Atomistic investigation on the failure of diffusion-bonded Aluminium-Nickel

M Zaenudin[1], M N Mohammed[2], A Sunardi[1], S Al-Zubaidi[3], H Wijaya[4]

[1] Department of Mechanical Engineering, Faculty of Information Sciences and Engineering, Institut Teknologi & Kesehatan Jakarta, Jakarta 17411, Indonesia
[2] Department of Engineering & Technology, Faculty of Information Sciences and Engineering, Management & Science University, 40100 Shah Alam, Selangor, Malaysia
[3] Department of Automated Manufacturing Engineering, Al-Khwarizmi college of Engineering, University of Baghdad, Baghdad 10071, Iraq
[4] Department of Information System, Faculty of Information Sciences and Engineering, Institut Teknologi & Kesehatan Jakarta, Jakarta 17411, Indonesia

E-mail: zaenudin@itkj.ac.id

Abstract. This study presents an investigation on the role of temperature on the failure of diffusion-bonded Aluminium and Nickel. During diffusion bonding processes, where the bulk materials is subjected to join at the temperature of 300 K, 500 K, and 700 K with pressure of 10 MPa for 200 ps, the applied temperature is significantly influencing the final result of diffusion-bonded Al-Ni both in term of qualitative analysis (diffusion behaviour) and quantitative calculation (concentration distribution). In this case, as the temperature increased, the thickness of the interfacial region/diffusion zone is increased. However, when it is subjected to tensile test, the applied temperature is only has a significant impact to the ultimate tensile strength, that as the temperature is increased the ultimate tensile strength is decreased, but the applied temperature during diffusion welding is not influencing both time and strain value of the sample when it starts to failure.

1. Introduction

Manufacturing processes is involved many machinery processes, including welding and joining for particular materials such as alloys and stainless-steel [1]. Welding processes involved several parameters that are mostly determine the quality of the welded materials. For example, specific on the semisolid diffusion joining of stainless-steel, welding temperature and holding time is one of the main contributions of the welding quality [2]. However, these welding parameters is quietly complex due to the fact that it is not only involved the apparatus that are used in welding, but also depends on the used materials [3]. For every pure material, such as Cu, Al, Ni, the applied parameters are complex due to the difference of each melting point and will be even more complex for the alloys and compounds, since in those materials consists mostly more than one phase. In this case, this complexity is hard to overcome due to the fact that experimental investigations are known take a very long time to be

finished and moreover they are costly. Numerical simulation such as molecular dynamics (MD) simulation is then introduced to fill the gap between theoretical prediction and experimental investigation, and has shown a very good advantage, especially when it comes to the insight that is necessary to study the phenomena that are hard to be achieved by both theoretical and experimental investigations. In brief, classical MD simulation is a method that solved numerically Newtonian equation of motion for every atom consisting in the system, while it also integrates the ensemble condition of atoms. One of the most used atomic ensembles is Nose-Hoover thermostat in which the applied temperature is statistically calculated and controlled. Combining the control of temperature, pressure, and also the number of the atoms inside the system, NPT ensemble is practically used many times by researcher when they perform MD simulation for their study. When it comes to the failure phenomena, it's critical to know whether or not the applied parameters are the optimum one, and if not which one is at least has the nearest value. The question of how to manage to prevent failure for certain extreme applications, such as with very high tension or compression, however, is still on debate, especially when it is not the perfect bulk material one, but those materials that are being joint.

MD simulation is now having a broad range application in giving some important insight of the phenomena during joining processes, including in several joining techniques such as diffusion welding, explosive welding, friction stir welding, linear friction welding, cold-welding, nano-joining and thermal bonding [3]. Specific for diffusion bonding, Chen et al. has demonstrated that diffusion bonding of two dissimilar materials is influenced by both temperature and pressure [4, 5]. They have shown that the thickness of the diffusion interfaces is could be associated with a function of time and that compared to the influence of temperature, the pressure has less significant impact. However, as demonstrated by Mohammed et al. [2] the important of pressure is even less significant when it comes to the very high applied temperature, especially when this high temperature causes the materials enters the "mushy" or semi-solid phase. The atomic diffusion interface of W/Cu has been conducted by Xiu and Wu revealing the dominant influence of diffusivity of both atoms due to the transformation of temperature and defects around the interface [6] and that the diffusivity of W atoms is higher compared to Cu atoms as shown by a greater number of W atoms diffused into Cu. These important diffusion bonding parameters could lead to a better resistance of failure of the joints, and ultimately could better prevent the crack that propagate along the interface of the joints. As shown by MD simulation performed Hu et al. [7] the tensile behavior that are mostly fail at the interface is characterized by the applied temperature, that lower temperature during diffusion bonding of Ni-Al could lead to a better ultimate tensile strength and a better prevention to failure for some degree. Thus, the role of diffusion bonding parameters to the failure at the interface of joints are worth to investigate.

