3D Microstructure-Based Finite Element Simulation of Cold-Sprayed Al-Al₂O₃ Composite Coatings Under Quasi-Static Compression and Indentation Loading

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Abstract This study developed microstructure-based finite element (FE) models to investigate the behavior of cold-sprayed aluminum–alumina (Al-Al₂O₃) metal matrix composite (MMC) coatings subject to indentation and quasi-static compression loading. Based on microstructural features (i.e., particle weight fraction, particle size, and porosity) of the MMC coatings, 3D representative volume elements (RVEs) were generated by using Digimat software and then imported into ABAQUS/Explicit. State-of-the-art physics-based modeling approaches were incorporated into the model to account for particle cracking, interface debonding, and ductile failure of the matrix. This allowed for analysis and informing on the deformation and failure responses. The model was validated with experimental results for cold-sprayed Al-34 wt.% Al₂O₃ and Al-46 wt.% Al₂O₃ metal matrix composite coatings under quasi-static compression by comparing the stress versus strain histories and observed failure mechanisms (e.g., matrix ductile failure). The results showed that the computational framework is able to capture the response of this cold-sprayed material system under compression and indentation, both qualitatively and quantitatively. The outcomes of this work have implications for extending the model to materials design and for applications involving

different types of loading in real-world application (e.g., erosion and fatigue).

Keywords Al-Al₂O₃ MMC coating · aluminum · compression test · damage mechanisms · finite element simulation · microstructure-based model

Introduction

Aluminum (Al)-based metal matrix composites (Al-MMCs) have been widely used to enhance surface performance (Ref 1–4) due to their superior mechanical properties such as high stiffness and strength (Ref 5), low coefficient of thermal expansion (Ref 6), improved wear (Ref 7) and corrosion resistance (Ref 8), and better creep–fatigue performance (Ref 9). To fabricate Al-MMCs, a wide range of reinforcing ceramic particles are added to an Al matrix (e.g., SiC (Ref 10), Al₂O₃ (Ref 1), TiC (Ref 11), TiB₂ (Ref 12), and B₄C (Ref 13)). Among these reinforcing particles, Al₂O₃ has been frequently used due to improved corrosion resistance and chemical stability (Ref 14). Recently, the Al-Al₂O₃ composites fabricated by the cold spray additive manufacturing process have been used as protective coatings against wear, erosion, corrosion, and high temperature degradation in aerospace and other industrial sectors (Ref 15, 16). Among many deposition routes for producing coatings made of pure Al, cold spray stands out due to minimal heat loading of the substrate during the deposition process (Ref 17). In addition, this additive manufacturing method provides the possibility of producing multi-phase coatings via mixing feedstock powders by which the hard phases such as SiC and Al₂O₃ can be incorporated effectively in the Al-MMCs coatings

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(Ref 18). These hard particles play a critical role in lowering the wear rate of the ceramic–metal coatings (Ref 19).

In research studies on experimental mechanics of ceramic–metal composite coatings, the behavior of cold-sprayed MMC coatings has been extensively addressed in terms of dry sliding wear (Ref 20), indentation (Ref 15), flexural properties (Ref 21), and erosion (Ref 16). However, there are a limited number of articles that investigate the response of MMC coatings through computational approaches, which is addressed in the current study. For example, Bolelli et al. (Ref 22) generated 2D RVEs based on the SEM images of WC–CoCr and WC–FeCrAl coatings to simulate ball-on-disk test and compression. The matrix and hard particles were modeled as elastic–plastic and pure elastic materials, respectively. The numerical results of Bolelli et al. (Ref 22) were compared with experiments based on the morphology of the worn surfaces and Young's modulus. In a separate study by Balokhonov et al. (Ref 23), 2D models at micro-, meso-, and macro-scales have been implemented by using the finite difference method for MMC coatings under tension and compression. It was found that curvilinear interfaces lead to stress concentration giving rise to the formation of shear bands in the Al matrix locally as well as cracking in the ceramic particles.

From a computational perspective, the majority of previous studies on Al-MMCs have focused on axial tensile loading, by which the microstructure has been modeled via 2D (Ref 24) and 3D (Ref 25) RVEs. In a large number of studies, the occurrence of the three competitive damage mechanisms in particulate-reinforced Al matrix composites (PRAMCs) subject to tension, such as matrix ductile failure, matrix/particle debonding, and particle cracking, has been mainly explored by using phenomenological ductile failure criteria (Ref 25), cohesive zone models (Ref 26), and a conventional brittle cracking model (Ref 13) (i.e., elastic cracking behavior which employs the Rankine criterion for failure initiation (Ref 48)), respectively. For example, Zhang et al. (Ref 25) investigated the behavior of a 7vol.% SiCp/Al composite made by a stir casting technique and incorporated the three damage mechanisms in a real microstructure-based 3D RVE. The numerical results revealed that particle fracture and interfacial debonding emerged as the initial failure mechanisms in the composite under tensile loading.

In contrast to the numerous numerical studies that explore the tensile behavior of Al-MMCs, limited efforts have been made to address the indentation and compressive behavior computationally, particularly with emphasis on damage mechanisms. For example, Park et al. (Ref 27) investigated Al-SiC MMCs under quasi-static compression up to 1% strain using a statistical synthetic RVE made by the DREAM.3D software—no damage mechanisms were

incorporated into the model. The indentation behavior of MMCs has been frequently explored via 2D models (Ref 28). More recently, Shedbale et al. (Ref 29) employed homogeneous and heterogeneous 3D FE models to study the ball indentation response of particulate-reinforced MMCs. The results showed that the heterogeneous model tends to overestimate the hardness compared to the experiments due to the local concentration of particles under the indenter.

