Atomistic Investigation on the Role of Temperature and Pressure in Diffusion Welding of Al-Ni

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Highlights:

- Mechanical properties of diffusion-bonded Al-Ni are more significantly influenced by temperature, while pressure has a less significant impact.
- A higher temperature applied during diffusion welding results in focusing the deformation around the diffusion zone.
- Molecular dynamics simulation is an effective method that can be used to gain an insight into the material's behavior at the atomic scale, which may improve the mechanical properties at the macro scale, especially those in which diffusion welding phenomena are involved.

Abstract. This paper presents an investigation of diffusion welding of aluminum and nickel at the atomic scale by utilizing molecular dynamics simulation. By employing several temperature and pressure values, the significant influence of the two could be obtained and thus the optimum parameter values could be obtained. The results showed that the bonding mechanism is mostly promoted by Al, in which the deformation and defects are involved. The results on both the mechanical properties and the evolution of the diffusion configuration showed that temperature has more impact compared to pressure. It was indicated that by raising the temperature to 700 K with the lowest pressure (50 MPa), both the mechanical properties and the evolution of the diffusion configuration showed a relatively significant difference. On the one hand, the deformation that occurs during welding, which is mostly caused by raising the temperature, obviously promotes joining and therefore more joining depth can be achieved, although it results in a curved diffusion zone at the interface. On the other hand, it also leads to a lower ultimate tensile strength. During the tensile test, raising the temperature also led to focusing the deformation in the diffusion zone, while a lower temperature resulted in a wider area of deformation.

Keywords: *Al-Ni; diffusion welding; molecular dynamics simulation; pressure; temperature.*

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1 Introduction

The Industrial Revolution 4.0 is creating huge differences, from an economic as well as a social perspective. This is related to several major manufacturing processes, including welding and joining processes in which two materials are combined to achieve particular shapes and properties, leading it to become one of the main activities in manufacturing processes [1]. However, now that several classical welding techniques that involve the metallic interlayer can successfully combine metals with relatively low complexity, we currently face a new problem. To achieve structural metals that can be used for various applications, ranging from automotive, aviation, industrial manufacturing tools, architectural buildings that involve a concrete structure, and so forth, metallic materials are now becoming more complex than ever before. This is due to new alloying designs that involve many different chemical compositions to achieve specific mechanical and physical properties. The complexity of materials that undergo several phase changes in which their structural properties change due to external conditions, such as temperature and pressure, poses new problems to the manufacturer when it comes to welding and joining. Classical welding techniques are no longer suited for these complex materials.

One of the advanced welding techniques that are now broadly used in manufacturing processes is solid-state welding, including diffusion welding. In diffusion welding, two materials are combined directly by introducing both high temperature and pressure. Thus, the interlayer that is used by classical welding techniques, most of which deteriorate the mechanical properties of the as-welded materials, is no longer necessary.

However, effectiveness and efficiency of diffusion welding have to be achieved first before it can be broadly applied in manufacturing processes to join particular materials. Optimum parameter values that introduce both effectiveness and efficiency can lead to the reduction of resources and the most desired properties of the as-welded material. Long-standing research has been conducted to develop this method. Unfortunately, experimental investigation to accomplish the best parameter values for this technique is costly and consumes a relatively large amount of time. To overcome this issue, several numerical methods are available to help in the determination of the best parameter values for a certain application. They are the Monte Carlo simulation, finite element method, continuum method, and molecular dynamics simulation. For a particular application, such as the investigation of welding of various materials at the atomic level, molecular dynamics (MD) simulation not only comes with several advantages but also has been proven to be reliable [2]. MD simulation has several major advantages over other methods, such as being able to be executed at the nano scale or even at the atomic scale [3].

The capability of handling various broad applications of materials investigations and the advantages offered by MD simulation has led many studies to adopt this method, including those that were conducted to figure out the influence of several parameters in various welding techniques that are critical during the process of welding and their impact on the mechanical properties. Specifically for the diffusion welding process, MD simulation has shown great results, which not only revealed atomistic behavior, as it can be visualized by several software tools [4,5], but some mechanical properties can also be estimated and validated by this method [6-17].

