

Wear

Computational Investigation of the Effect of Microstructure on the Abrasive Wear Resistance of Tungsten-Carbide Nickel Composite Coatings

--Manuscript Draft--

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Abstract:	<p>Sliding wear was simulated for tungsten carbide-nickel (WC-Ni) composites with different WC particle sizes and volume fractions under various normal forces. Johnson-Cook and Johnson-Holmquist models were employed to simulate the mechanical behaviour of the Ni and WC phases, respectively. Using high-powered parallel computing, a detailed parametric study was conducted to understand the effects of normal force, WC particle size, WC particle volume fraction, and their interaction on the worn volume and the material removal mechanisms in WC-Ni metal matrix composite coating materials. This allowed for investigation of the competition and transition between microploughing, microcutting, and microfatigue. The results revealed that the stress was distributed better in the composite coating with higher particle volume fraction and smaller particle size, which increased the ability of the composite coating to resist deformation and wear. It was also found that the material removal mechanism changed from microploughing to microcutting with an increase in particle volume fraction. The worn volume was calculated for different combinations of intrinsic (e.g., WC particle size and volume fraction) and external (e.g., normal force) parameters considered in this study. The data obtained was used to train a machine learning-based model using artificial neural networks. The trained model was further employed to predict the worn volume, and the results revealed that a mechanistic modelling approach can predict worn volume reasonably well.</p>
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October 22, 2020

Drs. A. Fischer, M. Papini
Co-Editors-in-Chief, Wear

Re: Manuscript Submission

Dear Drs. Fischer and Papini

We are pleased to submit a research paper entitled “Computational Investigation of the Effect of Microstructure on the Abrasive Wear Resistance of Tungsten-Carbide Nickel Composite Coatings”. This manuscript highlights our most recent findings regarding abrasive wear resistance of Tungsten Carbide (WC)-based metal matrix composite (MMC) coatings. To date, limited studies have focused on the effect of the external and intrinsic factors on the wear resistance of WC-Ni composites and overlays. In experiments, controlling the factors, particularly intrinsic factors, affecting the scratch resistance is difficult. A few studies have used numerical approaches to unravel the effects of reinforcing particles on the local scratch and the mechanisms involved in plastic deformation and material removal of composite coatings. Also, to the best knowledge of the authors, no 3-D numerical simulation has been conducted to evaluate the effect of WC reinforcing particles on scratch resistance in WC-Ni composites. No model has been developed to predict the scratch resistance of WC-Ni composite coatings. Thus, this paper aims to: (1) numerically analyze the effect of both external and intrinsic factors affecting the scratch resistance of WC-Ni composite coatings, and (2) develop a model to predict the scratch resistance of the composite under study using the a machine-learning based approach, Artificial Neural Network.

To accomplish this, a finite element (FE) model was developed to simulate the scratch resistance of WC-Ni composite coatings with consideration for relevant material and damage models needed for scratch simulation. The FE model was validated with an experimental study published earlier. The effects of WC particles size, volume fraction,

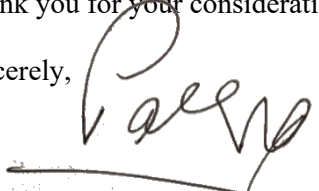
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and load on the scratch resistance of the composite coating were evaluated, and an ANNs model was developed to predict the scratch resistance of the composite coating, which could be employed to optimize the composite in terms of the material wear. It is worth-mentioning that this manuscript is the first public report that developed this machine-learning based model to predict the scratch resistance of WC-Ni composite coating.

If any additional material is needed, please contact me.

Thank you for your consideration.

Sincerely,



Mohammad Parsazadeh, Ph.D., M.Sc., B.Eng.
Postdoctoral Fellow
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Highlights

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- FE model was developed to analyze the wear loss of WC-Ni composite coating.
- The FE model was used to study the material removal mechanisms.
- Effects of intrinsic and external factors on the wear resistance were analyzed.
- A machine learning-based model, ANN, was developed to predict the worn volume.