Motivated by previous numerical studies, which primarily focus on the tensile response of MMCs, this work aims to investigate the compressive and indentation behavior of Al–Al₂O₃ coatings by using 3D RVEs produced by Digimat software based on microstructural characteristics obtained using scanning electron microscope images. To account for the damage mechanisms, the Gurson–Tvergaard–Needleman (GTN) model (Ref 30) was applied to the Al matrix and the matrix/particle debonding was modeled by the CZM method (Ref 31). For the ceramic particle phase, the Johnson–Holmquist II (JH2) model (Ref 32) was used to incorporate particle cracking into the FE model. The model was validated with the experimental data for Al-34 wt.% Al₂O₃ and Al-46 wt.% Al₂O₃ coatings in terms of stress–strain histories, failure mechanisms, and Vickers hardness. The results show that the model has the potential to be employed for future parametric studies for material design and optimization, which tailors concentration of reinforcing particles to balance strength and density for weight-sensitive applications.

Experimental Procedures

Material and Specimen Preparation

In this study, pure Al and Al–Al₂O₃ composite coatings were fabricated using a low-pressure cold spray system (SST series P, CenterLine Ltd., Windsor, ON, Canada), as shown schematically in Fig. 1(a), which was connected to a volumetric powder feeder (5MPE, Oerlikon Metco, Westbury, NY, USA). Based on previous studies (Ref 2, 33, 34), the air temperature and pressure were set to 375 °C and 620 kPa, respectively. The nozzle was manipulated by a robot (Motoman HP-20, Yaskawa Electric Corp., Waukegan, IL, USA). The cold spray nozzle traversed across the Al substrate at a speed of 15 mm/s to transfer the feedstock powder to the substrate, and the deposition process produced five layers of the coating. The feedstock powder blend was developed through a three-step process: gas atomization, sieving, and mixing (see Fig. 1a). Aluminum (99.0%) powder (CenterLine Ltd., Windsor, ON, Canada) and α -Al₂O₃ with a purity of 99.5% (Amdry 6060, Oerlikon Metco Inc., Westbury, NY, USA) were used in this

Fig. 1 Preparation, test, and characterization of Al-Al₂O₃ composite coatings: (a) A schematic illustration of the cold spray setup used for the fabrication of pure Al and MMC coating samples: The processing strategy for making the mixed powder includes gas atomization, sieving, and mixing using a rotated cylinder; (b) typical compressive cuboidal specimen with dimensions 2.3 mm × 2.7 mm × 3.5 mm cut from the composite depositions via wire electrical discharge machining, which was loaded in the direction of the 3.5 mm dimension. The green contour shows the region of interest defined on the specimen surface in VIC-2D software for monitoring the strain fields. The top

image shows an example of Al-Al₂O₃ coating deposited on an Al substrate from which the cuboidal specimens were cut; (c) SEM characterization of the microstructure of Al-34 wt.% Al₂O₃ composite coating showing the distribution and morphology of the reinforcing ceramic particles in the Al matrix; (d) SEM micrograph of Al-46 wt.% Al₂O₃ composite coating. Note that the black arrows on the SEM micrographs show the deposition direction. The darker regions correspond to the Al phase and the lighter regions correspond to the alumina phase

study. The Al and Al₂O₃ powders were sieved to obtain a size distribution of 40–60 and 30–45 μm, respectively. The Al and Al₂O₃ powders were admixed to produce powder blends containing 0, 60, and 90 wt.% Al₂O₃. This process was conducted using a cylinder with a 20 mm diameter whose angular velocity and operating time were set to 20 RPM and 30 minutes, respectively. As shown by Shao et al. (Ref 33), when deposited into coatings, the mixed powder

blend with 60 wt.% Al₂O₃ produced coatings that were Al-34 wt.% Al₂O₃ and the mixed powder blend with 90 wt.% Al₂O₃ produced coatings that were Al-46 wt.% Al₂O₃.

Mechanical Testing and Characterization

As shown in Fig. 1(b), the cold-sprayed coating deposits were cut into cuboidal specimens with dimensions of 2.3

mm in length, 2.7 mm in width, and 3.5 mm in height using wire electrical discharge machining. The samples were used for quasi-static compression testing, where the loading was applied in the direction of the 3.5 mm dimension. The experiments were conducted using the displacement control technique up to a maximum displacement of 1 mm at a constant rate of $1 \times 10^{-3} \text{ s}^{-1}$ using an Instron 3365 testing machine (Instron, Norwood, Massachusetts, USA). To visualize the features of the macroscopic deformation of the specimen surface, the machine was equipped with an AOS PROMON U750 high-speed camera with a full resolution of 1280×1024 and a VIC 900170WOF LED laser light guide for illumination. This assembly was coupled with digital image correlation (DIC) capabilities using VIC-2D (v6 2018) software (Ref 35) (Correlated Solutions Irmo, SC, USA) to monitor the strain fields, which is detailed in Shao et al. (Ref 33). The specimen was aligned between the loading platens made from M2-graded high-speed steel with a diameter of 1 inch (see Fig. 1b), and extreme pressure grease was applied on the interfaces to eliminate the effect of friction and allow free lateral expansion. The compression tests were carried out as per ASTM Standard C1424-15 (Ref 36) at room temperature and repeated four times for each coating with different reinforcing particle content. To inform the microstructure-based models as related to the reinforcing particle content, porosity, particle shape, size, and distribution, microstructural characterization was done using a field-emission SEM coupled with energy-dispersive x-ray spectroscopy (EDS) operated at 20 kV (Zeiss Sigma, Oberkochen, Baden-Württemberg, Germany), as shown in Fig. 1(c) for the Al-46 wt.% Al_2O_3 composite. The porosity of the samples was estimated using ImagePro software coupled with the SEM images, and the porosity was found to be $2.84 \pm 0.31 \text{ vol.}\%$ in pure Al, $0.23 \pm 0.04 \text{ vol.}\%$ in Al-34 wt.% Al_2O_3 , and $0.17 \pm 0.03 \text{ vol.}\%$ in Al-46 wt.% Al_2O_3 . In addition, the EDS analysis revealed that the feedstock powders with 60 and 90 wt.% Al_2O_3 led to depositions with 34 ± 2.56 and $46 \pm 2.04 \text{ wt.}\%$ of ceramic particles, respectively.