This study focuses on the revealing the role of temperature in preventing the failure of the joint interface, specifically for the diffusion-bonded Al-Ni, when it is subjected to high tension and compression load. By means of MD simulation, several simulations have been carried out and the results are presented. Discussions regarding its significant role are addressed in brief, and the conclusion has been drawn carefully.

2. Simulation modelling and method

The correctness and accuracy of an interatomic potential model are significantly determined the quality of the results that are carried out by MD simulation. Here, the author chooses interatomic potential model developed by Mishin [8]. This model, however, has been improved to accommodate the complexity of Al-Ni system in γ and γ' phase. Also, several investigations have shown successfully in giving an insight to the atomic phenomena during diffusion welding [7] and linear friction welding [9]. The simulation model consists of two monocrystalline Al & Ni with dimension of about 7.2 nm x 9.2 nm x 9.2 nm in x, y, and z direction, respectively, as shown in Figure 1. The fixed atoms are located at the edge of every slabs. The lattice constant as investigated by Mishin [8] is 3.52 and 4.05 for both Al and Ni, respectively. Periodic boundary condition is applied in all x, y, and z directions. Both Al and Ni monocrystalline are configured as [1 0 0] plane. These simulations are carried out with Verlet algorithm by using LAMMPS package, with the postprocessing software used

is OVITO. For the timesteps, here 1 fs timestep is applied for 200000 runs. It means that the total amount of the simulation is about 200 ps which are similar to those in [4–7, 10, 11]. The employed temperature is 300 K, 500 K, and 700 K with pressure is subjected with the same value which is 10 MPa. These differences in temperature are expected could reveal the role of temperature for certain range. Tensile test will be performed with strain rate value of 2.64e-9/s.

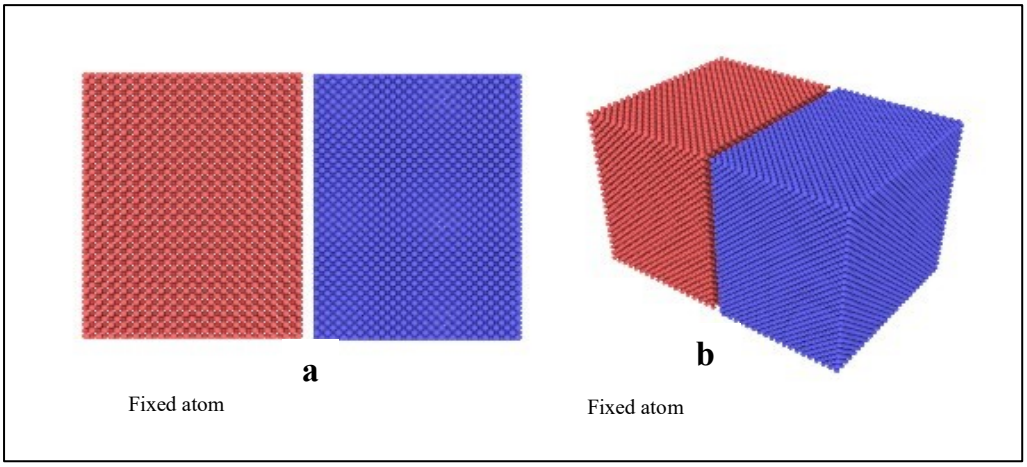

Figure 1. Two slabs of Al (red) and Ni (blue) with fixed atom each side with top (a) and angle (b) view.

