



# Atomistic Simulation of Temperature-Dependent Interfacial Diffusion between Solid Nickel and Liquid Aluminum

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**Abstract:** The performance and durability of welded joints are directly influenced by interfacial diffusion between the metals involved, making it essential to investigate the effect of temperature on these processes. The present research examines temperature-dependent diffusion mechanisms at the interface between solid nickel and liquid aluminum using molecular dynamics simulations. Investigations were conducted at 1200, 1300, 1400, and 1500 K to explore the influence of temperature on atomic mobility and interfacial mixing. Radial distribution function analysis revealed a significant increase in the diffusion of nickel atoms into the aluminum phase with increasing temperature, indicating enhanced atomic interactions at the interface. The mean square displacement analysis supported these findings, showing that aluminum atoms were more mobile than nickel atoms at lower temperatures, while nickel atoms exhibited a faster diffusion rate with increasing temperature, surpassing aluminum in mobility. This trend is reflected in the diffusion coefficients, which exhibit a temperature-dependent increase in the diffusion rate of the nickel atoms. These results emphasize the role of temperature in controlling the diffusion dynamics at the solid–liquid interface. The insights gained from this study are critical for optimizing processes, such as dissimilar metal welding, where precise control over interfacial diffusion is essential for achieving the desired material properties and ensuring the structural integrity of nickel–aluminum joints in high-temperature applications.

**Keywords:** Nickel–Aluminum Interface, Molecular Dynamics Simulation, Interfacial Diffusion, Temperature Dependent Diffusion.

## 1. INTRODUCTION

The joining of metals with different compositions, melting temperatures, and thermal expansion coefficients is referred to as dissimilar-metal welding. This process is essential in various industries and requires a change in the mechanical properties or performance [1]. The strength of dissimilar metal welds is significantly influenced by the diffusion of weld metals, where the parent metals have dissimilar thermal expansion coefficients [2]. Furthermore, the formation of

intermetallic compounds at the weld interface during fusion welding can result in poor strength because of the different chemical and mechanical qualities of the metals involved [3]. Studies have indicated that dissimilar metal welds may produce tensile residual stresses on both the inner and outer surfaces after welding, emphasizing the significance of understanding and managing such stresses for the structural soundness of the joint [4]. Moreover, the microstructure and mechanical properties of dissimilar metal welds can be influenced by welding parameters such as the heat

input, holding time, and post-weld heat treatment [5–7]. Metallurgical compatibility between the interlayer and base metals is crucial when selecting interlayers in dissimilar weld joints because it can have a significant impact on the overall quality and performance of the weld [8, 9]. In addition, the presence of weld residual stresses in dissimilar metal welds, even after post-weld heat treatment, highlights the importance of considering these stresses when evaluating potential welding defects and joint performances [10]. The direction of crack growth in dissimilar metal-welded joints can also influence the fracture toughness and fatigue crack growth rates, underscoring the need to elucidate crack propagation mechanisms in such joints [11].

Solid metal–liquid metal diffusion is of significant interest because of its implications in various fields including materials science, metallurgy, and electrochemistry. This diffusion process, in which atoms move between solid and liquid metals, is essential for processes such as alloy formation, electroextraction, and liquid-metal embrittlement. It should be noted that in the process of atom diffusion between solid and liquid metals, the diffusion coefficients of liquid metals are several times greater than those of solid metals [12], which is attributed to the excited states of the atoms in the liquid phase. The diffusion of metal atoms primarily occurs in the liquid phase rather than in the solid phase, which influences the characteristic contact melting time [13].