Numerical Methodology

A 3D FE model based on the coating microstructural features is presented to explore the behavior of Al- Al_2O_3 MMC coatings under quasi-static compressive loading. The 3D representative volume elements (RVEs) were generated by the Digimat software for Al-34 wt.% Al_2O_3 and Al-46 wt.% Al_2O_3 MMCs. The RVEs were imported into the ABAQUS/Explicit solver (release 6.14). For the micro-indentation test, the homogenization approach (Ref 29) was applied and experimental compression data were

used to extract the effective mechanical properties for each MMC coating sample.

Geometry and Model Description

RVEs with different sizes have been considered in previous studies (Ref 13, 37). For example, Ma et al. (Ref 37) found no significant difference in the tensile stress–strain responses by varying the RVE size from 20 μm to 50 μm . In this study, an RVE length of 100 μm was chosen based on the microstructural features (e.g., average reinforcing particle size of 15 μm). The SEM images (see Fig. 1c and d) were first used to extract the distribution of particle size in the composites (e.g., the size of the alumina particles range from 1 to 30 μm in the Al-46 wt. % Al_2O_3 composites (see Fig. 1c). Next, the measured range of distribution was incorporated into the RVE using a uniform distribution in the Digimat software, which accounts for the variation and uncertainty in the particle size distribution that is likely to be observed through the SEM images from different locations of the sample. Additionally, the reinforcing ceramic particles represent an irregular shape in the SEM micrographs. Here, an icosahedron geometry was used to account for the shape of the particles, which has also been used to represent the irregular-shaped particles in previous studies involving MMC coatings (Ref 37–39). The time step was set at 2 μs , which was found to meet the quasi-static loading condition (Ref 40). As shown in Fig. 2(a), the top and bottom boundary faces have been fully restricted to the reference points (RPs) by the kinematic coupling constraints to facilitate application of load/boundary conditions and obtain the stress–strain response of the RVE. A corner of the RVE was fully restricted to prevent the material from rigid boundary motion. The degrees of freedom of the bottom boundary face were fixed within all degrees of freedom, except for the in-plane displacements (i.e., Y- and Z-directions in Fig. 2b). The same boundary conditions for application of compressive loading were also used in other studies (Ref 41, 42). All of the constituents were discretized by 3D linear tetrahedral C3D4 elements. Following a mesh quality assessment to decrease the likelihood of element distortion at high strains, an average element size of 1.5 μm was used. On this basis, the RVE for Al-34 wt.% Al_2O_3 and Al-46 wt.% Al_2O_3 MMCs was meshed by 741,222 and 1,275,358 elements, respectively. Micro-indentation Vickers testing of the composite coatings was simulated via the homogenization approach (Ref 29). The effective mechanical properties, including the Young's modulus and flow stress, were extracted from the experimental compressive stress–strain histories for each particle concentration in the coatings and were an input into the approach. Figure 3 shows the FE model of the Vickers test. Due to symmetry, only

Fig. 2 (a) Application of kinematic coupling between the boundary faces and the reference points (RP) in yellow color to apply compressive load and boundary conditions: All degrees of freedom were coupled to each other; (b) the boundary conditions applied on the RVE: The displacement control technique was applied to the RP in red color using a smooth amplitude to meet the quasi-static condition

Fig. 3 Finite element model of the micro-indentation Vickers test. The block and the indenter were discretized by 30,276 first-order eight-node 3D elements with reduced integration (C3D8R) and 2104 quadrilateral four-node 3D rigid elements (R3D4), respectively

one quarter of the homogenized block with symmetric constraints was modeled. The size of the block was determined as per the work of Shedbale et al. (Ref 29) to achieve convergence in the indentation response.

As shown by Shedbale et al. (Ref 29), the Vickers indenter was considered as a discrete rigid body and fully confined, except for the vertical direction Y (see Fig. 3). The bottom surface of the block was fixed, and the lateral surfaces were free to deform. A frictionless contact was

defined between the indenter and the top surface of the block, which was implemented by the standard surface-to-surface contact algorithm (Ref 29). By using an average element size of 5 μm, the block and the indenter were meshed by using 30,276 first-order eight-node 3D elements with reduced integration (C3D8R) and 2104 quadrilateral four-node 3D rigid elements (R3D4), respectively.

Material Models

In this study, the micromechanical-based Gurson–Tvergaard–Needleman (GTN) model (Ref 30) was applied to capture the matrix failure. Given experimental evidence of particle cracking and interfacial debonding under compression, the Johnson–Holmquist II (JH2) model (Ref 32) for the failure of ceramic particles and the cohesive zone model (CZM) approach (Ref 31) for the matrix/particle debonding failure were incorporated into the model.

The GTN Model for Matrix Failure

Ductile failure of metals occurs as a result of a three-stage mechanism of nucleation, growth, and coalescence of voids. Voids are nucleated from an inclusion or as a consequence of either cracking or decohesion of second-phase particles and then grow due to the localization of plastic strain under a high stress triaxiality state (Ref 43). To analyze this phenomenon theoretically, the porous metal plasticity model proposed by Tvergaard and Needleman (i.e., the GTN model) (Ref 30), as a modified version of the Gurson model (Ref 44), has been widely used (Ref 45–47). The yield function of the GTN model is expressed as follows:

$$\emptyset(\sigma, f) = \left(\frac{\sigma_q}{\sigma_y} \right)^2 + 2q_1 f^* \cosh \left(\frac{3q_2 p}{2\sigma_y} \right) - (1 + q_3 f^{*2}) = 0, \quad (\text{Eq 1})$$

where $\emptyset$ denotes the non-dilatational strain energy and q_1 , q_2 , and q_3 are the constants proposed by Tvergaard (Ref 48) to account for the effects induced by void interaction due to multiple-void arrays and to provide better consistency with experimental data. Here, σ_q and σ_y represent von Mises stress and the flow stress of the undamaged material. To model the rapid deterioration of stress carrying capacity caused by void coalescence, the parameter, f^* , known as the effective porosity was first introduced by Tvergaard–Needleman (Ref 30). The function is specified as follows:

$$f^* = \begin{cases} f & f \leq f_c \\ f_c + \frac{f_u^* - f_c}{f_F - f_c} (f - f_c) & f_c \leq f \leq f_F \\ f_u^* & f \geq f_F \end{cases}, \quad (\text{Eq 2})$$

where f_c is the critical void volume fraction (VVF) at the onset of the coalescence, $f_u^* = \frac{1}{q_1}$ corresponds to zero stress carrying capacity, and f_F denotes the VVF when the material has completely failed, which governs the element deletion process. The increase in the VVF is deemed as the summation of the increment owing to void nucleation and the growth of existing voids. The function can be written as

$$df = df_{\text{nucleation}} + df_{\text{growth}}. \quad (\text{Eq 3})$$

Assuming plastically incompressible behavior for the material, the void growth rate (i.e., df_{growth}) can be expressed as a function of the plastic volume change as follows:

$$df_{\text{growth}} = (1 - f) d\bar{\epsilon}_{ii}^p, \quad (\text{Eq 4})$$

where $d\bar{\epsilon}_{ii}^p$ denotes the trace of the plastic strain rate tensor. The nucleation of voids is considered to be exclusively dependent on the plastic strain, and it was assumed that occurrence of void nucleation occurred only under hydrostatic tension (Ref 49, 50). On this basis, the function is written as

$$df_{\text{nucleation}} = A_n d\bar{\epsilon}_m^p, \quad \text{where} \quad (\text{Eq 5})$$

$$A_n = \begin{cases} \frac{f_N}{s_N \sqrt{2\pi}} e^{-0.5 \left(\frac{\bar{\epsilon}^p - \bar{\epsilon}_N}{s_N} \right)^2} & \text{if } p \geq 0, \\ 0 & \text{if } p < 0 \end{cases}, \quad (\text{Eq 6})$$

where p represents the hydrostatic stress, f_N is the void volume fraction of the nucleated void, $\bar{\epsilon}_N$ is the mean equivalent plastic strain for void nucleation, and s_N is the standard deviation of the distribution. Here, the rate of equivalent plastic strain, $d\bar{\epsilon}^p$, is obtained by enforcing equality between the matrix plastic dissipation and the rate of macroscopic plastic work as follows:

$$d\bar{\epsilon}^p = \frac{\sigma : d\bar{\epsilon}^p}{(1 - f)\sigma_y}. \quad (\text{Eq 7})$$

Table 1 summarizes the constants of the GTN model used in this study. The proposed values by Tvergaard (Ref 48) were utilized for the q_1 , q_2 , and q_3 constants. From SEM characterization, the initial porosity, f_0 , was assumed to be an average quantity of 0.0017 and 0.0023 for Al-34 wt.% Al₂O₃ and Al-46 wt.% Al₂O₃ composites, respectively. The parameters $\bar{\epsilon}_N$, s_N , and f_N were obtained from previous studies for pure Al (Ref 39, 51).

The JH2 Model for Particle Cracking

For damage modeling of ceramics, the phenomenological Johnson–Holmquist models have been commonly used (Ref 38, 52–54) to depict the behavior of these materials, including pressure-dependent strength, strain rate dependency, and dilation or bulking effects (Ref 32). The strength and damage are expressed as analytical functions of pressure and other parameters as (Ref 32)

$$\sigma^* = \sigma_i^* - D(\sigma_i^* - \sigma_f^*), \quad (\text{Eq 8})$$

$$\sigma_i^* = A(P^* + T^*)^N (1 + C \ln \bar{\epsilon}^*), \quad \text{and} \quad (\text{Eq 9})$$

Table 1 GTN model constants used in this study

q_1 (Ref 48)	q_2 (Ref 48)	q_3 (Ref 48)	f_0 (Ref 33)	f_c (Ref 51)	f_F (Ref 51)	ε_N (Ref 39)	S_N (Ref 39)	f_N (Ref 51)
1.5	1	2.25	0.0017	0.1	0.45	0.3	0.1	0.25

Here, the value of f_0 corresponds to the composites with 34 wt.% of reinforcing particles. For Al-46 wt.% Al_2O_3 composites, the initial porosity was determined to be 0.0023 on average, while all other constants remain the same as the 34 wt.% case

Table 2 The JH2 constants used for Al_2O_3 reinforcing particles (Ref 54, 55)

Parameter	Value	Unit
A	0.93	...
B	0.31	...
N	0.6	...
M	0.6	...
C	0	...
K_1	193	GPa
K_2	0	GPa
K_3	0	GPa
d_1	0.005	...
d_2	1	...
ρ	3890	kg/m ³
G	155	GPa
T	0.6	GPa
HEL	10.5	GPa
P_{HEL}	4.5	GPa
$\sigma_{i,\text{max}}$	12.2	GPa
$\sigma_{f,\text{max}}$	1.3	GPa
$\varepsilon_{f,\text{min}}$	0	...
$\varepsilon_{f,\text{max}}$	1.2	...
FS	0.2	...
β	1	...