Two investigations by Chen, *et al.* have conducted MD simulation of diffusion bonding of Cu-Ag [18] and Cu-Al [19], revealing a dominant impact of temperature on the final result of diffusion-bonded materials and a mechanism in which increasing the temperature leads to an increase in the interfacial region thickness and temperature has more impact than pressure to promote welding. The atomistic diffusion behavior of W-Cu revealed by Xiu & Wu [20] shows that the diffusivity of the materials is important in the diffusion bonding process. In their simulation, the activation energy of the W atoms was larger than that of the Cu atoms and thus the Cu atoms promoted more diffusion into W, promoted by defects in the crystal surface. Concerning the tensile behavior, Hu, *et al.* [20] have investigated the tensile strength of diffusion bonded Ni-Al and revealed that the deformation that occurred in the sample welded with higher temperature decreased the tensile strength.

However, a study that compares both the effect of temperature and pressure of diffusion welding between Ni and Al is still lacking. It is known that Al-Ni is a material that has a wide range of applications due to its excellent properties. It has been used as one of the main materials in several promising alloys for various applications, such as turbine airfoils [21], battery electrodes [22,23], an interlayer for joining dissimilar Ti-alloys [24,25], coating of tungsten layers [26], and so on. Long-standing Al-Ni research has shown the advantages of Al-Ni alloys so that more applications of it will be conducted soon, for instance in extreme ultraviolet (EUV) mask absorbers [27].

In several applications, the joining process must be performed so that it satisfies the shape of the materials and the manufacturing processes. Both advantages of molecular dynamics simulation and the excellent properties of Al-Ni led to this study. The purpose of this study was to compare the effect of two welding parameters, i.e. temperature and pressure, and to figure out the deformation of the materials that occurs during the welding processes of aluminum and nickel. Furthermore, the welding temperature and pressure that contribute to the tensile behavior are discussed in detail.

2 Simulation Modelling and Method

One of the most important aspects that contributed to the quality of the result of the molecular dynamics simulation method is their adopted interatomic potential. In this study, the interatomic potential proposed by Mishin, *et al.* [28] was adopted. This potential was constructed using experimental data and a large set of *ab initio* (LAPW) structural energies. The first developed interatomic models of EAM B2 Al-Ni have been improved to fit more complex systems of Ni-Al, such as for γ and γ′ phase. In this study, the latest interatomic potential of Al-Ni developed by Mishin in 2009 was used for the simulation. This interatomic potential also has been used in several investigations reported as successful that employed MD simulation, such as for diffusion-bonding of Ni-Al [20] and linear friction welding of Ni-Al [29].

The simulation system consisted of two slabs of monocrystalline Ni and Al with a dimension of approximately 7.2 nm x 9.2 nm x 9.2 nm for both the Al and the Ni slab. A fixed layer of atoms was configured on the edge of each atom, mimicking the boundary of the system, as shown in Figure 1. The lattice structure of Al and Ni was configured as a face centered cubic (FCC) with a lattice constant of 4.05 and 3.52, respectively, as investigated by Mishin in Ref. [28]. The periodic boundary condition (PBC) was applied in all three directions, x, y, and z. Both monocrystalline Al and Ni atoms were configured on [1 0 0] planes. In the present work, the LAMMPS software package was used, since it has many features and is very suitable for running MD simulations of metallic materials [30]. The calculation of the LAMMPS software is constructed by the Verlet algorithm and has several advantages such as that it can be optimized for a system with parallel processing and even for using a graphical processing unit (GPU) [31]. Furthermore, it is considered to be fairly accurate to evaluate pressure in a system [32].

