Effect of Pressure on Mechanical Properties and Structural Evolution of Diffusion-Bonded Al-Ni: Insight from Molecular Dynamics Simulation

Mohamad Zaenudin[1], Mohammed N. Abdulrazaq[2], Salah Al-Zubaidi[3] and Adhes Gamayel[1]
[1]*Jakarta Global University, Indonesia*
[2]*Gulf University, Bahrain*
[3]*University of Baghdad, Iraq*

Keywords: Al-Ni Alloy, Diffusion Bonding, Mechanical Properties, Structural Evolution.

Abstract: Molecular dynamics simulation is a method to investigate the behavior of material at atomic scale. The application of molecular dynamics in investigation of the phenomena in joining processes at atomic scale has significantly increased. One of the advanced joining methods that nowadays used in joining dissimilar materials is diffusion bonding. This paper discusses the effect of pressure on the mechanical properties and structural evolution of diffusion-bonded Al-Ni. The results showed that both concentration distribution profiles and ultimate tensile strength showed excellent joints with low applied pressure (10 MPa), while higher welding pressure does not come with more benefits but decreasing the material performance. Defects and deformation that occurs during diffusion welding process has affected to the lower ultimate tensile strength which caused by the remarkably high applied welding pressure (100 MPa and 150 MPa) while at low applied pressure (10 MPa) defects and deformation is relatively low and thus affect to an excellent result in ultimate tensile strength value.

SCITEPRESS
SCIENCE AND TECHNOLOGY PUBLICATIONS

1 INTRODUCTION

The joining of metallic materials in industrial processes is particularly important due to the need to create desired shapes which involve two dissimilar materials. However, it has several difficulties for the dissimilar materials mean different properties, which lead to the other different applied parameters in joining processes, like temperature, pressure, and holding time. Diffusion bonding is introduced to solve this kind of problem when the two dissimilar joining of materials is necessary (Akca & Gu Gürsel, 2015, Cooper & Allwood, 2014). To achieve optimum conditions using this method, several experimental investigations are necessary. It is well known that experiments on advanced material science take huge amount of cost and time, thus a few alternatives of numerical methods are introduced. These methods have shown promising advantages to enhance the needs of joining dissimilar materials with optimum condition.

Apart from the other numerical methods such as finite element method (FEM), continuum modeling, and Monte Carlo simulation, another numerical method like Molecular Dynamics (MD) simulation has shown an increasing interest by researchers extensively, especially in joining processes (Zaenudin et al., 2018, Zaenudin et al., 2022, Zaenudin et al., 2020). The core idea of this method is the solution of the Newtonian equation of motion numerically, which runs under a particular ensemble of atoms like microcanonical and canonical ensemble. These equations are then numerically integrated for a tiny range of time (about $2-3\,fs$), and through the observation of elapsed time the equilibrium of the statistical averages is computed as interim averages. This method offers a new way to observe and analyze the behavior of material at atomic scales, which nowadays become more important due to the requirement of precision and accuracy of the estimation properties and applied parameters for application like joining processes. Specific on joining process using diffusion bonding technique, MD simulations was able to deliver several phenomena and mechanisms that have significance influence to the final result of the as

Zaenudin, M., Abdulrazaq, M., Al-Zubaidi, S. and Gamayel, A.
Effect of Pressure on Mechanical Properties and Structural Evolution of Diffusion-Bonded Al-Ni: Insight from Molecular Dynamics Simulation.
DOI: 10.5220/0011770300003575
In *Proceedings of the 5th International Conference on Applied Science and Technology on Engineering Science (iCAST-ES 2022)*, pages 337-341
ISBN: 978-989-758-619-4; ISSN: 2975-8246
Copyright © 2023 by SCITEPRESS – Science and Technology Publications, Lda. Under CC license (CC BY-NC-ND 4.0)

welded materials, whether it is based on the structural evolution during joining processes, diffusion mechanism based on the self-diffusion of material, or even the phenomena that contribute to the mechanical properties and structural evolution of the as received material compared to the as received material. Chen et al. has conducted research on diffusion bonding of Cu-Ag (Chen et al., 2005) and Cu-Al (Chen, 2007) and has successfully investigated the dominant mechanism during diffusion bonding. Hu et al. (2013) have demonstrated the temperature-dependence of the mechanical properties of diffusion-bonded Ni-Al. The significance effect of temperature also has been demonstrated by Zhang and Jiang (Zhang and Jiang, 2013) on the stainless-steel and pure Ni materials by simply extracting the displacement of atoms into calculation of mean square displacement (MSD).