3. Results and discussion

To reveal the dominant mechanism of temperature, its role to the failure of the joint interface, first the diffusion bonding simulation is carried out for all three condition. These results are presented in Figure 2. For the ease in mentioning the sample, hereafter, sample with temperature of 300 K will be mentioned as S1, sample with 500 K will be mentioned as S2, and sample with temperature of 700 K will be mentioned as S3. Figure 2 has shown that even for the diffusion-bonded process itself, the temperature has shown relatively significant role. As the temperature is increased, the more deformation is created along the interface and the more diffusion between both Al and Ni atoms occurs. More detailed value of this phenomena is shown in Figure 3 that is the concentration distribution of diffusion-bonded Al-Ni correspond to S1, S2, and S3. For the sake of ease, the thickness of the diffusion interface is put together with the other data in Table 1. Based on the Figure 3, a region is defined as interfacial region if the concentration of Al and Ni atoms are both over at 5% [4]

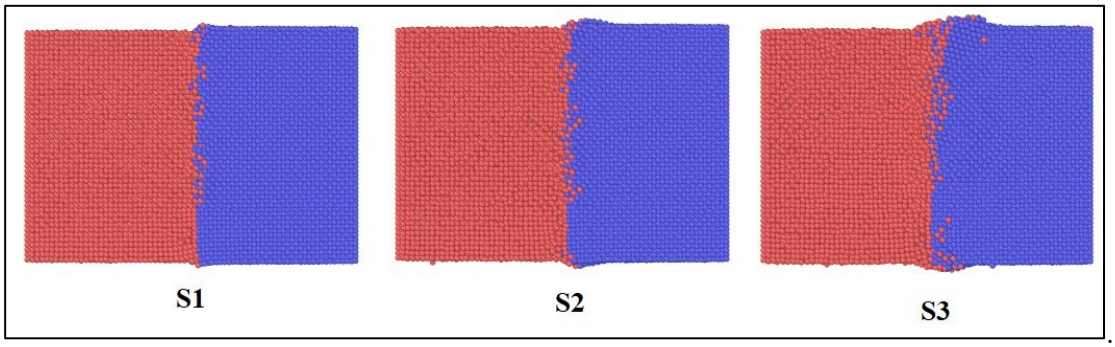

Figure 2. Diffusion-bonded of Al-Ni welded at pressure of 10 MPa with various temperature of (S1) 300 K, (S2) 500 K, and (S3) 700 K.

During diffusion bonding, the subjected temperature is very important, since the higher temperature will reduce the ability of bulk materials to prevent any deformation. As shown in Figure 1, the deformation is quite high for those with high temperature (S1 & S2) compared to the lower one (S1). As mentioned by ref. [6] the diffusion is mostly promoted by defects and are confirmed here. As the temperature is increased the bulk materials will become more sensitive to the subjected pressure and bonding of the other materials and finally the defects occur. These defects then promote the diffusion between both Al and Ni. In short, atomic diffusion between Al and Ni become higher as the temperature increased, since higher temperature results in defect that promote the mentioned atomic diffusion.

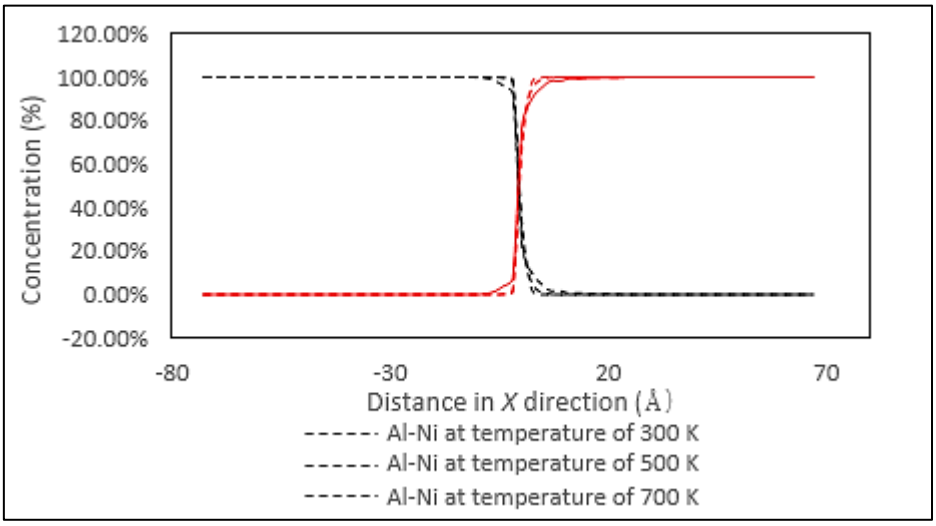

Figure 3. Concentration distribution of diffusion-bonded Al-Ni welded at pressure of 10 MPa with various temperature.