The diffusion of nickel and aluminum at the interface is a crucial process in various applications involving these materials; it occurs when atoms from one material move into another, resulting in the formation of intermetallic compounds and altered material properties. This phenomenon is particularly important for nickel and aluminum. Research has revealed considerable variations in the diffusion coefficients of these metals in nickel–aluminum systems. The rapid outward diffusion of nickel, in contrast to the slower inward diffusion of aluminum, led to the formation of Kirkendall voids. This process is commonly referred to as the Kirkendall effect [14] and is responsible for the generation of pores and vacancies within the crystal structure of the material owing to the disparity in diffusion rates. According to previous studies, interfacial diffusion between nickel and aluminum typically results in inward diffusion of aluminum

toward the nickel substrate. However, the presence of zirconium causes it to diffuse toward specific layers at the  $\beta$ -NiAl/ $\gamma'$ -Ni<sub>3</sub>Al interface, where it can be substituted for aluminum atoms in the  $\beta$ -NiAl phase [15]. This substitution can affect the microstructure and properties of the intermetallic compounds formed at the interface. Furthermore, studies on nickel diffusion in intermetallic compounds have revealed that nickel diffuses through compound layers and dissolves in the aluminum phase at the other end of the couple [16]. This process plays a crucial role in the formation and evolution of intermetallic phases at the nickel–aluminum interface. The role of nickel diffusion in practical applications, such as welding and coating processes, is essential for enhancing the bonding and mechanical properties of joints. In particular, the incorporation of a nickel interlayer can prevent the formation of brittle intermetallic compounds and improve the strength and ductility of joints between dissimilar metals, such as aluminum and steel [17].

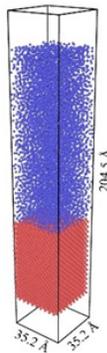
Despite extensive research on interfacial diffusion in dissimilar metal systems, the specific mechanisms driving atomic diffusion at solid nickel–liquid aluminum interfaces, particularly at elevated temperatures, remain inadequately understood. Although, Zhang *et al.* [18] employed molecular dynamics (MD) simulations to examine the interfacial diffusion between nickel and aluminum, their research was constrained to a single high-temperature condition of 1200 K. Despite offering valuable insights into diffusion mechanisms, their study did not explore how diffusion coefficients vary with temperature, creating a notable gap in understanding the impact of thermal changes on atomic mobility and interfacial dynamics in the nickel–aluminum system. Our research addresses this limitation by broadening the scope to include simulations at multiple temperatures: 1200, 1300, 1400, and 1500 K. This comprehensive approach allows for a thorough analysis of the diffusion coefficients and their temperature dependence, providing more extensive insights into the interfacial diffusion mechanisms across various thermal conditions. By analyzing the diffusion coefficients and structural evolution of Ni atoms at the interface, this research aims to provide a deeper understanding of how temperature and atomic interactions influence the diffusion processes. The findings of this study will contribute to optimizing

welding techniques and improving the performance of dissimilar metal joints in high-temperature applications, where precise control over diffusion is crucial.

## 2. SIMULATION DETAILS

Simulations were carried out using the LAMMPS software package [19, 20] to investigate the interfacial diffusion between solid nickel and liquid aluminum. The Embedded Atom Method (EAM) potential parameterized for nickel and aluminum [21] was used to ensure accurate interactions between the nickel and aluminum atoms. The simulation system, with dimensions of 35.2 Å × 35.2 Å × 204.5 Å, comprised 6,400 nickel atoms in a face-centered cubic structure, representing the solid phase, and 6,400 Al atoms as the liquid phase (Figure 1). The temperature dependence of diffusion was studied by conducting simulations at 1200, 1300, 1400, and 1500 K using the NVT ensemble with a Nosé–Hoover thermostat to maintain stability. The Velocity Verlet algorithm was used to integrate the equations of motion with a time step of 1 fs; each simulation was run for a total duration of 1,000,000 fs, allowing sufficient time for the diffusion processes to occur.

Structural analysis and visualization were performed using OVITO [22], allowing for a thorough examination of the atomic structure and interfacial diffusion. The atomic structure of the system was analyzed using the radial distribution function  $g(r)$ . The radial distribution function was calculated using Equation (1).



**Fig. 1.** Initial simulation configuration. The red and blue spheres represent nickel and aluminum atoms, respectively.

$$g(r) = \frac{1}{N} \sum_{i=1}^N \frac{n_i(r, r + \Delta r)}{\rho \cdot V(r, r + \Delta r)} \quad (1)$$

Where,

$N$  = Total number of atoms in the system

$n_i(r, r + \Delta r)$  = Number of atoms found within a spherical shell of radius  $r$  and thickness  $\Delta r$  around atom  $i$ .