$$\sigma_f^* = B(P^*)^M (1 + C \ln \dot{\varepsilon}^*) \leq \text{SFMAX}, \quad (\text{Eq 10})$$

where σ^* and σ_i^* represent the normalized intact equivalent stress, σ_f^* denotes the normalized fracture stress, and D is the damage variable, varying from 0 to 1. Here, $\sigma^* = \sigma/\sigma_{\text{HEL}}$, $P^* = P/P_{\text{HEL}}$, $T^* = T/P_{\text{HEL}}$, and $\dot{\varepsilon}^* = \dot{\varepsilon}/\dot{\varepsilon}_0$, where σ is the actual equivalent stress, σ_{HEL} is the equivalent stress at the Hugoniot elastic limit (HEL), P is the actual pressure, P_{HEL} is the pressure at the HEL, T is the maximum tensile hydrostatic pressure tolerated by the material, $\dot{\varepsilon}$ is the actual strain rate, and $\dot{\varepsilon}_0 = 1$ is the reference strain rate. A , B , C , M , and N are material constants which need to be calibrated for each material. The maximum value of σ_f^* is defined by SFMAX (i.e., the maximum limitation of the normalized fractured strength). Once the yield function is met as per Eq 11, the damage begins to accumulate based on the incremental equivalent plastic strain defined as

$$\emptyset(\sigma, f) = \sigma_q - \sigma_{\text{HEL}} \sigma^* \geq 0, \quad (\text{Eq 11})$$

$$D = \sum \frac{\Delta \varepsilon_{\text{eff}}^p}{\varepsilon_f^p}, \text{ and} \quad (\text{Eq 12})$$

$$\varepsilon_f^p = D_1 (P^* + T^*)^{D_2}, \quad (\text{Eq 13})$$

where σ_q , D_1 , and D_2 are deemed as material constants. To calculate pressure, P , a polynomial equation of state (EOS) is employed, which is defined as

$$P = \begin{cases} K_1 \eta + K_2 \eta^2 + K_3 \eta^3 + \Delta P & \eta > 0 \\ K_1 \eta & \eta \leq 0 \end{cases}, \quad (\text{Eq 14})$$

$$\Delta P_{t+\Delta t} = -K_1 \eta_{t+\Delta t} + \sqrt{(K_1 \eta_{t+\Delta t} + \Delta P_t)^2 + 2\beta K_1 \Delta U}, \quad (\text{Eq 15})$$

$$\Delta U = U_t - U_{t+\Delta t}, \text{ and} \quad (\text{Eq 16})$$

$$U = \frac{\sigma_y^2}{6G}, \quad (\text{Eq 17})$$

where K_1 denotes the bulk modulus, K_2 and K_3 are material constants, η is the specific volume, U represents the internal energy which is related to the equivalent plastic flow stress σ_y by a quadratic expression, β is the fraction of the elastic energy loss converted to potential hydrostatic energy, and the shear modulus is shown by G . The 21 constants of the JH2 model for Al_2O_3 were obtained from previous studies (Ref 54, 55) and are summarized in Table 2.

The Cohesive Zone Model for the Interfacial Debonding

The cohesive zone model (CZM) was first proposed by Barrenblatt (Ref 31) and Dugdale (Ref 56) and is now widely used as an effective approach for modeling the fracture process in materials such as polymers, metals, ceramics, concretes, and laminated composites (Ref 57). It was assumed that matrix/particle interface debonding occurs when the quadratic interaction function involving the nominal stress ratios attains unity as follows (Ref 58):

$$\left(\frac{T_n}{T_n^0}\right)^2 + \left(\frac{T_s}{T_s^0}\right)^2 + \left(\frac{T_t}{T_t^0}\right)^2 = 1, \quad (\text{Eq 18})$$

where T_n , T_s , and T_t represent the tractions acting on the

interface at a load increment in normal and in two in-plane shear directions, respectively. Likewise, T_n^0 , T_s^0 , and T_t^0 denote the tractions at the onset of damage initiation in normal and in two in-plane shear directions. Note that the normal traction is tensile and pure compressive stress does not lead to decohesion. The components of the traction–separation law are written as follows:

$$T_n = \begin{cases} (1-D)T_n^* & T_n^* \geq 0 \\ T_n^* & T_n^* < 0 \end{cases}, \quad (\text{Eq 19})$$

$$T_s = (1-D)T_s^*, \text{ and} \quad (\text{Eq 20})$$

$$T_t = (1-D)T_t^*, \quad (\text{Eq 21})$$

where T_n^* , T_s^* , and T_t^* are the stress components calculated by the elastic traction–separation behavior for the current strain prior to the damage initiation. D denotes the damage variable which begins to gradually increase from 0 to 1 with further loading once the debonding initiation criterion expressed by Eq 18 is met. The damage variable is defined as (Ref 58)

$$D = \begin{cases} 0 & \delta_m^{\max} \leq \delta_m^0 \\ \frac{\delta_m^f(\delta_m^{\max} - \delta_m^0)}{\delta_m^{\max}(\delta_m^f - \delta_m^0)} & \delta_m^0 < \delta_m^{\max} < \delta_m^f \\ 1 & \delta_m^{\max} > \delta_m^f \end{cases}, \quad (\text{Eq 22})$$

where δ_m^0 and δ_m^f represent the effective separations at damage initiation and complete failure, respectively. The maximum value of the effective displacement during the loading process at each increment is shown by $\delta_m^{\max}$. The effective separation at each load increment δ_m is calculated as (Ref 58)

$$\delta_m = \sqrt{\delta_n^2 + \delta_s^2 + \delta_t^2}, \quad (\text{Eq 23})$$

where δ_n , δ_s , and δ_t are the nominal separations in normal and in two in-plane shear directions, respectively. To obtain the effective separation at complete decohesion, one can use the fracture energy G_c , which is given as

$$\delta_m^f = \frac{2G_c}{T_n^0}. \quad (\text{Eq 24})$$

The CZM constants used in this study are presented in Table 3. For Al-MMC composites, the CZM constants have been reported in different ranges in the previous studies (Ref 13, 59–62). For example, the reported values for the

interface strength vary from a quantity on the order of MPa (Ref 61) to GPa (Ref 62). The values in Table 3 were selected to establish the best match between the experimental and numerical outcomes in this research study.