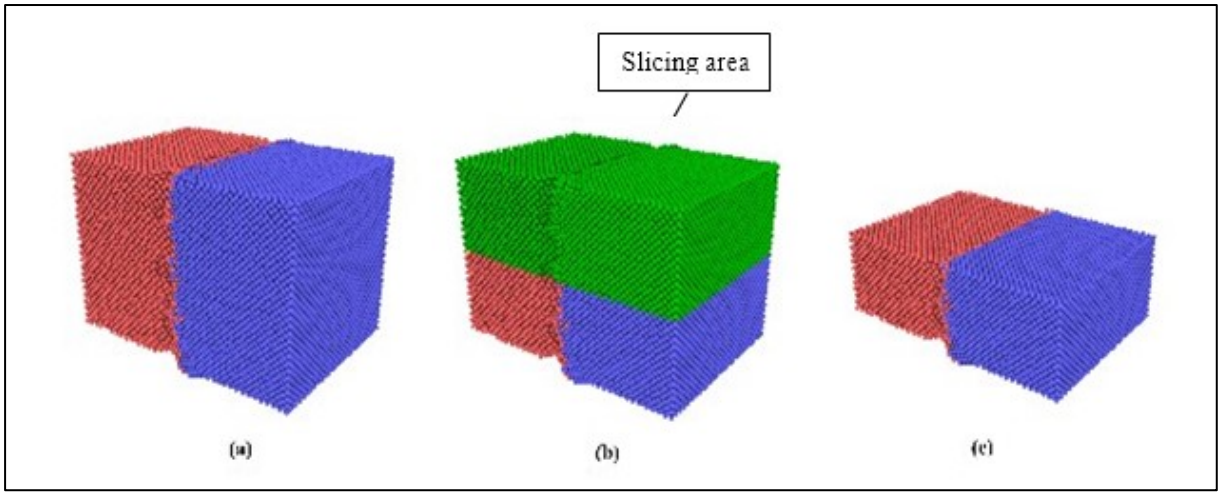

Figure 4. Slicing in the middle of diffusion-bonded Al-Ni.

Both qualitatively (Figure 2) and quantitatively (Figure 3) has shown the significant role of temperature on diffusion-bonded Al-Ni. However, to induce more specific results, here the sample is sliced in the middle of the sample as shown in Figure 4, to reveal the phenomena inside the bulk

materials. This technique allows us to reveal what is happening inside the bulk materials of Al and Ni, especially when it is subjected to tensile test. During tensile test, as shown in Figure 5, at time of 25 ps of tensile test, the bulk material has shown to be disordered and based on the data, for the sample of S2, its failure occurs when approximately at strain of 0.07128 at time of 27 ps. For the second line of figures in Figure 5, slip vector analysis techniques is used to view the magnitude of displacement. As the displacement is high, the more orange-red value it resulted.

For the sake of completeness, all three samples' stress-strain curve is depicted in Figure 6. It is shown that plastic deformation is not occur since most pure materials are not generating enough slip to accommodate indentation and deformation, thus it is brittle until a certain degree. However, since experimental works shows to deal with variation of grains, grain boundary, and including the slip analysis, the perfect crystalline used in this study is hard to be validated with most experimental data. Table 1 shows the results of the simulations. Although the temperature significantly influencing ultimate tensile strength, however, it is not influencing both time and strain values of samples when it begins to failure. Most of the three samples are in the same or at least has only a slight difference in terms of both time and strain values of the samples when it starts to fail. Instead of depending on the temperature, this strain value is most probably depending on the used materials. In this case, as we could see in Figure 5, the fracture site is located around the interface, and occurs in the Al side. However, concluding as discussed is not quietly proper and further study is necessary.