A timestep of 1 fs was used in this simulation. In the first step, the system was relaxed for 10 ps to reach equilibrium state in room temperature at 300 K. Low pressure was applied in all three directions at this stage, i.e. controlled at atmospheric pressure. After the system was relaxed, in the second step the system consisting of Ni and Al slabs was subjected to diffusion welding for 200 ps at various temperature and pressure levels. Three levels of temperature and pressure were considered, i.e. 300 K, 500 K, and 700 K for temperature and 50 MPa, 100 MPa, and 150 MPa for pressure. The temperature design was based on the melting point of the two materials, i.e. 933.47 K for Al and 1728 K for Ni, since in diffusion welding the temperature ranges from 0.6 to 0.8 of its melting point. The simulation parameters matrix is given in Table 1. The diffusion-bonded Al-Ni from the system in the previous stage then performed a tensile test with a strain

rate of 2.64e9/s at room temperature (300 K) for 100 ps. All of the stages were run under the isothermal-isobaric (NPT) ensemble.

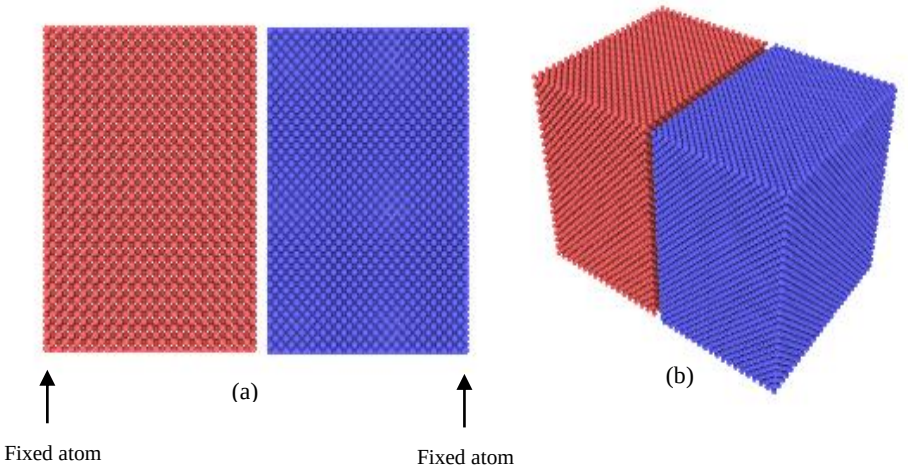

Figure 1 Top (a) and angle (b) view of Al (red) and Ni (blue) slabs with fixed atoms on each side.

Table 1 Simulation parameters matrix.

Parameter / Parameter	Temp 300 K	Temp 500 K	Temp 700 K
Press 50 MPa	**S1**	**S2**	**S3**
Press 100 MPa	**S4**	**S5**	**S6**
Press 150 MPa	**S7**	**S8**	**S9**

3 Results and Discussions

In order to investigate the effect of temperature and pressure on the diffusion welding of Al-Ni in the MD simulation, Figure 2 visualizes the diffusion-welded Al-Ni after holding for 200 ps for different parameter values with respect to the simulation matrix in Table 1. At a glance, Figure 2 indicates that the differentiation of pressure did not change very much to the diffusion-bonded Al-Ni configuration, as shown in S1, S4, and S7. On the other hand, differentiation of temperature influenced the diffusion-bonded Al-Ni configuration relatively more than pressure. Figure 2 was arranged to simplify the comparison of all of the specimens. Vertically it compares the effect of pressure (e.g. S1, S4, and S7) and horizontally it compares the effect of temperature (e.g. S1, S2, and S3).