Results

Quasi-Static Compression

The numerically predicted results for Al-34 wt.% Al_2O_3 and Al-46 wt.% Al_2O_3 coatings under quasi-static compression are compared with those of the experiments in terms of the stress versus strain histories and observed failure mechanisms. This can provide insights for establishing an accurate computational framework to further explore the behavior of the material that can eventually give rise to a tool for material design and optimization. Figure 4 shows the predicted stress–strain responses in comparison with those measured by experiments. The pure Al and MMC samples were all experimentally tested in different directions, namely the nozzle traverse (travel) direction, the second in-plane direction perpendicular to the nozzle travel direction, and the deposition direction represented by X, Y, and Z, respectively, in Fig. 4.

For the pure Al matrix, the results based on the data for the Z-direction were compared to experiments, as shown in

Fig. 4 Numerical (Num) and experimental (Exp) stress–strain responses under quasi-static compression for different weight percentage of alumina in the Al matrix. The cuboidal samples were all tested in three different directions denoted by X, Y, and Z corresponding to the nozzle moving direction, the second in-plane direction perpendicular to the nozzle moving direction, and the deposition direction, respectively. The dashed curves correspond to the experimental responses for each coating, and the solid curves represent the associated numerically predicted behavior

Table 3 Summary of the matrix/particle interface properties

Parameter	K_{nn}, K_{ss}, K_{tt}	T_n^0, T_s^0, T_t^0 (Ref 61)	δ_m^f (Ref 61)
Value	2E7 MPa mm ⁻¹	705 MPa	0.00035 mm

the red solid curve in Fig. 4. The predicted curve for the pure Al matrix aligns with the experimentally measured one, which shows the accuracy of the approach for modeling the pure Al coating. Regarding the predicted responses for the MMCs, the model can reasonably capture the stiffness (i.e., the Young's modulus) and the maximum load bearing capacity of the composite coatings with different reinforcing particle concentrations. In addition, the experimental trend toward decreasing ductility with an increase in reinforcing particle content from 34 to 46 wt.% is reasonably reflected in the numerically predicted curves. Namely, plastic deformation in the Al-34 wt.% Al_2O_3 composite coating begins to take place in the model at a strain of 0.6%, which leads to a yield stress of 141 MPa. The experimental yield strain ranges from 0.53% to 0.65% and the yield stress ranges from 135 MPa to 178 MPa based on the different coordinate directions that were explored. The model tends to slightly underestimate the yield stress of the MMC with 34 wt.% of the reinforcing inclusions. This is likely due to cold working, which introduces a hardening and strengthening effect in the matrix during the cold spray process. This is a result of the high-velocity hard ceramic particles impacting on the Al grains (Ref 18, 63), which is not yet considered in the model. In addition to cold working, there are also other mechanisms that are likely to cause the deviations observed between the predicted and experimental stress versus strain histories as it relates to strain hardening behavior and elongation at failure. Among these mechanisms, grain size effects (Ref 64, 65) (e.g., Hall–Petch relationship (Ref 66)), which require implementation of strain gradient plasticity models (Ref 67) in the model of this study, may also play a role.

Figure 5 illustrates the contour of the plastic deformation (Ref 68), interfacial failure (Ref 26), and particle cracking (Ref 24) at two different axial strains during the loading process for the Al-34 wt.% Al_2O_3 composite. With the further application of load, the plastic strain begins to accumulate in the ligament between the particles closely aligned together (see Fig. 5a), which has been reported in previous studies of 2D RVEs (Ref 68). The localization of plastic strain leads to the growth of the void volume fraction in the matrix resulting in a gradual decrease in matrix flow stress. (See the solid black curve in Fig. 4.) In addition, as the strain exceeds 4%, matrix/particle debonding and a particle cracking failure mechanism manifest and develop with the increase in applied load within the RVE (see Fig. 5b and c), particularly at the sharp corner and concaves of the particles (Ref 68). This behavior can be attributed to the mismatch between the mechanical constants as well as the stress concentration at the curvilinear interfaces (Ref 23). Consequently, the flow stress remains almost constant from 5% strain to a strain of 15% and then

rises slightly with a further increase in load up to the end of the loading cycle. This behavior is also reflected in the experimental curves, as matrix failure happens locally and does not lead to fracture of the sample (Fig. 4—the dashed curves for the 34 wt.% Al_2O_3 MMCs). From simulation, it can be implied that the spatial distribution of the particles affected by the number of particles and the mean free path parameter (i.e., inter-particle spacing of the reinforcing phase) (Ref 69)—which is determined by the weight percentage of the inclusions—does not lead to fracture of the Al-34 wt.% Al_2O_3 MMC sample, since the number of thin ligaments is not critical enough to develop a 45° shear band (Ref 13, 68), fracturing the specimen. This numerical implication (i.e., the microcracks in the matrix do not evolve to fracture the sample) is also corroborated by the experimental observation of the deformed sample at the end of the loading and the corresponding SEM micrograph shown in Fig. 5(d). As shown, damage mechanisms such as ductile matrix failure and interfacial decohesion emerge locally, leading to the formation of dispersed microcracks that do not coalesce to cause failure in the sample at macro-length scales. For the Al-46 wt.% Al_2O_3 composite, the predicted yield strain and yield strength are 0.7% and 253 MPa, respectively, while the measured yield strain varies between 0.79% and 0.83%, and the yield strength varies between 298 MPa and 317 MPa for the different coordinate directions. The larger discrepancy in the predicted yield stress of the Al-46 wt.% Al_2O_3 MMC compared to that of the Al-34 wt.% Al_2O_3 MMC can be another indication of the importance of including the cold spray-induced hardening and strengthening effect in the model in order to produce more accurate numerical results, especially for MMCs with a high percentage of particle reinforcement. Additionally, the earlier onset of the debonding failure mechanism in the model compared to the experiments can also play a role in the loss of stiffness prior to achieving peak load.

