

Finite element modelling and simulation of the multiscale crystalline structure of aluminium deposit produced by helium cold spray additive manufacturing

J. Qi¹, R. N. Raoelison^{2, *}, J. Li¹, M. Rachik¹

¹ Alliance Sorbonne Université, Université de Technologie de Compiègne, Laboratoire Roberval, Centre de Recherche Royallieu, CS 60319,60203 Compiègne Cedex, France

² Université Marie et Louis Pasteur, Université de Technologie de Belfort-Montbéliard, Laboratoire ICB-UBE, UMR 6303 CNRS, 90010 Belfort Cedex, France

*Corresponding author. Email: rija-nirina.raoelison@utbm.fr

Abstract

This study addresses an experimental analysis with a multiscale modelling of a pure Aluminium deposit produced by helium cold spraying. The grain morphology and the crystallographic texture of the deposit revealed a significant grain refinement along with a formation of strong metallurgical bonding. Complementing the experiments, a two-part multiscale modelling framework is developed, integrating a simulation of the particle upon impact and a crystal plasticity finite element model for analysing the consolidation and deformation mechanisms across multiple scales. Using Johnson-Cook equations and coupled Eulerian-Lagrangian approach, the particle impact model effectively captures high-velocity impact behaviour, deformation mechanisms, and thermal interactions at the particle-substrate interface. The influence of intergranular interactions and phase heterogeneities on the overall mechanical response, at the mesoscale level, is investigated. The crystal plasticity-based approach can simulate the behaviour of individual grains within a representative volume element (RVE), with a prediction of the anisotropic mechanical properties and stress-strain relationships between various grains. The results pave the way for a better understanding of the microstructural evolution and mechanical behaviour of Aluminium deposits produced by helium cold spraying.

Keywords

Cold Spray, Microstructure, Modelling, Aluminium, Additive Manufacturing, Crystal Plasticity Simulation.

1 Introduction

Additive manufacturing (AM) has emerged as a transformative technology across various industries, offering the potential for rapid prototyping, complex geometrical freedom, and reduced material waste. Among AM techniques, cold gas dynamic spray (CGDS), also known as cold spraying, stands out due to its unique capability of depositing metals, composites, and ceramics at relatively low temperatures. This process involves the acceleration of solid particles to supersonic velocities, allowing them to adhere and consolidate upon impact with a substrate, thereby forming dense, well-bonded deposits [1]. Such characteristics make CGDS an attractive method for producing coatings, repairing components, and fabricating parts in diverse fields ranging from aerospace to biomedical applications. An intriguing advancement in cold spraying is its ability to achieve a high strain rate self-consolidation, where material bonding occurs through severe plastic deformation induced by high-velocity particle impacts [2]. Aluminium and its alloys, renowned for their high strength-to-weight ratio, corrosion resistance, and thermal conductivity, are widely used in aerospace, automotive, and defence industries. However, the fabrication of Aluminium components via conventional manufacturing processes often poses challenges related to porosity, residual stresses, and microstructural inhomogeneity. CGDS offers a promising solution to these challenges through high-strain-rate self-consolidation, which facilitates the formation of dense, defect-free structures with tailored mechanical properties [3].

This study explores the microstructural evolution and modelling of Aluminium deposits produced via high strain rate self-consolidation using helium CGDS. The paper is structured as follows. First, a review of the principles of CGDS and its application to Aluminium is presented, highlighting the challenges and opportunities. Next, a series of characterization experiments are performed on helium cold spray-fabricated pure Aluminium sample. Following microstructure characterization, particle impact simulations are conducted to detail the complex features of the particle-substrate interface, particularly in its vicinity. By analysing the interplay between particle deformation, interfacial bonding, and thermal effects, we aim to elucidate the underlying mechanisms driving the formation of dense and cohesive deposits. At the same time, in order to uncover the intrinsic mechanisms of the observed behaviours, a crystal plasticity finite element model is developed to provide insights into the interplay between grains and strain rate effects. It is worth noting that the RVE model is derived from the real EBSD microstructure of the CS deposit through image processing. Crystal plasticity modelling helps in elucidating the localized deformation behaviours and stress-strain responses under various loading conditions, bridging the gap between process parameters and material performance. This work emphasizes the viability of CGDS as an advanced manufacturing technique for producing high-quality Aluminium components with tailored properties.