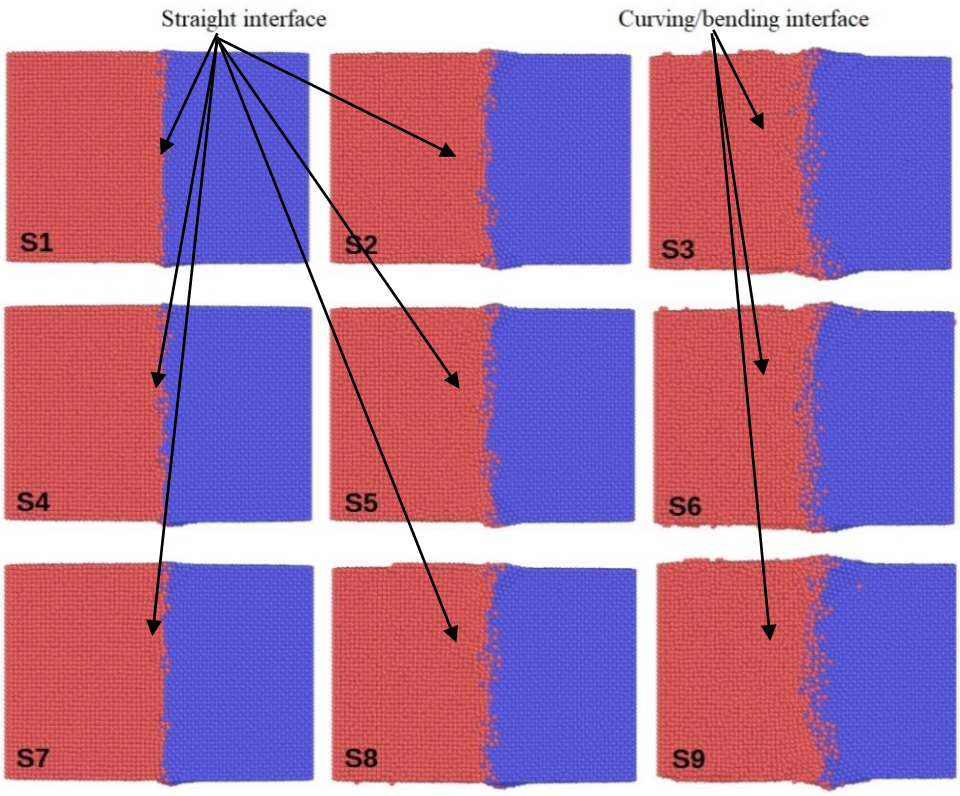

Figure 2 Diffusion-welded Al-Ni after holding for 200 ps at various parameter values with respect to the simulation matrix.

By directly analyzing Figure 2, an interesting phenomenon of curving/bending lines at the interface is visible. It is worth addressing the influence of temperature as demonstrated in Ref. [18,19], which first observed this phenomenon. First of all, better joints are achieved by increasing the temperature until a certain degree. However, when the temperature is too high (700 K), as can be seen in samples S3, S6, and S9, the Al slab that had a lower melting point severely deformed, thus introducing a curving line at the interface. Secondly, the ability of the Ni slab to maintain its structure, even at a very high temperature compared to Al, gave rise to this curving phenomenon that did not occur when the applied temperature was lower (300 K and 500 K). The unexpected phenomenon started to occur when the applied parameter values exceeded the ability of the sample materials to maintain their structure, especially when they were extremely pressed (150 MPa) and hence the Al slab deformed over a wide area. This may be critical for certain applications since this curving line would lead to a lower ability to prevent

fracture of the as-welded material when it is exposed to extreme conditions. This phenomenon could be further investigated by a creep test.

3.1 Time Evolution of Diffusion Configuration

During diffusion welding, the sample evolution is captured to see the differentiation of the materials as influenced by the applied parameter values. As previously analyzed and compared in Figure 2, the temperature dominantly influenced the configuration of the diffusion-bonded Al-Ni. Increasing the temperature means more joining depth will be achieved. When the temperature was relatively low, the sample kept its crystalline structure, leading to only a small number of atoms that diffuse into each other. The evolution of diffusion welding of Al-Ni under conditions S1, S2, and S3 is shown in Figure 3. Under these conditions, since the temperature is not high enough to promote joining, the pressure takes action. But, as discussed before, pressure only has a relatively small impact on the process so no significant effect can be seen in the time evolution in this condition.