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10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65

Sliding wear was simulated for tungsten carbide-nickel (WC-Ni) composites with different WC particle sizes and volume fractions under various normal forces. Johnson-Cook and Johnson-Holmquist models were employed to simulate the mechanical behaviour of the Ni and WC phases, respectively. Using high-powered parallel computing, a detailed parametric study was conducted to understand the effects of normal force, WC particle size, WC particle volume fraction, and their interaction on the worn volume and the material removal mechanisms in WC-Ni metal matrix composite coating materials. This allowed for investigation of the competition and transition between microploughing, microcutting, and microfatigue. The results revealed that the stress was distributed better in the composite coating with higher particle volume fraction and smaller particle size, which increased the ability of the composite coating to resist deformation and wear. It was also found that the material removal mechanism changed from microploughing to microcutting with an increase in particle volume fraction. The worn volume was calculated for different

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22 combinations of intrinsic (e.g., WC particle size and volume fraction) and external (e.g., normal
23 force) parameters considered in this study. The data obtained was used to train a machine learning-
24 based model using artificial neural networks. The trained model was further employed to predict
25 the worn volume, and the results revealed that a mechanistic modelling approach can predict worn
26 volume reasonably well.

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28 **Keywords:** Artificial neural networks (ANNs), Finite element modelling, Johnson-Cook model,
29 Johnson-Holmquist model, Machine learning, Nickel, Metal matrix composite coating (MMC),
30 Scratch test, Tungsten carbide, Wear

31
32 **1. Introduction**

33 The development of advanced coating materials with increased longevity [1] is important in the
34 petroleum [2], aerospace [3], mining [4], and manufacturing industries [5,6], where high
35 temperatures [7], corrosion [2], and wear [8] are common. Among types of coating materials used
36 in these applications (e.g., silicon carbide (SiC) [9], boron carbide (B₄C) [10], titanium carbide
37 (TiC) [11]), tungsten carbide (WC)-based metal matrix composite (MMC) coatings and overlays
38 are suitable choices given their unique combination of hardness and fracture toughness [12]. In
39 these applications, WC is commonly combined with Ni-based alloys to serve as a metallic binder
40 to effectively resist against wear damage [12–14].

41 The main factors influencing the abrasive wear performance of metal matrix composite coatings
42 and overlays can be categorized as intrinsic or external factors [15]. Intrinsic factors include
43 mechanical properties of both reinforcing particles and the matrix and microstructure of the
44 composite coating and overlay (e.g., volume fraction [12,16], size [16,17], shape, and size