2 Material and fabrication

The feedstock material used in this study is a pure aluminium powder (purity $\geq 99.5\%$) commercialized by Toyal company. The granulometry ranges in between 15 and 45 μm . The high purity of aluminium ensures minimal contamination and promotes a better bonding during deposition, which is critical for the high strain rate self-consolidation process inherent to cold gas dynamic spray additive manufacturing. The deposition of the aluminium powder was carried out using a closed-loop cold spray system [4]. The substrate is Al 7075 substrate. Helium was used as the carrier gas to ensure optimal velocity for the cold spray deposition. Additionally, the process gas was preheated to 350 °C and delivered at a pressure of 28 bar.

3 Experimental procedure and results

The cold spray samples were sectioned for microstructural and mechanical analysis. The metallographic preparation included mounting, grinding, polishing, and etching using Keller's reagent [5]. Scanning electron microscopy (SEM) and optical microscopy (OM) are used to examine the microstructure, focusing on particle deformation and bonding characteristics.

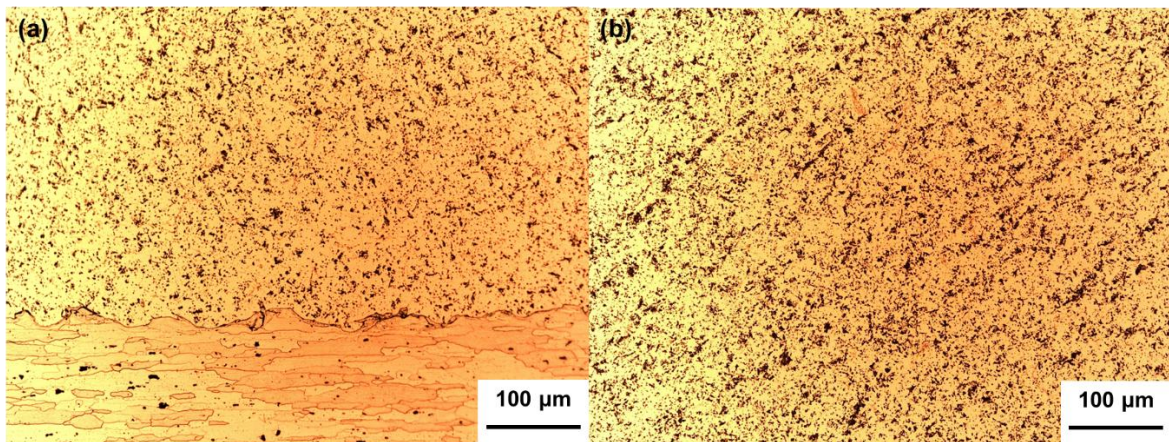


Figure 1: OM image of the helium CSed Aluminium deposit: (a) cross section; (b) top section.

The microstructural analysis of the aluminium deposit shows distinct features associated with the processing conditions. The as-deposited samples exhibited a dense microstructure with a very low porosity ($<2\%$), as observed through OM and scanning electron microscopy SEM. High-resolution SEM micrographs revealed the presence of localized bonding interfaces between the individual particles, characterized by flattened and elongated grain structures indicative of severe plastic deformation. These observations revealed a significant plastic deformation of the aluminium particles upon impact. The particle interfaces were characterized in the as-deposited state using Electron backscatter

diffraction (EBSD). The results show equiaxed grains with an average size of 2 μm , indicating substantial grain refinement compared to the original feedstock material.