Based on the broad range application of Ni-Al materials like turbine blades (Darolia et al., 2012), batteries (Mukherjee, 1998, Young, 2013, Young, 2013), multilayers for joining of different Ti-alloys (Simões et al., 2010, Simões et al., 2018), coating with a tungsten layer (Ramos et al., 2017), and mask absorber of extreme ultraviolet (EUV) radiation [17], this paper presents an investigation on the effect of applied pressure on the structural evolution and mechanical properties of diffusion bonding between Al and Ni. The structural analysis is obtained by employing a vector displacement analysis tool (Stukowski, 2010) based on its slip vector properties (Zimmerman et al., 2001) and the other properties, such as mechanical and physical properties, are presented in curves and tables.

2 SIMULATION PROCEDURE

This study has been performed by using LAMMPS software package (Plimpton, 1994). Every movement and energy of atoms in the molecular dynamics simulation system is defined by an interatomic potential model, thus the importance of interatomic potential is crucial. Embedded atom method is one of the well-established interatomic potentials. In EAM, the total energy of a binary system A-B is defined as:

$$E_{tot} = \frac{1}{2}\sum_{ij}\Phi_{a_i-a_j}\left(r_{ij}\right) + \sum_{i}F_{a_i}\left(\underline{\rho}_i\right) \qquad (1)$$

Here $\Phi_{\square_{\square}-\square_{\square}}$ is the interaction of pair potential as a function of distance r_{ij} between atoms $\square$ and $\square$ that have chemical sorts $\square_{\square}$ and $a_j(= A\ or\ B)$ and $\square_{\square_{\square}}$ is the embedding energy of an atom of chemical sort a_i as a function of the host electron density $\underline{\rho}_{\square}$ induced at site $\square$ by all other atoms in the system. The well-established EAM developed by Mishin (Mishin, 2002) is adopted in this simulation.

In this simulation, two slabs of Al and Ni is deployed in this simulation with approximate dimension of $7.2\ nm\ x\ 9.2\ nm\ x\ 9.2\ nm$ for both Al and Ni slabs and followed by fixed atoms in the edge of each slab as shown in Figure 1. Lattice constant of both monocrystalline Al and Ni slabs are 4.05 and 3.52, respectively, as reported by refs. (Mishin et al., 2022, Mishin et al., 2004). Boundary condition is set to periodic in all three directions x, y, and z. This configuration allows atoms pass through the sides of the cell and entering on the opposite side with the exactly with the same condition and properties such as velocity and internal energy, and the system can also maintain the number of atoms. In addition, each atom in the simulation cell interacts with the closest image of the remaining atoms. This would then avoid the boundary effects on the simulation. Isothermal-isobaric ensemble with Number, Pressure, and Temperature (NPT) controlled is employed in this simulation.

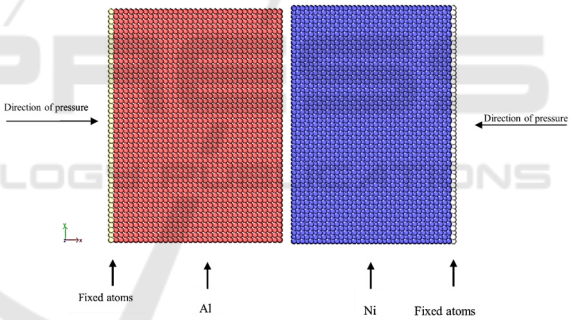

Figure 1: Planar view of simulation model of Al (red) and Ni (blue) slabs paired with fixed atoms in each edge of the slab.

The initialization process is started with low temperature and pressure and maintained for 10 picoseconds. This initialization process is a key to the achieve an equilibrated system before the production process. Equilibrium state is indicated by the minimal amount of potential and kinetic energy. For production process, the temperature is designed at $500\ K$, while the pressure is set to three different levels, they are $10\ MPa$, $50\ MPa$, $100\ MPa$, and $150\ MPa$ in x direction for $200\ ps$. Finally, the structure is cooled down from temperature of $500\ K$ to an ambient temperature to perform a tensile test with a strain rate of $2.64e9/s$. The timestep of all simulation process is set to $1\ fs$.