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4 45 distribution of the reinforcing particles). External factors include the loading condition [18], the
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6 46 shape and size of the abrasive particles [19, 20], temperature [21], and sliding velocity [22]. In the
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9 47 literature, models have been developed to describe the wear performance of MMCs [10, 23, 24].
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11 48 The simplest and most fundamental model that was derived from complex abrasive wear
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14 49 conditions is the one-cycle interaction of a single abrasive particle and material [17, 18, 25, 26].
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16 50 Commonly, this interaction is evaluated in a controlled scratch test [27], which is an experiment
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19 51 used by many researchers to evaluate the mechanical and wear behaviour of different materials
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21 52 (e.g., polymers [28], ceramics [29], metals [30], metal-matrix composites [9, 29, 30], and coatings
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24 53 [31, 32]). In this type of experiment, the scratching deformation [34] is a consequence of a
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26 54 combination of failure processes: 1) microploughing [35], 2) microcutting [36], 3) microfatigue
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29 55 [37], and 4) microcracking [37]. The competition of these mechanisms is material-dependent [38]
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31 56 and manifests as measurements of penetration and residual scratch depth [38]. These can be
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34 57 induced by controlling the normal load, indenter shape, and scratch speed. This study aims to
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36 58 explore these mechanisms through physics-based modelling of a scratching action of a rigid
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39 59 indenter with a predefined radius over a WC-Ni composite surface.
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42 60 Scratch test experiments allow for better understanding of the mechanisms of wear and the effect
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44 61 of the intrinsic and external factors on the wear performance [39]. For example, ploughing was
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46 62 found to be dominant in a study conducted by Varga, *et al.* [40] to evaluate the effects of load and
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49 63 temperature on scratch mechanisms of austenitic steel, a cast steel with a carbide network, and a
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51 64 Ni-based material with a carbide network. The adhesion and hardness of electrodeposited Ni
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54 65 coatings were improved by heat treatment in another study conducted by Ul-Hamid, *et al.* [41],
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56 66 and the surface mechanical properties of Ni were evaluated at different progressive loads.
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59 67 Microscratch test of Ni coatings revealed that cracking and decohesion of Ni coatings do not occur
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4 68 at the highest final loads (30 N) that were considered in their study. Also, the deformation
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7 69 mechanisms were evaluated at different scratch velocities in nanostructured Ni [42] and
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10 70 nanostructured Ni with bimodal grain size distributions [43] and were found to be different
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12 71 compared with conventional coarse grain counterparts due to the different strain rate sensitivity of
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14 72 these materials. The effects of different grades of WC reinforcing particles and volume fraction on
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16 73 the microstructure and material removal behavior of the WC-Ni composite, for example, were
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19 74 analyzed by Alzouma *et al.* [17]. It was found that the composite becomes more wear-resistant
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21 75 when the reinforcing volume fraction is increased, which results in protection and strengthening
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24 76 of the matrix. Plastic deformation of the metal matrix was also reduced [17]. The results from these
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26 77 previous studies will be important in the present investigation on the effects of microstructure,
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29 78 mechanical properties, and loading conditions on the scratch response of WC-Ni composites.
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32 79 Studying the effect of microstructure on wear mechanisms is difficult to analyze experimentally
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34 80 since fully controlling the intrinsic and external factors is challenging. Numerical simulation is an
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37 81 alternative to evaluate the contribution of individual factors on scratch resistance separately [18].
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39 82 For example, the effect of the attack angle and load on the wear performance of glass fibre
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41 83 reinforced polyester composites were evaluated in a numerical study by Mzali, *et al.* [44].
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44 84 Consideration was given to the cohesive zone between the fibre and matrix. The results revealed
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46 85 the significant effect of attack angle on the transition of wear mechanisms during ploughing to
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49 86 result in composite damage. Also, the effects of the size and volume fraction of WC particles on
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51 87 scratch resistance in WC-Ni composites were evaluated in a two-dimensional numerical model by
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54 88 Hu, *et al.* [45]. They later expanded their initial study [45] to analyze the effect of other parameters
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56 89 on material removal, such as WC particle shape, distribution of reinforcement, and their interaction
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59 90 with their volume fraction [46]. Hu, *et al.* [46] concluded that the composite material might benefit
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91 from the increase in hardness at the expense of toughness by increasing the volume fraction of the
92 reinforcing particles. Among the studies reviewed above, a few of them numerically evaluated the
93 scratch resistance of the composites; however, no model has been developed to predict the scratch
94 resistance of WC-Ni composite coatings, as is pursued here.

95 As an alternative modelling approach to finite element analysis, artificial neural networks (ANNs)
96 have attracted increasing interest due to the high capability of modelling highly nonlinear and
97 complex problems [47–51]. To predict wear rates using ANNs, one of the first efforts was
98 conducted by Jones, *et al.* [47] based on a limited set of experimental data. ANNs were also
99 employed to predict the tribological properties of Al7075-Al₂O₃ composites [48], epoxy
100 composites [49], rice husk ash reinforce aluminum alloys [50], and also to predict wheel and rail
101 wear rates [51]. The results of these studies revealed that ANNs could be an appropriate approach
102 to predict the scratch resistance of composite materials, as is pursued here.

103 To date, limited studies have focused on the effect of the external and intrinsic factors on the wear
104 resistance of WC-Ni composites and overlays. In experiments, controlling the factors, particularly
105 intrinsic factors, affecting the scratch resistance is difficult. A few studies have used numerical
106 approaches to unravel the effects of reinforcing particles on the local scratch and the mechanisms
107 involved in plastic deformation and material removal of composite coatings. Also, to the best
108 knowledge of the authors, no 3-D numerical simulation has been conducted to evaluate the effect
109 of WC reinforcing particles on scratch resistance in WC-Ni composites. No model has been
110 developed to predict the scratch resistance of WC-Ni composite coatings. Thus, this paper aims to:
111 (1) numerically analyze the effect of both external and intrinsic factors affecting the scratch
112 resistance of WC-Ni composite coatings, which could also be applied to reasonably thick overlays,
113 and (2) develop a model to predict the scratch resistance of the composite under study using the

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ANNs approach. To accomplish this, a finite element (FE) model was developed to simulate the scratch resistance of WC-Ni composite coatings with consideration for relevant material and damage models needed for scratch simulation in Section 2. In the same section, the FE model was validated with an experimental study conducted by Ul-Hamid, *et al.* [52]. The effects of WC particles size (d_p), volume fraction (ϕ), and load on the scratch resistance of the composite coating were evaluated in Section 3, and an ANNs model was developed to predict the scratch resistance of the composite coating, which could be employed to optimize the composite in terms of the material wear.