$\rho$  = Atomic number density (atoms/Å<sup>3</sup>)

$V(r, r + \Delta r)$  = Volume of the spherical shell (Å<sup>3</sup>)

The mean square displacement (MSD) of the nickel and aluminum atoms at the interface was calculated from the atomic trajectories to quantify the diffusion behavior. The MSD was calculated using Equation (2).

$$MSD = \frac{1}{N} \sum_{i=1}^N \langle |\vec{r}_i(t) - \vec{r}_i(0)|^2 \rangle \quad (2)$$

Where,

MSD = Mean square displacement (Å<sup>2</sup>)

$N$  = The total number of atoms

$t$  = Time (fs)

$\vec{r}_i(t)$  = position of atoms  $i$  at time  $t$

$\vec{r}_i(0)$  = position of atoms  $i$  at time  $t = 0$

This study specifically focused on interfacial atoms, as they are essential for understanding the diffusion process at the solid–liquid boundary. The diffusion coefficients for nickel and aluminum were estimated from the slope of the plots of MSD versus time, utilizing the Einstein relation for diffusion, as expressed in Equation (3).

$$D = \frac{1}{2d} \lim_{t \rightarrow \infty} \frac{MSD}{t} \quad (3)$$

Where,

$D$  = Diffusion coefficient (Å<sup>2</sup>/ps)

$d$  = Dimension of the system

## 3. RESULTS AND DISCUSSION

This section presents and examines the results of MD simulations using visual and quantitative methods. The structural evolution of the nickel–aluminum interface was analyzed to illustrate the diffusion processes at various temperatures. Additionally, we employed the radial distribution function,  $g(r)$ , to analyze atomic interactions (Figure 2), MSD to quantify atomic mobility, and diffusion coefficients to assess the rate of diffusion.

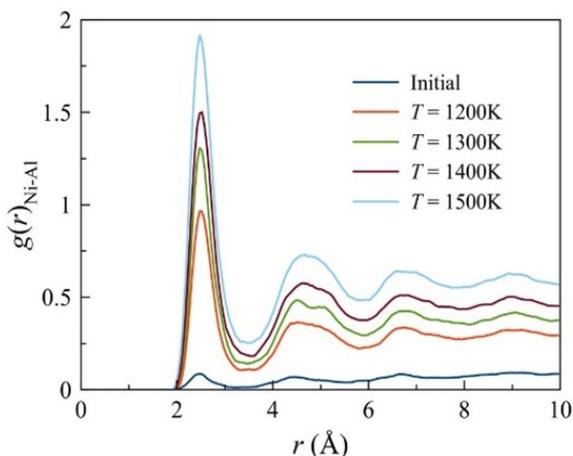


Fig. 2. Radial distribution function,  $g(r)_{\text{Ni-Al}}$ .

In Figure 2,  $g(r)_{\text{Ni-Al}}$  depicts the distribution of the distances between nickel and aluminum atoms in the system in both the initial and final states of the MD simulations at temperatures of 1200, 1300, 1400, and 1500 K.  $g(r)$  is an essential tool for elucidating the local atomic structure and degree of atomic interactions within a material, particularly at the interface between two distinct phases. At the beginning of the simulation,  $g(r)_{\text{Ni-Al}}$  exhibits a very low first peak, indicating that only a few nickel atoms are within a close range of aluminum atoms. This initial condition reflects the configuration of the system, in which the nickel atoms are primarily confined to the solid phase and the aluminum atoms are in the liquid phase, with minimal intermixing at the interface. The low intensity of the first peak suggests that the atomic interactions between nickel and aluminum are limited, primarily occurring at the solid–liquid boundary, with most of the atoms remaining in their respective phases.

When the temperature is increased to 1200 K, a notable transformation occurred in the  $g(r)_{\text{Ni-Al}}$  curve. After  $10^6$  fs, the first  $g(r)_{\text{Ni-Al}}$  peak became more pronounced, which indicated that a larger number of nickel atoms moved closer to the aluminum atoms, suggesting an increase in atomic diffusion at the interface. The higher intensity of the first peak at 1200 K suggests greater mobility of atoms at the interface, allowing for greater intermixing between the solid nickel and liquid aluminum phases. The elevated degree of atomic interaction at this temperature arises from enhanced diffusion, resulting in a higher number of nickel atoms coordinating with aluminum atoms.