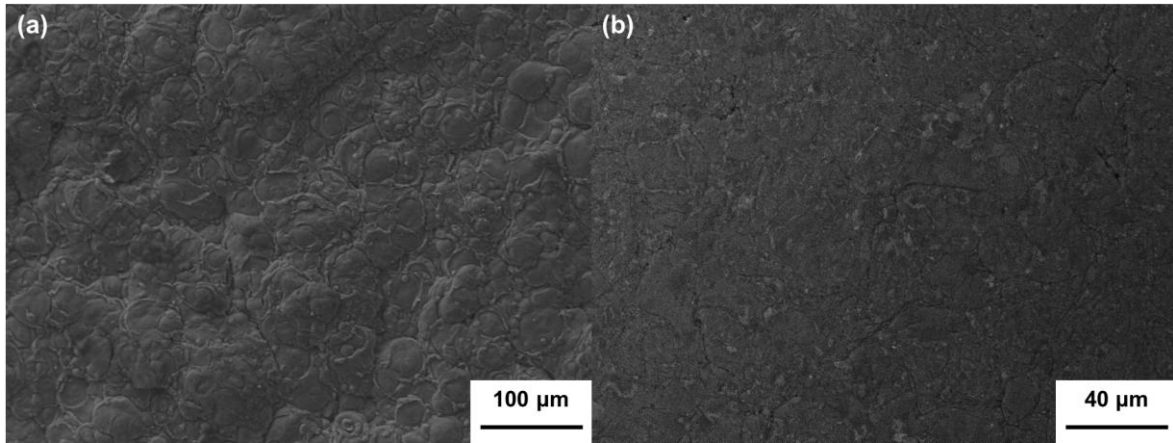


Figure 2: SEM image of CSed Aluminium deposit: (a) top section without polishing; (b) top section with polishing.

The interface between the Aluminium deposit and the substrate displays a transition zone with recrystallized or deformed grains as shown in Figure 3. The grain size varies from large to fine across the interface. The EBSD analysis provides insights into the understanding of the grain structure and recrystallization phenomena. Figure. 3 shows the cross sectional EBSD image which exhibits equiaxed or elongated grains. It shows significant grain refinement compared to the feedstock powder.

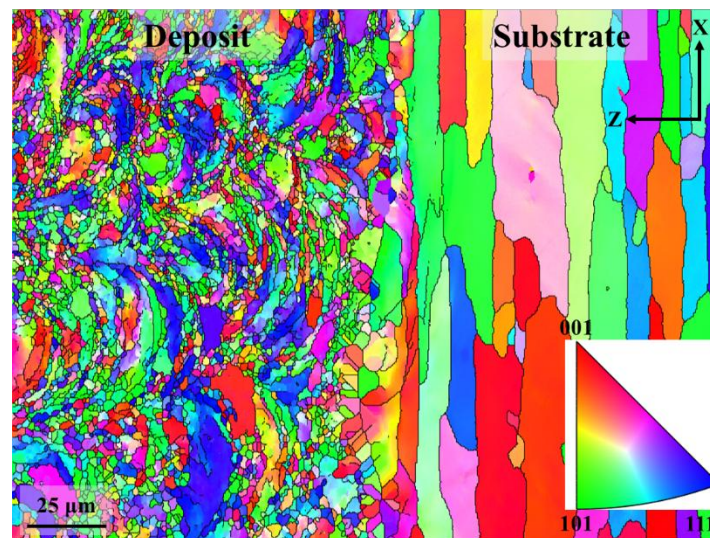


Figure 3: EBSD image of the helium CSed Aluminium deposit: cross section of the bonded interface. (Z presents building direction, X presents nozzle traverse direction)

The average grain size was reduced from approximately 25 μm in the feedstock to sub-micron levels ($<1 \mu\text{m}$) within the deposit. The formation of equiaxed grains at the immediate

vicinity of the interface reveals a thermal recrystallization process upon impact, due to plastic work produced by the several plastic deformations. The fine but elongated grains are attributed to the dynamic recrystallization due to the high strain rates deformation at the interface upon impact.