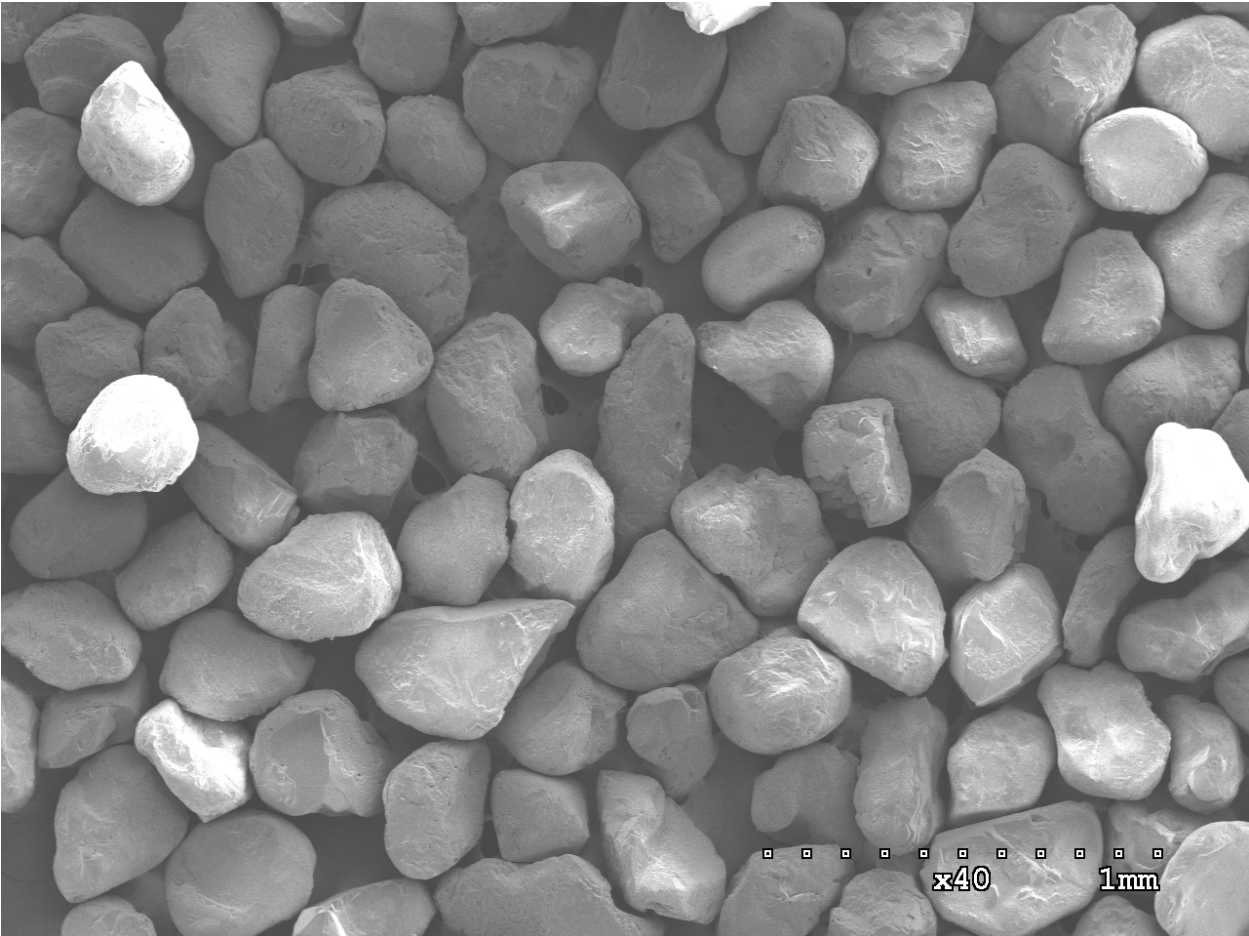
2. Model and Theory

2.1. Physical Model

To evaluate the effects of various tribological scratch parameters (load, volume fraction, and particle size), a 3D model for scratch test simulation was developed. The scratch particle geometry was modelled on sand sizes observed in the Albertan oil sands, where the size distribution of these sands shown in Fig. 1 (a) was obtained using ImageJ software. It was found that the diameter of the sand varies from 55 μm to 505 μm , and more than 75 % of these sands have a diameter range between 55 and 205 μm , as shown in Fig. 1 (b). The average sand diameter and the standard deviation were found to be 140 μm and 78 μm , respectively. This average sand diameter was chosen as the diameter of the spherical indenter used in simulating scratch testing resistance. To reduce the computation time, the geometry size was also considered to be $0.40 \times 0.25 \times 0.60 \text{ mm}^3$. This geometry size was chosen according to the criterion introduced by Bucaille, *et al.* [53] and Tabor [54]. In this criterion, the geometry thickness must be four times greater than the scratch depth, and also the geometry width must be ten times greater than the scratch width. With these

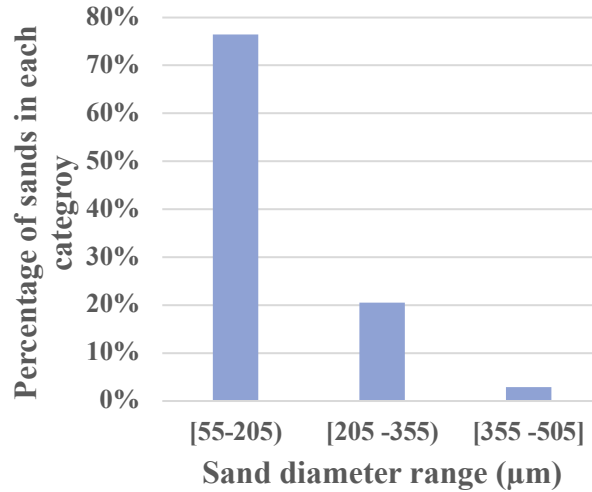
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136 points in mind, the width and depth of the geometry were estimated by considering the scratch
137 depth and width obtained for Ni in the studies conducted by UI-Hamid, *et al.* [52] and Zhu, *et al.*
138 [43].



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(a)