Figure 6 and 7 shows a comparison between the predicted and experimentally observed failure mechanisms in the Al-46 wt.% Al_2O_3 composite. As shown, the FE model can capture the occurrence of the three competitive damage mechanisms (i.e., matrix ductile failure, matrix/particle debonding, and particle cracking) of metal–ceramic coatings under compressive loading. In comparison with the MMC coating with 34 wt.% alumina reinforcement, the plastic strain is severely localized in the thin ligaments between the particles (see Fig. 6a) in the model. The model predicts the formation of 45° shear cracks passing through the Al matrix between the particles as observed in SEM images, as shown in Fig. 7. Once the strain exceeds 4%, particle cracking and matrix/particle debonding are initiated at the sharp corners of the particles (see Fig 6b and c)—which have been experimentally observed, as shown in

Fig. 5 The numerically predicted manifestation and evolution of the damage mechanisms in Al-34 wt.% Al_2O_3 MMC at an axial strain of 4% and 10%: (a) The equivalent plastic strain (PEEQ), which reveals the evolution of plastic deformation in the thin ligaments between the ceramic particles; (b) the data show the scatter of matrix/particle debonding failure criterion demonstrating the initiation of interfacial failure at the sharp corners of inclusions; (c) the distribution of the JH2 damage parameter shows the accumulation of damage and

element removal in the concaves of particles either at the boundary surfaces or considerably close to each other; (d) SEM micrograph of the Al-34 wt.% Al_2O_3 MMC subject to quasi-static compression showing the localized occurrence of damage mechanisms (e.g., matrix ductile failure and matrix/particle decohesion) at a micro-length scale, which does not lead to the coalescence of microcracks and global failure of the composite at the macroscale

Fig. 6 The numerical qualitative results for the Al-46 wt.% Al_2O_3 MMC shown at an axial strain of 4% and 10%: (a) The contour shows the distribution of void volume fraction in the Al matrix, which accumulates in the thin ligaments between the alumina particles forming $\sim 45^\circ$ shear cracks as the strain reaches 10%; (b) the spatial distribution of matrix/particle decohesion damage variable (CSDMG)

which illustrates more severely debonding failure compared to the Al-34 wt.% Al_2O_3 MMC (see Fig. 5b). This results in loss of stiffness and load sustaining capacity as shown in Fig. 4 (see the solid blue curve); (c) the data illustrates the evolution of particle cracking initiating from the sharp corners within the RVE as the axial strain increases from 4% to 10%

Fig. 7 SEM micrograph of the Al-46 wt.% Al_2O_3 MMC subject to quasi-static compression showing the simultaneous occurrence of failure mechanisms, namely matrix ductile failure, matrix/particle interfacial failure, and particle cracking. The 3D numerical predictions of the failure mechanisms (see Fig. 6 for more details) have been

correspondingly shown, which confirm the qualitative validity of the model. The damaged areas are shown in black. Note that this micrograph represents the cuboidal sample loaded in the Y -direction and has been observed through X (i.e., the nozzle moving direction) direction

Fig. 7—and then propagate within the RVE. These failure mechanisms are accompanied by matrix failure due to void growth in the thin ligaments (see Fig. 6a). Once the strain exceeds 5%, the stress bearing capacity starts to decrease slightly and then remains constant up to a strain of 12% (Fig. 4—the solid blue curve). This is a consequence of the development of the damage modes. The elements of the Al matrix in which the porosity has exceeded the critical value are removed from the mesh, leading to an abrupt decrease in load sustaining capacity (see Fig. 4—the solid blue curve at a strain of $\sim 12\%$). This behavior is in agreement with the experimental trend that the material's load sustaining ability decreases after a given strain is reached. Overall, the reasonable agreement between the numerical and experimental findings in terms of stress–strain behaviors and failure mechanisms reveals the applicability of the model to conduct parametric studies that translate into tailoring particle and concentration size to control competition between failure mechanisms toward improving strength–density trade-offs.

Vickers Micro-indentation

The numerical outcomes of the homogenization approach were validated by Vickers hardness experiments. In the experiments, Vickers micro-indentation was applied to the samples with a load of up to 10 N as per ASTM Standard E384 (Ref 70). Figure 8(a) shows the plastically deformed area after complete unloading for the homogenized model of each MMC composite. From the figure, the diagonal

length of the indented area decreased as the particle concentration increased, which results in a higher hardness. In other words, at a critical load, the composite material with a higher particle content is less deformed due to the enhanced stiffness and flow stress induced by the hard alumina particles.

Figure 8(b) illustrates the residual von Mises stress distribution for a load of 10 N after unloading in the homogenized model of Al-34 wt.% Al_2O_3 MMC. The distribution pattern for different particle concentrations is the same, and the magnitude of the residual stress rises with an increase in the percentage of alumina particles. From Fig. 8(b), the residual stress follows a continuous distribution as the model does not explicitly account for the microstructure, while the observations reported after using 2D heterogeneous models (Ref 28, 71) showed that the residual stress is localized between the particles. This implies that 3D microstructure-based models are needed to study how the residual stress is developed in the material more realistically. The Vickers hardness of the numerical data was computed using (Ref 72):

$$\text{HV} \approx 0.1891 \frac{F}{d^2} [\text{Kgf} \cdot \text{mm}^{-2}], \quad (\text{Eq 25})$$

where F represents the applied load and d is the diagonal length of the indented area. Figure 9 shows the numerically predicted Vickers hardness results in comparison with the experimental ones measured in three different directions, namely the nozzle travel direction, the deposition direction, and the third perpendicular direction represented by X , Z ,

Fig. 8 (a) Numerical prediction of the indented area for the MMC composites based on the homogenization approach. The numerically measured diameter, d , of the indented profile is substituted into Eq 25

to calculate the Vickers hardness; (b) the distribution of the residual von Mises stress in the homogenized block of Al-34 wt.% Al_2O_3 composite after unloading

Fig. 9 Comparison of experimental and numerical Vickers hardness of the MMC coatings. The X, Y, Z on the horizontal axis represent the direction over which the Vickers indentation was carried out on the samples which correspond to the nozzle travel direction, the deposition direction, and the third perpendicular direction, respectively. Unlike the experimental results, there is no variation in the predicted hardness values due to the homogenization approach

and Y, respectively. As shown, the homogenized model predicts the hardness of MMCs with an error of $10 \pm 3\%$ compared to the measured values. The heterogeneous modeling approach was reported to overestimate the hardness of MMCs in previous studies (Ref 28, 29, 71, 73) due to particle consolidation (Ref 74), which required

calibration of a significant number of parameters to reach acceptable agreement with the experiments, when compared to the homogenization approach. However, a 3D microstructure-based model allows flexibility to investigate the effect of the size, randomness, and morphology of the particles on the indentation behavior and hardness of cold-sprayed MMC coatings.

