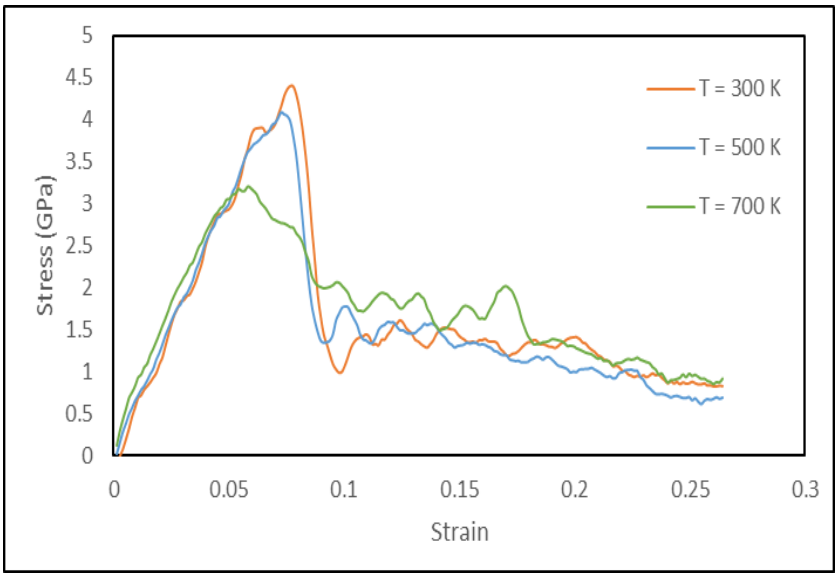

Fig 5 - Stress-strain curve of diffusion-bonded Al-Ni at a pressure of 100 MPa and hold for 200 ps with various temperatures referred to as S1-S3

Table 2 - Ultimate tensile strength of diffusion-bonded Al-Ni of condition S1-S3

Condition	Ultimate tensile strength (GPa)
S1	4.403
S2	4.085
S3	3.2

4. Conclusions

Molecular dynamics simulation of diffusion welding between Al and Ni has been performed and the effect of heating temperature during the welding process on the structural evolution, concentration profiles, and mechanical properties have been studied and the following conclusions can be outlined:

1. In terms of structural analysis, the increases in temperature promoting better bonding structure show by the wider diffusion zone on the concentration profiles. Point defects that are introduced at the interface of the two slabs, promoted by both temperatures make the deformation during the tensile test occur at the Al base metal and never at the interface.
2. As the temperature is increased, better concentration profiles are achieved and the interfacial region thickness becomes thicker. It also can be concluded that the system of Al-Ni becomes more sensitive at high temperature, thus it has to be precisely estimated.
3. Tensile examination showed that as the temperature is increased, the ultimate tensile strength is decreased. At low temperature (i.e. 300 K) the rising-phase of the stress-strain curve is fluctuating while it became better at the higher temperatures (i.e. 500 K and 700 K).

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