3 RESULT AND DISCUSSION

Figure 2 shows the structural evolution of diffusion-bonded Al-Ni of four different conditions namely S1, S2, S3, and S4. On the planar view (bottom) of the as welded Al-Ni, it can be observed that there is no major difference between all four different conditions. However, at the respective diffusion interface (above) it can be observed that the applied pressure is shown to deform the Al slab (top) as the pressure is increased. Even though higher pressure influences the diffusion interface by deforming it, the atomic exchange which is mostly shown by red-colored atoms has no significant difference. It can be concluded that the applied pressure (50 MPa to 150 MPa, S2-S4), instead of promoting into a better bonding structure, mostly only deformed the Al slab due to the lower strength of Al compared to Ni. In addition, most of both Al-Ni slabs maintain their FCC structure which is shown by the blue-colored atoms. It indicates the applied pressure and temperature for 200 ps has an excellent bonding structure, except for the highest applied pressure which can be observed had significant defects and deformations located on the interface. At this step, it is suggested to apply low pressure if the temperature is high enough to allow diffusion between two dissimilar materials to be joined.

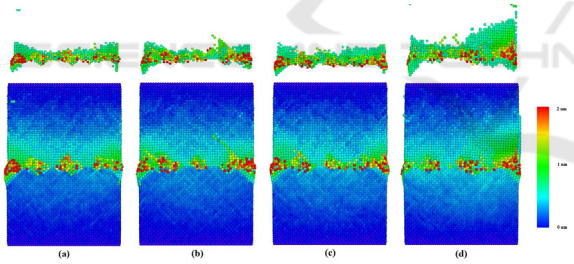

Figure 2: Planar view of displacement vector analysis of diffusion-bonded between Al and Ni at temperature of 500 K and hold for 200 ps with pressure at (a) 10 MPa, (b) 50 MPa, (c) 100 MPa, and (d) 150 MPa (upper image) and its respective diffusion interface (lower image).

The concentration distribution curve is depicted in Figure 3 and Table 1 shows its corresponding interfacial region thickness. Interfacial region is defined as the area within the diffusion zone in which the concentration of a material is more than 5%. Table 1 is obtained from the concentration distribution data with proper estimation. Even though the highest value applied pressure shown has the widest interfacial region area as listed in Table 1, the difference between the other values of interfacial region thickness is small. For the lowest value of applied pressure (i.e., S1 with 10 MPa) to the highest value of applied pressure (i.e., S4 with 150 MPa), the difference in interfacial region thickness is only about 0.1 Angstrom. While S1 also has the highest value among the other two conditions namely S2 and S3 (50 and 100 MPa). The applied pressure at this level of temperature (500 K) has no significant effect on the result of diffusion bonded Al-Ni, thus the lowest applied pressure and vast amount of heat is suggested.

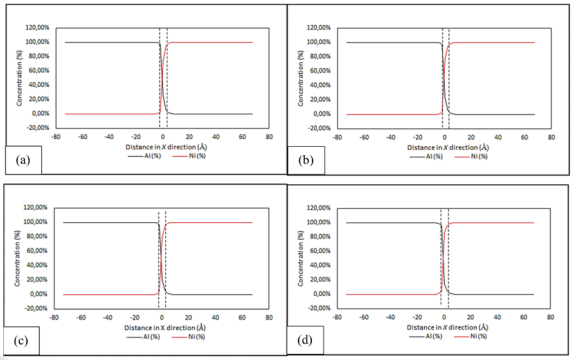

Figure 3: Curve of concentration distribution of four different welding conditions at temperatures of 500 K with holding time of 200 ps and variation on pressure (a) 10 MPa, (b) 50 MPa, (c) 100 MPa, and (d) 150 MPa referred as sample $S1$, $S2$, $S3$, and $S4$, respectively.

Table 1: Approximated interfacial region thickness of four different conditions namely S1, S2, S3, and S4.

Condition (s)	Interfacial region thickness (Å)
S1	4,485838854
S2	4,383252102
S3	4,474520861
S4	4,585924319

After the final diffusion-bonded result is acquired, the system is then subjected to a tensile test. The structural evolution of diffusion-bonded Al-Ni depicted in Figure 4. The image is captured when the as-welded Al-Ni subjected to tensile test at the time of 25 ps, 50 ps, 75 ps, and 100 ps. At time of 25 ps, condition S4 showed the worst behavior owing to the huge number of defects and deformations during the welding process and thus influencing the sample during tensile test. While the other sample namely S1-S3 still maintain their structure, the sample S4 deformed at the interface. This behavior proves that during diffusion welding, the applied welding pressure of 150 MPa is too high and is not suggested. As the tensile test goes on to time of 50 ps to 100 ps, sample with the lowest applied welding pressure

which is 10 MPa (S1) has the best behavior, as shown it mostly maintain the structure and the deformation during tensile test shown relatively small compared to the other sample. For the tensile test result, the stress-strain curve is presented in Figure 5. The ultimate tensile strength is obtained from the lowest applied pressure. The route with the lowest applied pressure has the best results and behaviors, while the highest one shows the worst. However, an inverted behavior is obtained for pressures of 50 MPa and 100 MPa which indicate the sensitivity of the system as the pressure is increased. The behavior of the system becomes harder to estimate as the pressure is increased.