At 1300 K, the diffusion process is further accelerated, as evidenced by the more pronounced first peak of the  $g(r)_{\text{Ni-Al}}$  curve. This suggests that more nickel atoms can migrate into the liquid aluminum phase because of the higher thermal energy, which provides the atoms with the necessary kinetic energy to overcome barriers to diffusion. Additionally, the increased peak intensity indicates that the nickel atoms not only entered the aluminum phase but also found more stable positions within the liquid structure, leading to more defined atomic interactions.

At 1400 and 1500 K, the first  $g(r)_{\text{Ni-Al}}$  peak exhibits a noteworthy increase in intensity, which suggests that the diffusion of nickel atoms into the aluminum phase becomes more pronounced as the temperature increases. As the temperature increased, the atomic mobility also improved, leading to more significant interfacial mixing and the formation of a more ordered interfacial region. The observed trend indicates that, as the temperature increases, the atoms gain sufficient thermal energy to surmount any remaining diffusion barriers, resulting in a more homogeneous distribution of nickel atoms within the liquid aluminum phase.

Figure 3 validates the results of the  $g(r)_{\text{Ni-Al}}$  analysis, demonstrating that higher temperatures lead to increased diffusion of nickel atoms into the liquid aluminum region. As the temperature increased, the kinetic energy of the atoms increased, enhancing their mobility and leading to a

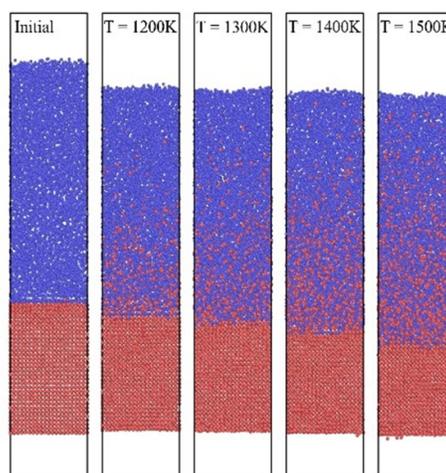


Fig. 3. Snapshots of the initial and final MD configurations. The red and blue spheres represent nickel and aluminum atoms, respectively.

more significant interfacial mixing. This increased diffusion is visually evident in Figure 3, where the simulation snapshots show a greater number of nickel atoms migrating from the solid phase to the liquid phase as the temperature increases from 1200 to 1500 K. Moreover, Figure 3 reveals another critical aspect of the diffusion process: the erosion of nickel layers from the solid phase. Initially, the solid nickel structure in the simulation comprised 32 layers; after  $10^6$  fs, the number of layers progressively decreased with increasing temperature. At 1200 K, the solid Ni was reduced to 28 layers, indicating the diffusion of four layers of nickel atoms into liquid aluminum. As the temperature increased to 1300 K, the number of Ni layers further decreased to 26, and at 1400 K, only 24 layers remained. At the highest temperature of 1500 K, the solid nickel structure was reduced to 22 layers, indicating significant erosion owing to the high rate of diffusion.

Figure 4 presents the MSD of nickel and aluminum atoms at the solid-liquid interface at various temperatures, including 1200, 1300, 1400, and 1500 K. The MSD curves offer insights into atomic mobility and diffusion behavior under different thermal conditions. At 1200 K, the slope