4 Modelling of particle impact behaviour and results

The finite element modelling of the cold gas dynamic spray process provided further insights into the high strain rate self-consolidation mechanism [6]. A model incorporating particle impact dynamics, plastic deformation, thermal evolution, and inter-particle bonding mechanisms is of interest. In this study, a finite element model is performed to simulate the stress, strain and temperature distribution during the particle impact process based on coupled Eulerian-Lagrangian approach. The uses of the Johnson-Cook plasticity constitutive law allow for accounting for the strain hardening, the strain rate sensitivity, and the thermal softening. The detailed J-C equations and parameters of pure Aluminium can be seen in the literature [7]. The impact velocity of particle is 700 m/s. A mesh size of 0.5 μm was employed for both the particle and the refined region of the substrate adjacent to the interface to ensure simulation accuracy.

The residual stress distribution is also investigated by analysing the compressive stresses near the substrate-deposit interface due to collision. The spatial and dimensional agreement between the simulated high-strain/high-temperature band and the experimentally observed dynamically recrystallized belt validates the model's ability to couple deformation and microstructure evolution during cold spray single-particle deposition. The modelling results also highlighted the critical role of thermal softening and adiabatic heating in facilitating particle bonding. A combination of localized thermal softening and adiabatic shear at the particle interfaces facilitated the metallurgical bonding.

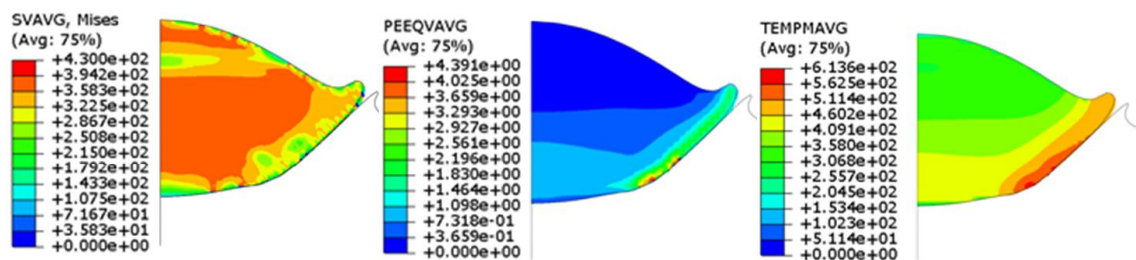


Figure 4: Simulation of single particle impact behaviour: distribution of stress, strain, and temperature, respectively.

5 Modelling of microstructural evolution and results

The modelling of microstructural evolution of due to the cold sprayed deposition depicts the inhomogeneous deformation mechanisms resulting from high strain rate self-consolidation. Figure. 5 shows the RVE modelling using the crystal plasticity framework.

From the EBSD map in Figure 5 (a) and the microstructural experiments mentioned above, it can be seen that the Aluminium deposit has a bimodal polycrystalline microstructure consisting of recrystallized ultrafine grains (UFG) and deformed coarse grains (CG). The significant size disparity between CGs and UFGs requires a multiscale modelling approach. To this end, it is essential to distinguish these domains when constructing the microstructural RVEs and conducting the simulations. We adopt an image-based RVE model, explicitly representing these domains as polycrystalline ensembles, incorporating particle boundary regions (UFG domain) as shown in Figure 5 (c). Figure 5 (d) shows the final RVE model for the Aluminium prepared by cold spraying, thus combined with the crystal plasticity equation. We analysed the impact of the topology on the plastic behaviour of the heterogeneous structure using a 2D representative volume elements ($90\ \mu\text{m} \times 60\ \mu\text{m}$) with an element size of $0.35\ \mu\text{m}$. For the FEM simulation, quadrilateral quadratic plane strain elements with reduced integration (CPE8R) were utilized in combination with a user-defined material subroutine. Periodic boundary conditions were applied in the RVE model to simulate an upward tensile loading scenario.