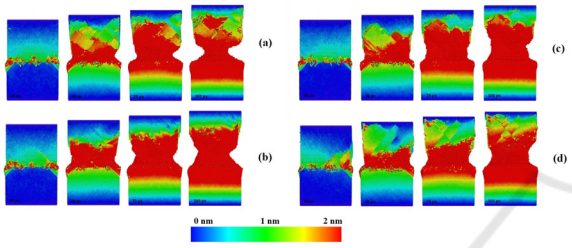

Figure 4: Planar view of displacement vector analysis of structural evolution of diffusion-bonded Al-Ni with four different welding conditions (a) S1, (b) S2, (c) S3, and (d) S4 subjected to tensile test.

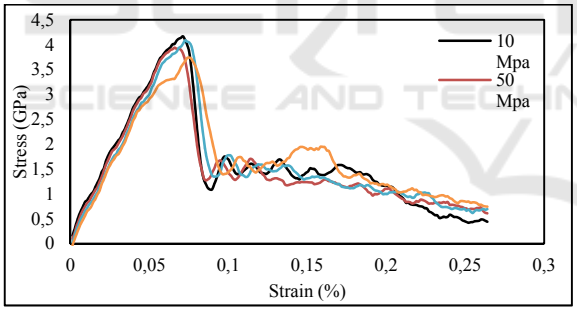

Figure 5: Stress-strain curve of as-welded Al-Ni with four different welding conditions (S1-S4) subjected to tensile test.

During diffusion welding, there are at least three parameters that contribute to the result of the as welded materials, they are temperature, holding time, and pressure. The effect of pressure in this study indicates significant to the performance of the as welded material. For example, when the applied welding pressure is too high, even before being subjected to tensile test defects and deformations has occurred and it has affected the lower ultimate tensile strength during tensile test. Thus, diffusion welding with relatively high pressure is not suggested. Another aspect to be considered when the applied welding pressure too high is the ability of the welded materials to recover their structure is not utilized, which means if defects are occur during diffusion bonding, the structure will keep the defects or even make it bigger and thus affecting the ultimate tensile strength of the as welded material. Instead of applying high welding pressure which has no significant difference in term of benefits, applying low welding pressure, such as 10 MPa, is suggested because it has indicates resulting the highest ultimate tensile strength and excellent bonding structure while interfacial region thickness shown indication the ability to maintain its bonding that can avoid any dissolving phenomena. This low-pressure diffusion-bonding could be used for nano-scale welding (Lu et al., 2010) to macroscale. Even though the applied welding pressure is low, the other parameters like temperature and pressure still need to be estimated properly. Here, at a temperature of 500 K, good joints are achieved with a relatively wide enough interfacial region and relatively high ultimate tensile strength. As reported in refs. (Chen et al., 2007, Hu et al., 2013), the influence of temperature will decrease the ultimate strength, thus the applied heating temperature has to be considered properly. If the temperature is high enough to promote diffusion between the two dissimilar materials, thus avoiding making the temperature higher is reasonable.

4 CONCLUSIONS

This study has successfully examined the effect of pressure on diffusion bonding between Al and Ni. The conclusions are drawn as listed below:

1. From the concentration distribution profiles, the welding at low pressure with high enough holding time (200 ps) and temperature (500 K) shows good joints and it is enough to avoid any dissolving phenomena indicated by the high value of thickness of the interfacial region. Instead of performing at high pressure that shows no significant impact, the welding of Al-Ni is better selecting high enough temperature and long enough holding time.

2. If the pressure is high enough to perform diffusion bonding of Al-Ni and has shown satisfactory results on concentration profile, it is a good decision to consider the lowest value of pressure to avoid deformation/defect and efficiency of resources. Another reason to consider the lowest possible applied pressure is that with the lowest value, as discussed in this section, the highest value of ultimate tensile strength is achieved.

ACKNOWLEDGEMENTS

The authors would like to acknowledge the support from Jakarta Global University and Management & Science University throughout this project.

REFERENCES

Akca, E., & Gürsel, A. (2015). The importance of interlayers in diffusion welding-A review. *Periodicals of Engineering and Natural Sciences (PEN)*, *3*(2).

Liu, Z., Nouraei, H., Papini, M., & Spelt, J. K. (2014). Abrasive enhanced electrochemical slurry jet micro-machining: Comparative experiments and synergistic effects. *Journal of Materials Processing Technology*, *214*(9), 1886-1894.