of the curve for nickel atoms at the interface was notably smaller than that for aluminum atoms. This suggests that, at this temperature, aluminum atoms exhibit higher mobility and, consequently, a higher diffusion rate than nickel atoms. This observation is corroborated by the diffusion coefficients presented in Table 1, with a value of  $0.23 \text{ \AA}^2/\text{ps}$  for aluminum atoms compared to  $0.18 \text{ \AA}^2/\text{ps}$  for nickel atoms at 1200 K. The higher mobility of aluminum atoms at this lower temperature can be attributed to the liquid state of aluminum, which facilitates atomic movement compared with the more rigid solid structure of nickel. However, as the temperature increases to 1300, 1400, and 1500 K, a reversal in this trend is observed: the MSD curves for nickel atoms at the interface are steeper (with larger slopes) than those for aluminum atoms, indicating a more rapid diffusion of nickel atoms compared to aluminum atoms. This shift is also reflected in the diffusion coefficients listed in Table 1. At 1300 K, the diffusion coefficient for nickel is  $0.30 \text{ \AA}^2/\text{ps}$ , slightly higher than that of aluminum ( $0.28 \text{ \AA}^2/\text{ps}$ ). The difference becomes more pronounced at 1400 and 1500 K, with nickel exhibiting diffusion coefficients of  $0.39$  and  $0.43 \text{ \AA}^2/\text{ps}$ , respectively, compared to  $0.30$  and  $0.40 \text{ \AA}^2/\text{ps}$  for aluminum. The simulation results indicate that the diffusion

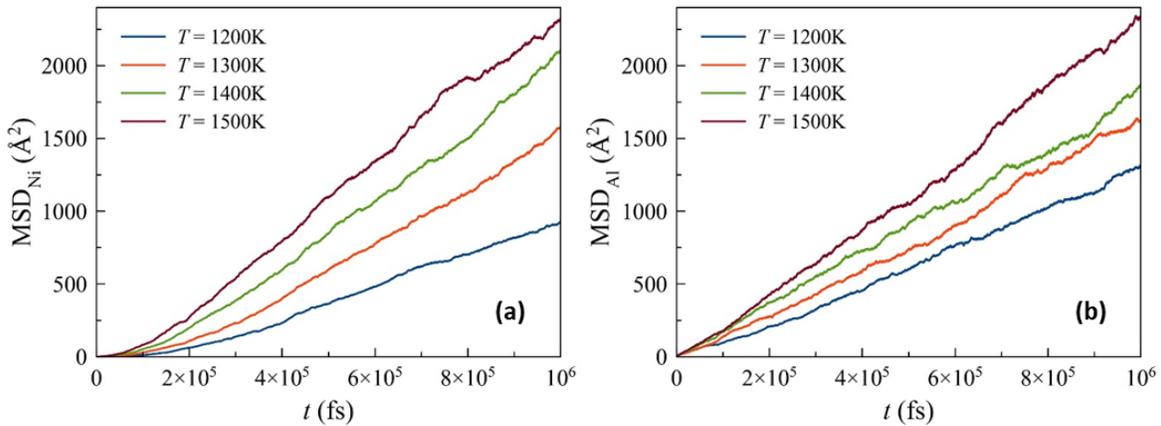


Fig. 4. MSD plots of (a) nickel and (b) aluminum atoms at the surface.

Table 1. Diffusion coefficients of surface atoms at the nickel-aluminum interface.

No.	Temperature (K)	Nickel diffusion coefficient ( $\text{\AA}^2/\text{ps}$ )	Error (%)	Aluminum diffusion coefficient ( $\text{\AA}^2/\text{ps}$ )	Error (%)
1	1200	0.18	0.3	0.23	0.2
2	1300	0.30	0.2	0.28	0.5
3	1400	0.39	0.3	0.30	0.4
4	1500	0.43	0.4	0.40	0.4

coefficient of aluminum is lower than its self-diffusion coefficient in pure liquid form ( $0.88 \text{ \AA}^2/\text{ps}$ ) [23], which can be attributed to interfacial effects at the solid nickel-liquid aluminum boundary. In the pure liquid state, aluminum atoms exhibit higher mobility in a homogeneous environment. However, at the nickel-aluminum interface, aluminum atoms interact with nickel atoms, creating a nonhomogeneous environment that constrains their movement. These interactions, in conjunction with the ordered structure induced by the solid nickel substrate, increase the energy barriers for diffusion and decrease atomic motion. Consequently, the interfacial dynamics significantly reduce the effective diffusion of aluminum compared with its behavior in a pure liquid state.