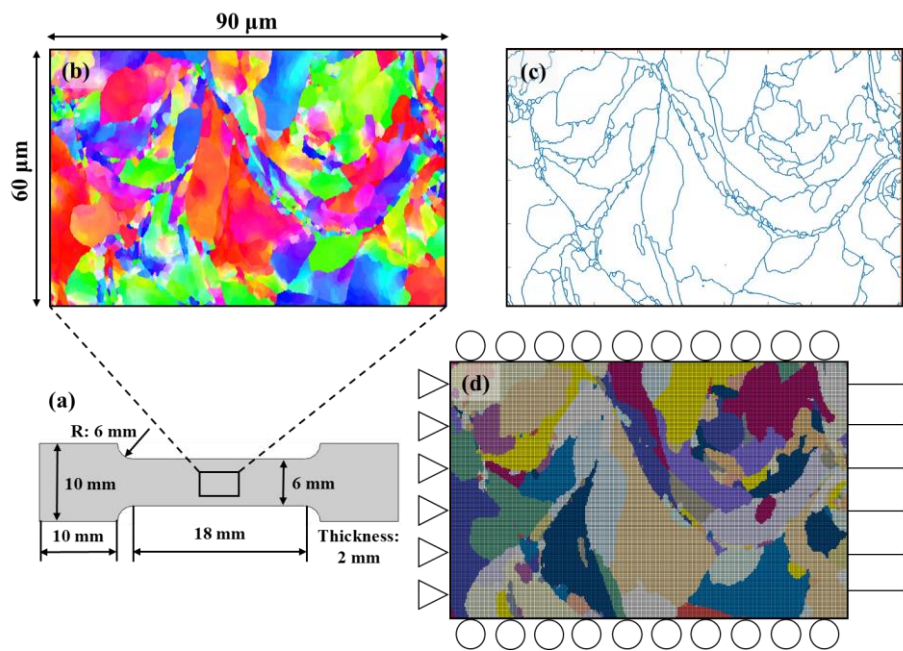


Figure 5: Process of configuration reconstruction: (a) sketch of tensile test sample with selected region for EBSD characterization; (b) EBSD IPF map; (c) grain boundary map; (d) EBSD-based RVE model with load condition.

The identification of elastic and plastic properties of materials from indentation tests has been extensively studied in the literature [8]. The classical dislocation density-based crystal plasticity theory equations can be found in the literature [9]. To enhance computational efficiency, the parameter identification for the constitutive model was conducted using the lsqnonlin algorithm in MATLAB. The target parameters were first assembled into a vector and initialized with estimated values. ABAQUS was then invoked from within the MATLAB working environment to perform simulations, and the parameters

were iteratively optimized using a nonlinear least squares approach. Once the deviation fell within an acceptable tolerance range between the experiment and simulation, the corresponding parameters were regarded as the optimal solution. The identified parameter values are presented in Table 1.

Table 1: Fitted crystal plasticity parameters of cold sprayed Aluminium.

Parameter	Variable	Unit
Reference slip rate	1435	1/s
The first obstacle profile	0.7	-
The second obstacle profile	1.3	-
Activation energy	5.00E-19	J
Lattice Boltzmann constant	1.38E-23	-
Absolute temperature	298	K
Lattice friction	37	MPa
Geometric factor in Taylor's strength	0.25	-
Shear modulus	29	GPa
Burgers vector per slip system	0.000286	μm
SSD density multiplication rate	200	1/ μm
SSD annihilation rate	1000	-
Initial dislocation density per slip system	1.4	μm^{-2}