In condition S2, the temperature is high enough to promote more joining depth and promote diffusion into each slab, indicated by the deformation of monocrystalline Al since it has a lower melting point than Ni. Additionally, the condition of S3 with the highest temperature showed more joining depth than S1 and S2. In all three conditions, however, the Ni slab kept its structure better than Al. In condition S3, monocrystalline Ni deformed only at the interface because of the pressure. Meanwhile, the other atoms that were far from the interface kept their FCC crystalline structure, while the Al atoms deformed in all of their parts. Furthermore, after 50 ps, there was no significant difference in diffusion configuration. These configurations are more clearly described by Figure 4, which shows the respective concentration distributions of diffusion-welded of Al-Ni after holding for 200 ps.

A smoother transition line of both slabs when the temperature is increased indicates the increase of atoms diffused from one side to the other. Therefore, it can be concluded that an increase in temperature influences the diffusivity of the materials and ultimately influences the thickness of the interfacial region, as indicated by the concentration distribution depicted in Figure 4. For the sake of completeness, all of the interfacial region thicknesses, defined as the area of the interfacial region for which the number of atoms exceeds 5%, is presented in Table 2 along with the ultimate tensile strength data. The joinging depth can be quantitatively interpreted by the interfacial region thickness value. As the interfacial region thickness value is higher, the atomic exchange between the two slabs is higher and consequently the joining depth also increases.

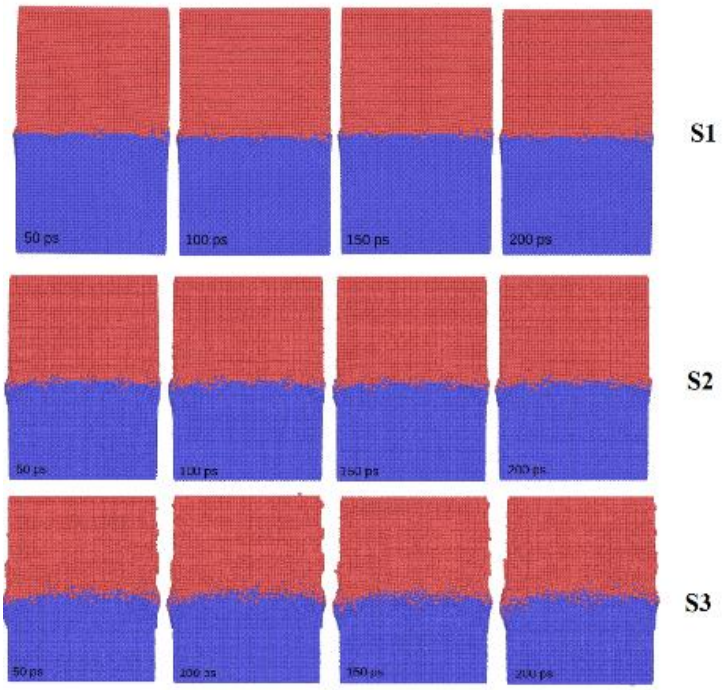

Figure 3 Time evolution of diffusion bonding Al-Ni of condition S1, S2, and S3 at 50 ps, 100 ps, 150 ps, and 200 ps.

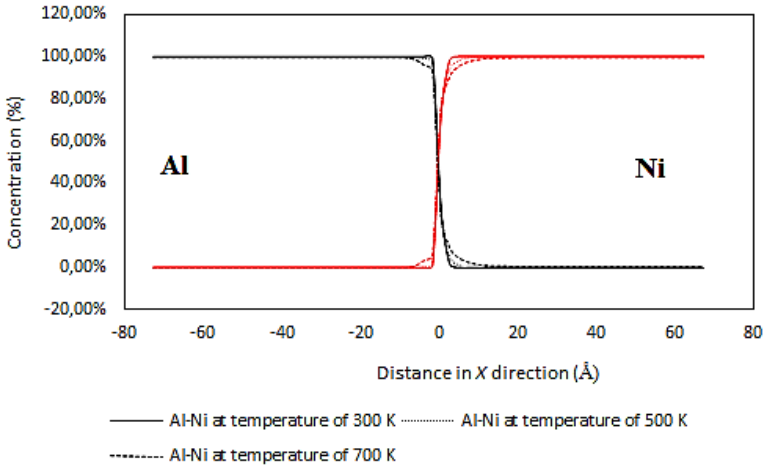

Figure 4 Concentration distribution of diffusion-bonded Al-Ni after 200 ps at a pressure of 50 MPa and various temperatures.