Discussion

This study is the first of its kind to develop 3D finite element models to explore the compressive behavior and hardness of Al- Al_2O_3 composite coatings fabricated by low-pressure cold spray. The presented microstructure-based models for the MMC coatings were built on previous studies of 3D modeling of tensile behavior (Ref 10, 11, 13, 37, 75–78) and 2D modeling of the compressive response (Ref 54, 68) of particulate-reinforced metal matrix composites. Our model culminated in an acceptable consistency between the numerical and experimental findings, both quantitatively (i.e., based on yield strain, yield strength, and stiffness) and qualitatively (i.e., based on initiation and propagation of damage mechanisms as well as the trends of stress versus strain histories), which lays the foundation to fill the gap in our computational

knowledge of ceramic–metal composite coatings. The extended 3D models of Al–Al₂O₃ MMC coatings were generated by Digimat software, where microstructural characteristics obtained by SEM micrographs and EDS analysis (Ref 33) were incorporated into the model, including the distribution of size, shape, and weight fraction (i.e., ~ 34wt. % and ~ 46wt. %) of reinforcing ceramic particles. Once the RVEs were generated, the models were validated using the experimental outcomes in terms of quantitative (i.e., stress versus strain histories) and qualitative (i.e., failure mechanisms) comparisons. This method of validation has also been used in previous studies (Ref 41, 42, 59, 79). The experimental measurements linked with the DIC technique showed that the compressive strength of the material was between 135 and 178 MPa for the composite with 34wt. % of alumina and between 298 and 317 MPa for the composite with 46wt. % of alumina. These are among the highest values reported in the literature (Ref 80–83) due to the fabrication strategy in this research that employs both matrix strengthening and dispersion strengthening mechanisms (Ref 33). In addition, the measured stiffness of our coatings varied from 28 GPa to 62 GPa for the Al–34 wt. % Al₂O₃ composites and from 48 GPa to 63 GPa for the Al–46 wt.% Al₂O₃ composites. The developed model predicted the strength of the material with an error based on the average experimental quantities of 9.6% and 17.6% for the 34wt. % alumina and the 46wt. % alumina samples, respectively. As well, the numerical prediction of the stiffness yielded a value of 38 GPa and 53 GPa for the 34wt. % alumina and the 46wt. % alumina MMCs, respectively, resulting in an error of 15.5 % and 4.5% with respect to the average measured values. With the maximum error of 17.6%, the model is reasonably in quantitative agreement with the experimental outcomes. Qualitatively, for the first time to the best of our knowledge, the manifestation and evolution of experimentally observed failure mechanisms in ceramic–metal coatings under compression (i.e., matrix ductile failure, matrix/particle debonding, and particle cracking) were all numerically captured through a 3D micromechanical finite element framework. This improves upon previous studies using 2D models (Ref 23, 54, 68) or single-particle 3D models (Ref 11). Additionally, the necessity of developing 3D models in this study was illustrated by Böhm et al. (Ref 84) and Soppa et al. (Ref 85) to adequately capture the plastic strain distribution in two-phase materials.

Finally, the deviations between the simulation and experimental results can stem from the differences between the assumed and real boundary conditions (Ref 86), the complexities of the real microstructures such as reinforcing particle clustering (Ref 79) that are not yet incorporated into the generated RVEs, the fracture of reinforcing

particles during the cold spray deposition process (Ref 18) leading to damage accumulation, and the increase in porosity due to interface decohesion and particle cracking (Ref 87), which are not considered in the GTN model implemented in the present study. In addition, the work hardening effect (Ref 88) induced in the Al matrix by the high-velocity impact of hard ceramic particles gives rise to a significant increase in dislocation density (Ref 89), which results in higher strength and hardness in the experimental samples when compared to the model material systems. To account for these crystallographic orientation effects (Ref 90) in the model, electron backscatter diffraction (EBSD)-based RVEs (Ref 91, 92) can be employed in the future as a promising future direction to numerically explore the micromechanical behavior of MMC coatings. Altogether, the presented model established a reasonable match between the predicted and measured outcomes which allows for further exploration of the microstructure–property relationships of the material (i.e., the effect of matrix porosity (Ref 93) as well as particle size (Ref 2, 94), shape (Ref 95), and distribution (Ref 96) of particles on the macroscale behavior). This paves the way to create a 3D computational tool for the design and optimization of ceramic–metal cold-sprayed composite coatings via tailoring the microstructure.

Conclusion

This study explored the behavior of Al–Al₂O₃ composite coatings under quasi-static compression and indentation loading via FE analysis, both quantitatively (i.e., stress versus strain response) and qualitatively (i.e., the manifestation of damage mechanisms, including matrix ductile failure, interfacial debonding, and particle cracking). For the FE models, 3D RVEs were generated by Digimat software based on the microstructural features of the MMC coating samples with different particle concentrations, and the homogenization approach was employed for modeling the Vickers micro-indentation test. To account for the matrix ductile failure and the matrix/particle decohesion, the GTN model and the CZM approach were employed, respectively. The ceramic particles were modeled using the phenomenological JH2 model to incorporate particle damage accumulation. The FE model was validated by stress–strain histories, Vickers hardness, and damage mechanisms obtained experimentally, and a reasonable agreement was observed between the results. Altogether, the outcomes of this study confirm the applicability of the model to be used as a computational tool for spatially tailoring matrix and particle properties and geometries to develop high-performing gradient coating structures.

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