The results indicate that increasing the temperature increases the thermal energy available to the nickel atoms, which surpasses the energy barriers associated with diffusion and leads to increased atomic mobility. Elevated temperatures result in higher diffusion rates for nickel atoms and their stronger inclination to migrate into the liquid aluminum phase, leading to enhanced interfacial mixing and structural changes. These findings align with those of previous studies conducted on liquid metal systems such as liquid nickel and liquid titanium, where nickel displayed a higher diffusion coefficient than titanium [24]. The results of the present study highlight the significance of controlling the temperature during processing to ensure optimal material properties as well as the critical role of elevated temperatures in influencing the stability and performance of dissimilar metal interfaces under various thermal conditions.

#### 4. CONCLUSIONS

This study investigated the diffusion dynamics at the interface between solid nickel and liquid aluminum via MD simulations at temperatures ranging from 1200 K to 1500 K. The results showed that, as the temperature increased, the diffusion of nickel atoms into the aluminum phase became more pronounced, leading to enhanced interfacial mixing. The  $g(r)_{\text{Ni-Al}}$  analysis indicates a significant increase in atomic interactions at higher temperatures, correlating with the greater mobility of nickel atoms observed in the MSD analysis. At lower temperatures, aluminum atoms exhibit more mobility, but as the temperature increases, nickel atoms display faster diffusion,

surpassing aluminum in mobility. This shift is reflected in the diffusion coefficients, indicating the temperature-dependent acceleration of nickel atom diffusion. These findings highlight the critical role of temperature in controlling atomic diffusion at the solid-liquid interface and have implications for processes such as dissimilar metal welding.

#### 5. ACKNOWLEDGEMENTS

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#### 6. CONFLICT OF INTEREST

The authors declare that they have no conflicts of interest.

#### 7. REFERENCES

1. B. Belkessa, D. Miroud, B. Cheniti, N. Ouali, M. Hakem, and M. Djama. Dissimilar Welding Between 2205 Duplex Stainless Steel and API X52 High Strength Low Alloy Steel. *Diffusion Foundations* 18: 7–13 (2018).
2. R. Chaudhari and A. Ingle. An Empirical Research on Dissimilar Metal Weld of SA335 P11 and SA312 TP304 Formed by Metal Inert Gas (MIG) Welding. *International Journal of Recent Technology and Engineering* 8(2): 5008–5012 (2019).
3. S. Murugan, P. Sathiya, and A.N. Haq. Rotary Friction Welding and Dissimilar Metal Joining of Aluminium and Stainless Steel Alloys. *Annals of Dunarea De Jos University of Galati Fascicle Xii Welding Equipment and Technology* 32(1): 85–92 (2021).
4. W. Dong, D. Gao, and S. Lu. Numerical Investigation on Residual Stresses of the Safe-End/Nozzle Dissimilar Metal Welded Joint in CAP1400 Nuclear Power Plants. *Acta Metallurgica Sinica (English Letters)* 32: 618–628 (2018).
5. S. Ismadi. Study Effect of Holding Time at Post Weld Heat Treatment (PWHT) on Joint Dissimilar Welding ASTM 335 P11 to ASTM 304L Under Controlled Condition. *Key Engineering Materials* 975: 9–20 (2024).
6. M.A. Hayatu, E.T. Dauda, O. Aponbiede, K.A. Bello, and U. Abdullahi. Evaluation of Microstructure and Impact Toughness of Shielded Metal Arc Dissimilar Weldments of High Strength Low Alloy Steel and Austenitic Stainless Steel. *Fuoye Journal of Engineering and Technology* 5(2): 171-174 (2020).
7. M. El-Shennawy, H.A. Abdel-Aleem, M.M.