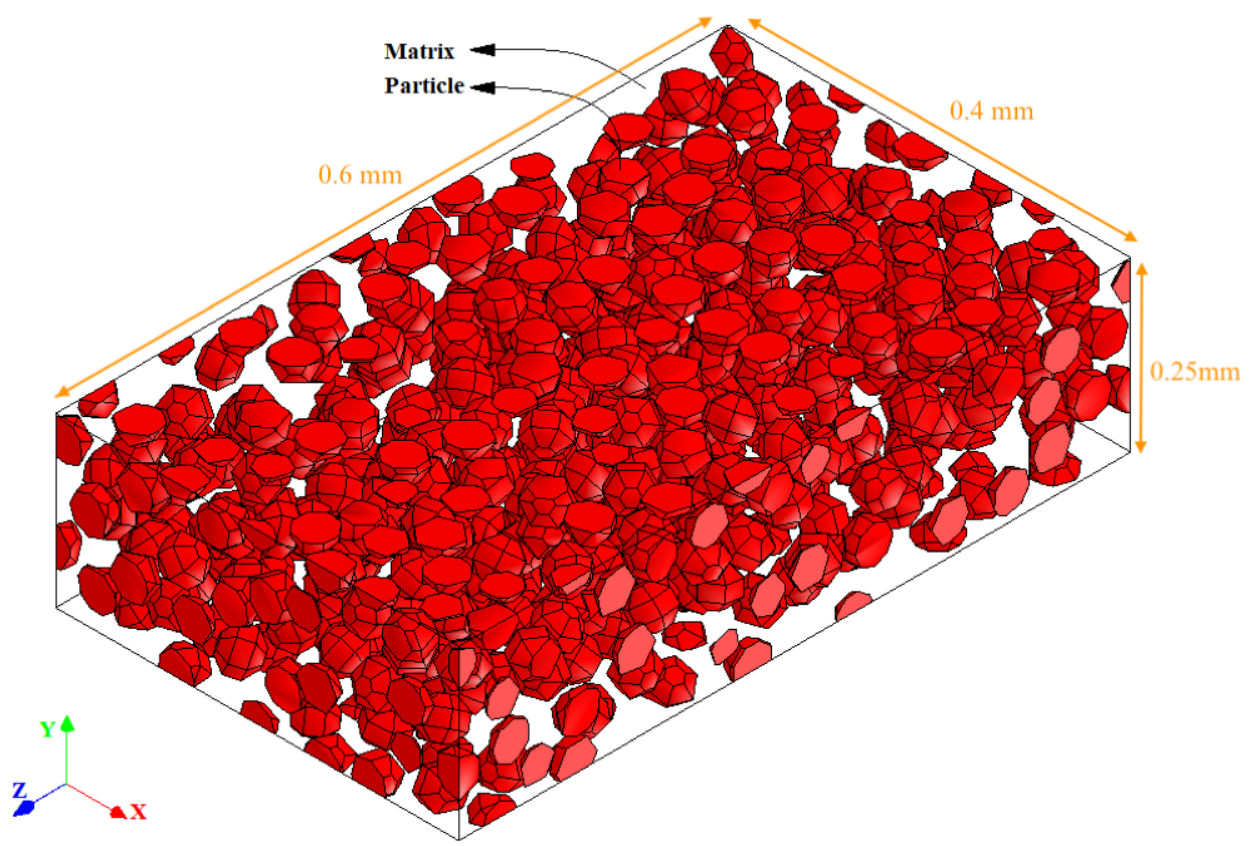


(b)

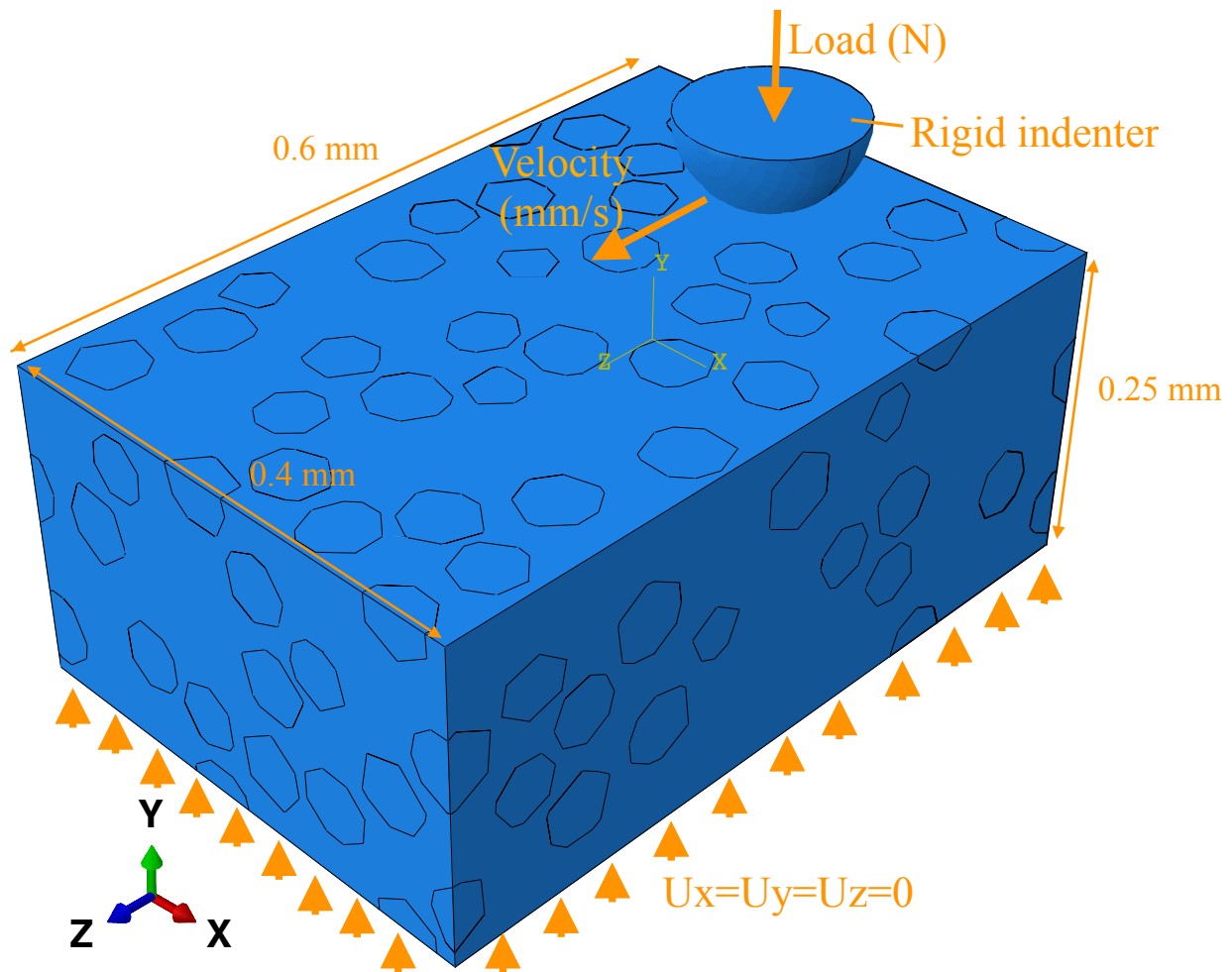
Fig. 1 (a) SEM images of different Alberta mine site sands (b) Sand size distribution.