3.2 Tensile Testing

The tensile test is a mechanical test that applies tension to a material (which can be an as-welded material) to see the stress-strain curve for which the mechanical behavior of the material during tension and its tensile strength can be determined or at the very least estimated. Besides influencing the diffusion configuration as described in the concentration distribution, the applied temperature and pressure during the diffusion welding process also contribute to the tensile behavior when a tensile test is performed. The deformed material indeed will have lower strength compared to materials that keep their crystalline structure.

As previously mentioned, the tensile test in this study was run for 100 ps and, henceforward, to see the sample evolution during the tensile test, four different times were chosen. Figure 5 shows the time evolution of the tensile test at 25 ps, 50 ps, 75 ps, and 100 ps. It is indicated that at the lowest welding temperature, the deformation which occurred when the diffusion-welded of Al-Ni was subjected to the tensile test showed a uniform deformation that was not only focused in the interfacial region. As the applied temperature was increased, the deformation was focused only in the interfacial region (diffusion zone), while other parts that were far from the interface maintained an FCC crystalline structure. Since Al has lower strength, the deformation tended to occur in the Al slab in all nine conditions. This is due to the fact that the Al slab has a lower melting point and lower tensile strength.

In order to quantitatively compare the performance of each sample, the stress-strain curve is depicted in Figure 6. It is clear that the temperature very much influenced the mechanical properties of the diffusion-welded of Al-Ni, indicated by the ultimate tensile strength reached at the lowest temperature. As the applied temperature is increased, the ultimate tensile strength became lower. In the structural material, deformation due to plastic deformation is mostly accommodated by various mechanisms that may be responsible, i.e. dislocation motion, vacancy motion, twinning, phase transformation, or viscous flow of amorphous materials. However, the mechanism that occurred here was dislocation motion, due to the monocrystalline structure and did not accommodate any sort of other complex grain structure, thus it is reasonable to conclude that the absence of a grain structure is what caused the two slabs not to be separated at this very low temperature of welding, i.e. 300 K.

Welding, in general, is not done at such a low temperature, because most welding methods are performed to weld relatively larger samples that always come with a grain structure. One example of this is low-temperature welding, which can only be used on a relatively small sample, such as nanowire, as demonstrated in Ref. [33].