- Ghanem, and A.M. Sehsah. Effect of Welding Parameters on Microstructure and Mechanical Properties of Dissimilar AISI 304 / Ductile Cast Iron Fusion Welded Joints. *Scientific Reports* 14: 19827 (2024).
8. R.R. Gabbasov, E.V. Galieva, E.Y. Klassman, and V.A. Valitov. Effect of pressure welding temperature on the microstructure and mechanical properties of solid-state joints of wrought nickel-based EK79 and EP975 superalloys. *Letters on Materials* 14(2): 155–160 (2024).
  9. A.U. Rehman, N.K. Babu, M.K. Talari, S. Anwar, Y. Usmani, and A.M. Al-Samhan. Dissimilar Rotary Friction Welding of Inconel 718 to F22 Using Inconel 625 Interlayer. *Applied Sciences* 11(22): 10684 (2021).
  10. B. Spisák, Z. Bézi, and S. Szávai. Study of the Stress State of a Dissimilar Metal Weld Due to Manufacturing and Operational Conditions. *Periodica Polytechnica Mechanical Engineering* 66(2): 120–128 (2022).
  11. T. Saju and M. Velu. Analysis of Fracture Toughness and Fatigue Crack Growth Rates of Electron Beam-Welded Dissimilar Nickel-Based Superalloys: Mode-I Cracks Oriented Normal to the Weld. *Proceedings of the Institution of Mechanical Engineers Part L Journal of Materials Design and Applications* 237(8): 1699–1714 (2023).
  12. O.B. Girin. Review-Electrochemical Phase Formation via a Supercooled Liquid State Stage: Metastable Structures and Intermediate Phases. *Journal of the Electrochemical Society* 169(9): 092511 (2022).
  13. A.V. Melkikh. Contact Melting of Metals Explained via the Theory of Quasi-Liquid Layer. *Applied Sciences* 11(1): 51 (2021).
  14. M. Zagula-Yavorska, J. Morgiel, J. Romanowska, and J. Sieniawski. Nanoparticles in Zirconium-Doped Aluminate Coatings. *Materials Letters* 139: 50–54 (2015).
  15. J. Romanowska, M. Zagula-Yavorska, M. Góral, and J. Sieniawski. Zirconium Modified Aluminate Coatings Obtained by the CVD Method. *Solid State Phenomena* 227: 174–177 (2015).
  16. M. Khieokae, R. Hanamornroongruang, R. Ramasoot, A. Taechakaesaree, P. Ngamchaliew, and T. Luangvaranunt. Diffusion Coefficient of Nickel in  $\text{Ni}_2\text{Al}_3$  Intermetallic Compound. *Advanced Materials Research* 1025–1026: 731–736 (2014).
  17. Z. Nurisna, A. Supriyanto, N. Muhyat, and T. Triyono. Thermal Spray Application on the Dissimilar Metals Weld Between Aluminum and Steel. *Defect and Diffusion Forum* 402: 27–32 (2020).
  18. C. Zhang, H. Wang, and Y. Qiu. Study of Ni/Al Interface Diffusion by Molecular Dynamics Simulation. *Engineering* 3(3): 227–232 (2011).
  19. S.J. Plimpton. Fast Parallel Algorithms for Short-Range Molecular Dynamics. *Journal of Computational Physics* 117(1): 1–19 (1995).
  20. A.P. Thompson, H.M. Aktulga, R. Berger, D. Bolintineanu, M.W. Brown, P.S. Crozier, P.J. in 't Veld, A. Kohlmeyer, S.G. Moore, T.D. Nguyen, R. Shan, M.J. Stevens, J. Tranchida, C. Trott, and S.J. Plimpton. LAMMPS - a flexible simulation tool for particle-based materials modeling at the atomic, meso, and continuum scales. *Computer Physics Communications* 271: 108171 (2022).
  21. G.P. Purja Pun and Y. Mishin. Development of an interatomic potential for the Ni-Al system. *Philosophical Magazine* 89(34-36): 3245–3267 (2009).
  22. A. Stukowski. Visualization and analysis of atomistic simulation data with OVITO—the Open Visualization Tool. *Modelling and Simulation in Materials Science and Engineering* 18: 015012 (2009).
  23. F. Kargl, H. Weis, T. Unruh, and A. Meyer. Self diffusion in liquid aluminium. *Journal of Physics: Conference Series* 340: 012077 (2012).
  24. R. Arifin, Y. Winardi, Y.A. Wicaksono, L. Poriwikawa, Darminto, A. Selamat, W.T. Putra, and M. Malyadi. Atomic diffusion at the Ni–Ti liquid interface using molecular dynamics simulations. *Canadian Metallurgical Quarterly* 61(3): 359–365 (2022).