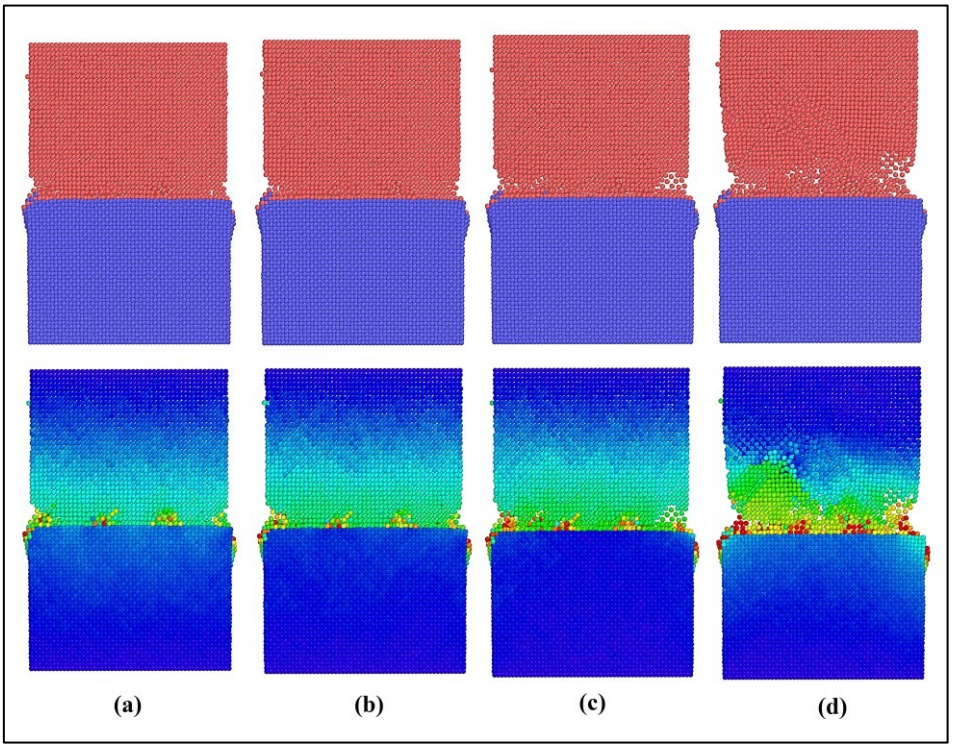

Figure 5. Sliced shows time evolution of the bulk diffusion-bonded Al-Ni for S2 during tensile test at time of (a) 15 ps, (b) 20 ps, (c) 25 ps, and (d) 30 ps.

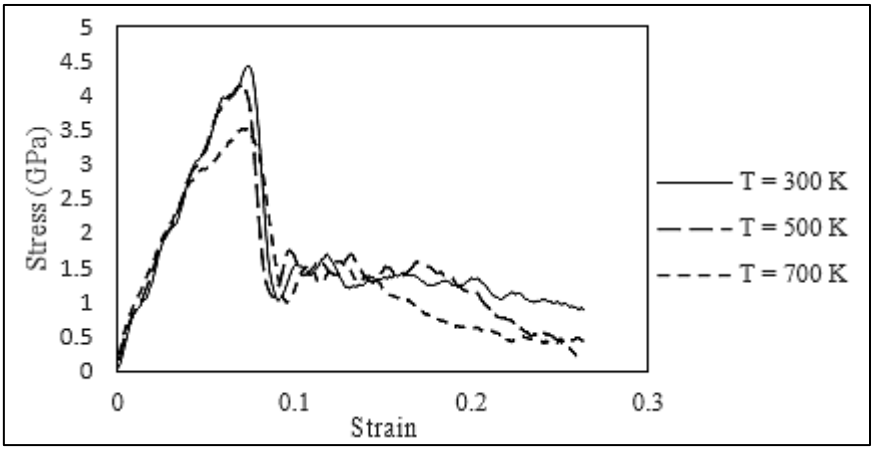

Figure 6. Stress-strain curve of diffusion-bonded Al-Ni in various temperature.

Table 1. Thickness of the diffusion interface, time value and strain value of the sample when it begins to failure and its corresponding ultimate tensile strength

Sample	Thickness of the diffusion interface (A)	Time value of failure (ps)	Strain value of failure	Ultimate tensile strength (GPa)
S1	3.997	28	0.07392	4.415
S2	4.485	27	0.07128	4.166
S3	8.087	27	0.07128	3.511

4. Conclusions

The role of temperature on the failure of diffusion-bonded Al-Ni has been conducted in terms of MD simulation and the results have been discussed. Although, several mentioned limitations are addressed clearly, however, this study conclude that temperature has significant impact on the result of diffusion-bonded Al-Ni, both in terms of diffusion behaviour as shown qualitatively and concentration distribution that quantitatively calculated. Although, the role of temperature during diffusion-bonding processes has shown significant impact on the bulk materials during tensile test, some values are not agreed to that results, that temperature is significantly influence the ultimate tensile strength, but is not significantly influence both strain and time value of the sample when it starts to failure.

5. References

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