Zaenudin, M., Mohammed, M. N., & Al-Zubaidi, S. (2018). Molecular dynamics simulation of welding and joining processes: an overview. *Int. J. Eng. Technol*, *7*(4), 3816-3825.

Zaenudin, M., Abdulrazaq, M. N., & Al-Zubaidi, S. S. (2022). A Review on Molecular Dynamics Simulation of Joining Carbon-Nanotubes and Nanowires: Joining and Properties. *International Journal of Integrated Engineering*, *14*(4), 137-159.

Zaenudin, M., Abdulrazaq, M. N., Al-Zubaidi, S., & Sunardi, A. (2020). Atomistic Investigation on the Role of Temperature and Pressure in Diffusion Welding of Al-Ni. *Journal of Engineering & Technological Sciences*, *52*(2).

Chen, S. D., Soh, A. K., & Ke, F. J. (2005). Molecular dynamics modeling of diffusion bonding. *Scripta Materialia*, *52*(11), 1135-1140.

Chen, S., Ke, F., Zhou, M., & Bai, Y. (2007). Atomistic investigation of the effects of temperature and surface roughness on diffusion bonding between Cu and Al. *Acta Materialia*, *55*(9), 3169-3175.

Hu, Z., Zhang, J., Yan, Y., Yan, J., & Sun, T. (2013). Molecular dynamics simulation of tensile behavior of diffusion bonded Ni/Al nanowires. *Journal of Mechanical Science and Technology*, *27*(1), 43-46.

Zhang, Y., & Jiang, S. (2018). Atomistic investigation on diffusion welding between stainless steel and pure Ni based on molecular dynamics simulation. *Materials*, *11*(10), 1957.

Darolia, R., Walston, W. S., & Nathal, M. V. (1996). NiAl alloys for turbine airfoils. *Superalloys*, *1996*, 561-570.

Mukherjee, A. B. (1998). Nickel: a review of occurrence, uses, emissions, and concentration in the environment in Finland. *Environmental Reviews*, *6*(3-4), 173-187.

Young, K. H. (2016). Research in nickel/metal hydride batteries 2016. *Batteries*, *2*(4), 31.

Simões, S., Viana, F., Ventzke, V., Koçak, M., Sofia Ramos, A., Teresa Vieira, M., & Vieira, M. F. (2010). Diffusion bonding of TiAl using Ni/Al multilayers. *Journal of Materials Science*, *45*(16), 4351-4357.

Simões, S., Viana, F., Ramos, A. S., Vieira, M. T., & Vieira, M. F. (2018). Microstructural characterization of dissimilar titanium alloys joints using Ni/Al nanolayers. *Metals*, *8*(9), 715.

Ramos, A. S., Maj, L., Morgiel, J., & Vieira, M. T. (2017). Coating of Tungsten Wire with Ni/Al Multilayers for Self-Healing Applications. *Metals*, *7*(12), 574.

Luong, V., Philipsen, V., Hendrickx, E., Opsomer, K., Detavernier, C., Laubis, C., ... & Heyns, M. (2018). Ni-Al alloys as alternative EUV mask absorber. *Applied Sciences*, *8*(4), 521.

Stukowski, A. (2009). Visualization and analysis of atomistic simulation data with OVITO–the Open Visualization Tool. *Modelling and simulation in materials science and engineering*, *18*(1), 015012.

Zimmerman, J. A., Kelchner, C. L., Klein, P. A., Hamilton, J. C., & Foiles, S. M. (2001). Surface step effects on nanoindentation. *Physical Review Letters*, *87*(16), 165507.

Prieve, D. C., & Russel, W. B. (1988). Simplified predictions of Hamaker constants from Lifshitz theory. *Journal of Colloid and Interface Science*, *125*(1), 1-13.

Mishin, Y., Mehl, M. J., & Papaconstantopoulos, D. A. (2002). Embedded-atom potential for B 2− NiAl. *Physical review B*, *65*(22), 224114.

Mishin, Y. (2004). Atomistic modeling of the γ and γ′-phases of the Ni–Al system. *Acta Materialia*, *52*(6), 1451-1467.

Lu, Y., Huang, J. Y., Wang, C., Sun, S., & Lou, J. (2010). Cold welding of ultrathin gold nanowires. *Nature nanotechnology*, *5*(3), 218-224.

Plimpton, S., & Root, J. (1994). Materials and strategies that work in low literacy health communication. *Public Health Reports*, *109*(1), 86.