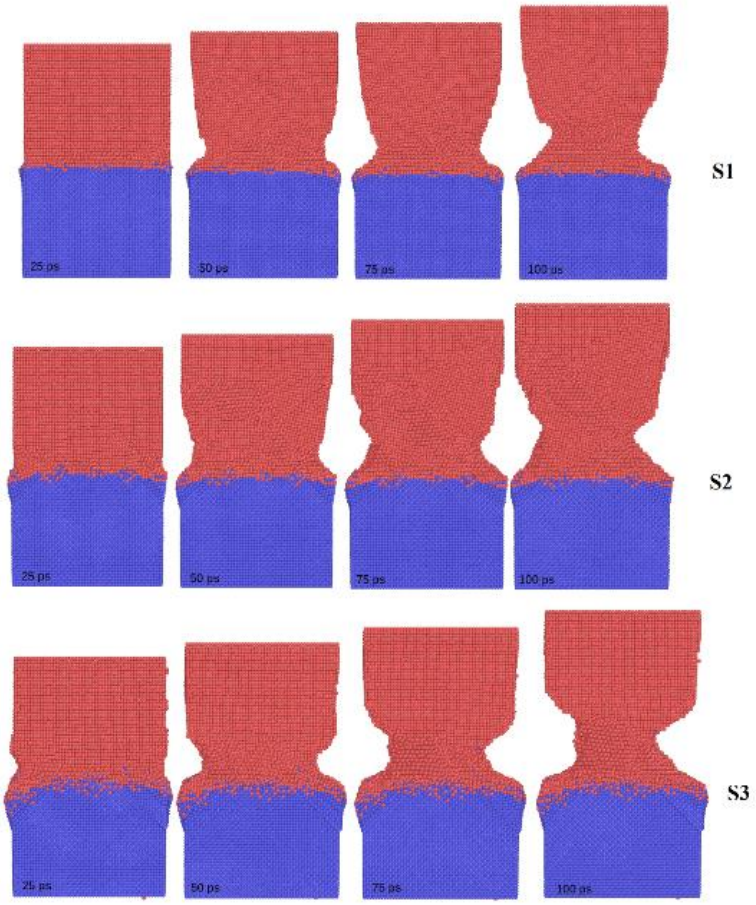

Figure 5 Time evolution of the tensile test of the diffusion-bonded Al-Ni.

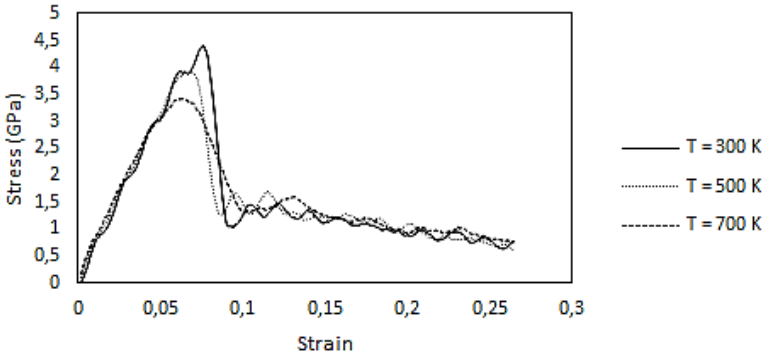

Figure 6 Stress-strain curve of the tensile test of the diffusion-bonded Al-Ni at a pressure of 50 MPa and various temperatures.

For the samples with higher temperatures, i.e. 500 K and 700 K, the ultimate tensile strength was lower but showed a structure with great bonding as can be seen from the concentration distribution (Figure 4) together with the relatively small deformation (Figure 3).

The ultimate tensile strength for all nine conditions (S1-S9) is shown in Table 2. When the temperature was higher, the fluctuation in tensile behavior decreased, which means that the whole slab was deformed uniformly, only in a more specific location, i.e. the interface of the diffusion zone. Meanwhile, when the temperature was relatively low (i.e. 300 K), the material tended to deform over a wider area than with higher temperatures (i.e. 500 K and 700 K). This behavior makes it easier to conclude whether or not the optimum condition is achieved. The fracture of the samples at high temperatures (500 K and 700 K) shows the same phenomenon, while for the lowest applied temperature (300 K), the dislocation mechanism has a higher value, which is promoted by its superior maintained crystalline structure.

Table 2 Ultimate tensile strength & interfacial region thickness of all nine sample conditions S1-S9.

Sample condition	Ultimate tensile strength (GPa)	Interfacial region thickness (Å)
S1	4.407	3.937
S2	3.938	4.383
S3	3.413	7.381
S4	4.403	3.937
S5	4.085	4.474
S6	3.200	7.996
S7	4.239	4.207
S8	3.738	4.586
S9	3.500	8.217

3.3 Optimum Parameter Values

Determining the optimum parameter values is not a simple task. The analysis derived here was based on a comparison of all nine samples for all of the aspects, including time evolution (whether or not the sample showed severe deformation), the final result of diffusion-welded Al-Ni (if the final result and its corresponding concentration distribution showed a good result as indicated by the thickness of the interfacial region and its diffusion between the two of Al-Ni slabs), and its mechanical properties (the evolution in the tensile test, the stress-strain curve, and its corresponding ultimate tensile strength). Considering all of these aspects, condition S5 was considered the optimum condition.

Figure 7 shows the structural and mechanical properties of the S5 sample. The deformation (one of the most important indicators of a weld joint's strength) that

occurred in this particular condition during the welding process showed relatively small defects. The concentration distribution indicates a smooth transition of the Al and Ni slabs, which means that the diffusion zone of Ni-Al had a uniform composition of diffusion of both materials.