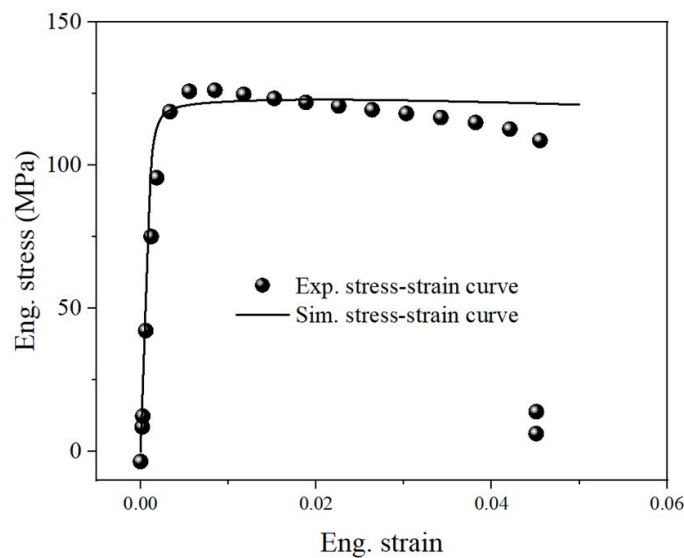


Figure 6: Comparison of tensile curve between simulation and experiment.

Virtual tensile deformation simulations of the cold-sprayed Aluminium crystals were conducted using the commercial finite element software ABAQUS/Standard, with single crystal plasticity models as material constitutive framework. Each integration point requires assigning a specific number of grains to represent a polycrystalline coarse or fine-grain material point, with each grain defined by its orientation and size. A macroscopic engineering strain of 0.05 was applied in for the virtual test. Figure 6 presents the comparison of experiment and simulation curve. The curve obtained from crystal plasticity parameter fitting aligns well with the experimental results. While the experimental curve shows a downward trend, the simulation does not replicate this behaviour. This difference may result from the simulation not accounting for process-induced defects—such as porosity, variations in inter-particle bonding, and residual stresses—that are typical of cold-sprayed materials and can impact their mechanical response.

Figures 7 and 8 present the computed stress and strain distributions based on a real microstructure-based representative volume element model using the crystal plasticity constitutive law. The results reveal significant inhomogeneity in both stress and strain fields. Notably, high stress concentrations—up to 433 MPa—are observed near particle impact zones characterized by ultrafine grains. These stresses tend to localize at particle boundaries, particularly in regions with smaller grains. The areas of high stress correspond to localized strain bands, which are critical drivers of microstructural evolution. As shown in Figure 8, the strain distribution exhibits clear localization along grain boundaries and within grains possessing specific crystallographic orientations, underscoring the influence of crystal anisotropy on the deformation behaviour. In coarse-grained regions, strain localization leads to the formation of distinct 45-degree shear bands, indicative of plastic instability. Conversely, lower strain levels are observed in mechanically harder or more constrained regions. These findings suggest that microstructures promoting stress and strain localization—such as weak inter-particle bonding or pronounced grain boundary activity—may facilitate failure initiation at particle interfaces. Overall, the non-uniform strain distribution highlights the critical role of microstructural features, including grain orientation, grain boundary interactions, and particle-particle interfaces, which are intrinsic to the cold spray additive manufacturing process.

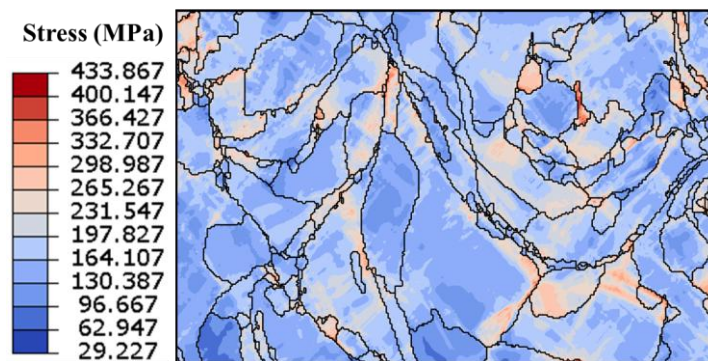


Figure 7: Contours of stress distribution.