Some other samples showed domination of only one of the two materials, i.e. Ni, and showed relatively significant deformation indicated by the curved interfacial region at a higher temperature. Furthermore, the tensile test showed great ultimate tensile strength since most of the parts kept their crystalline structure. Overall, the applied temperature and pressure of S5 showed a decent combination of diffusion welding parameter values with ultimate tensile strength reaching up to 4.08 GPa.

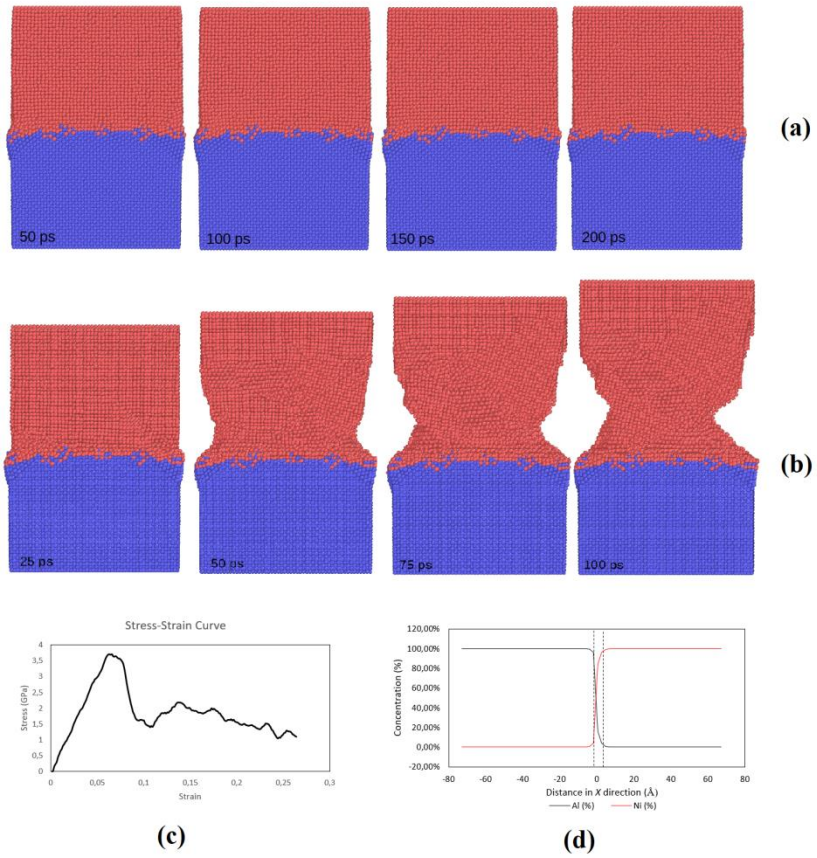

Figure 7 Result of diffusion-bonded Al-Ni for S5 (temp. 500 K, press. 100 MPa). (a) Time evolution of diffusion welding, (b) time evolution of the tensile test, (c) concentration distribution curve, (d) stress-strain curve.

4 Conclusions

A molecular dynamics simulation of diffusion welding between Al and Ni was performed to study the mechanical properties of the weld. The effect of welding temperature and pressure on the final as-welded materials was discussed in detail. The conclusions can be summarized as follows:

1. Temperature has a more significant impact on diffusion welding of Al-Ni compared to pressure. This is indicated by both the concentration distribution (i.e. interfacial region thickness) and ultimate tensile strength.
2. A curving line phenomenon at the interface line occurred due to the extremely high temperature and pressure, particularly when it exceeded the ability of the sample materials to maintain their structure.
3. As the temperature was increased, the ultimate tensile strength of diffusion-welded Al-Ni became lower. It should be considered to use the lowest possible temperature in diffusion welding in order to avoid severe deformation and consequently lower ultimate tensile strength.
4. Higher temperatures also focused the deformation on the diffusion zone of the diffusion-welded Al-Ni, while lower temperatures made the deformation occur in a wider area.

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