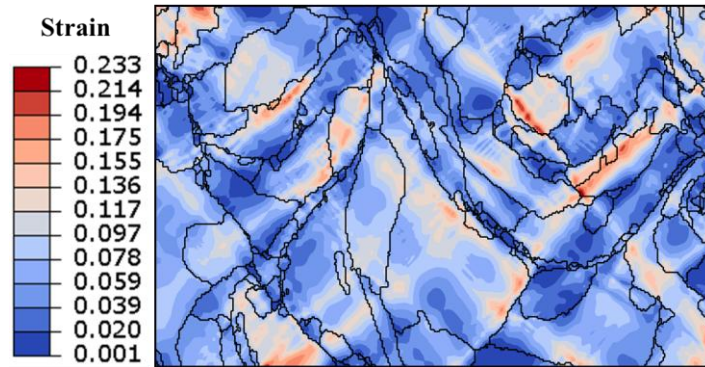


Figure 8: Contours of logarithmic strain distribution.

6 Conclusion

In this study, the microstructural analysis and multiscale modelling of an Aluminium deposit produced by the high-strain-rate self-consolidation in cold gas dynamic spray additive manufacturing were investigated. The combination of experimental results and modelling emphasizes the advantage of using a crystal plasticity model applied to a RVE microstructure which was built from the EBSD characterization of the deposit. The microstructure consists of fine equiaxed recrystallized grains mixed with fine elongated grains attributed to a dynamic recrystallization. This computational approach helps for understanding the stress and strain development within the fine microstructure generated by the high-speed collision of cold spraying. The results revealed stress concentrations at the boundaries between particles in the regions of fine grains due to localized strain bands. The strain distribution maps evidenced strain localization along the grain boundaries and within the grains with specific crystallographic orientations, confirming the role of crystal anisotropy in producing the deformation patterns.

Acknowledgement

The authors acknowledge the help of C. Verdy for the cold spray samples preparation. The authors also acknowledge the financial support by the China Scholarship Council (No. 202106220028).

References

- [1] Raelison, R. N., Verdy, C., & Liao, H., 2017. *Cold gas dynamic spray additive manufacturing today: Deposit possibilities, technological solutions and viable applications*. Materials & Design, 133, pp. 266-287.
- [2] Raelison, R. N., Xie, Y., Sapanathan, T., et al, 2018. *Cold gas dynamic spray technology: A comprehensive review of processing conditions for various technological developments till to date*. Additive Manufacturing, 19, pp. 134-159.

- [3] Rokni, M. R., Widener, C. A., & Champagne, V. R., 2014. *Microstructural evolution of 6061 aluminum gas-atomized powder and high-pressure cold-sprayed deposition*. Journal of thermal spray technology, 23, pp. 514-524.
- [4] Koithara, L. L., Raoelison, R. N., Costil, S., 2020. *Flow phenomenon of micron-sized particles during cold spray additive manufacturing: High-speed optic observation and characterization*. Adv. Powder. Technol. 31(3): pp. 1060-1079.
- [5] Lama, A., Sarvesha, R., John, D., et al, 2024. *Role of nitrogen and helium gases on microstructure and anisotropic mechanical properties of cold-sprayed scalmalloy deposits*. Journal of Materials Research and Technology, 30, pp. 1341-1353.
- [6] Adaan-Nyiak, M. A., Tiamiyu, A. A., 2023. *Recent advances on bonding mechanism in cold spray process: A review of single-particle impact methods*. Journal of Materials Research, 38(1), pp. 69-95.
- [7] Manap, A., Okabe, T., Ogawa, K., et al, 2019. *Experimental and smoothed particle hydrodynamics analysis of interfacial bonding between aluminum powder particles and aluminum substrate by cold spray technique*. The International Journal of Advanced Manufacturing Technology, 103, pp. 4519-4527.
- [8] Zhuang, Q., Yue, Z., Zhou, L., et al, 2022. *Study on Microstructural Evolution of DP Steel Considering the Interface Layer Based on Multi Mechanism Strain Gradient Theory*. Materials, 15(13), pp. 4590.
- [9] Qi, J., Yue, Z., Tuo, Z., et al, 2020. *Investigation on the Evolution of Subsequent Yield Surface of Pure Aluminum Under Changing Loading Paths Considering Microstructure Effects*. Journal of Materials Engineering and Performance, 29, pp. 303-314.