The matrix and the reinforcing particles chosen in this study were considered as Ni and WC, respectively. This material was selected because of its unique combination of hardness and fracture toughness [12]. To evaluate the effect of the reinforcing particle size to the indenter size ratio on the material removal, three different WC particle diameters (60 µm, 140 µm, and 220 µm) were chosen to have the size ratio smaller, equal, and larger than one. These different size ratios help better understand the different competing mechanisms that may affect material removal due to different reinforcing particle size to the indenter size. The volume fraction range of the WC particles was also considered to be 10–50 Vol.%, with an increment of 20 Vol.%. The arrangement of the WC particles was also depicted for $\phi = 50$ Vol.% in Fig. 2 (a), and this range of reinforcing particles was motivated based on practical considerations and our applications of interest. A schematic diagram of the indenter and the composite coating is depicted in Fig. 2 (b). The bottom surface of the substrate was kept motionless, while an indenter carrying a certain load moved toward the z -direction.

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(a)



(b)

Fig. 2 The schematic diagram of (a) arrangement of the WC particles in the FE model ($\phi = 50$ Vol.%) (b) the indenter and the composite coating.

2.2. Finite Element Modelling

A finite element (FE) scratch model has been developed using Abaqus software. The model consists of a spherical rigid indenter and a flat deformable surface, as shown in Fig. 2 (b). The indenter was considered under a normal load varying between 1–9 N pushing the indenter toward

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168 the substrate in the y -direction, and the indenter also moved in the z -direction with a constant
169 velocity of 100 mm/s. The load range selected in this study will help understand the mechanisms
170 affecting the material removal at small and large loads [18, 32, 54], and the indenter velocity was
171 chosen large enough to avoid making the simulation computationally expensive. The substrate
172 movement was constrained in all directions to evaluate the effect of the indenter over the substrate.
173 The scratch simulation was completed under four steps. In the first step, surface-to-surface contact
174 [18] was established between the indenter and the substrate, followed by increasing the normal
175 load gradually until the load reached its maxima at the end of the second step. In the third step, the
176 indenter moved with a constant velocity along the scratch length. During the last step, the indenter
177 was unloaded and gradually lifted up by imposing a small magnitude of load in the opposite
178 direction. The plastic deformation and material removal have been considered in the scratch model
179 developed in this study using the Explicit option in Abaqus. The element types chosen to mesh the
180 substrate and the indenter were a ten-node modified quadratic tetrahedron (C3D10M in ABAQUS
181 FEA notation) and a 3-node 3-D rigid triangular facet (R3D3 in ABAQUS FEA notation),
182 respectively. Compute Canada clusters were employed and paralleled to perform high-powered
183 parallel computing, with typical run times of 15 hours on two nodes, each with 48 CPUs.

2.3. Constitutive Models

186 Two main approaches drawn from fracture mechanics [55, 56] and damage mechanics [57–59]
187 were employed to model the material response under scratch loading. The matrix was modelled as
188 an elastoplastic hardening material. To model the plasticity and damage behaviour of the Ni matrix
189 under varying normal loads, the Johnson-Cook (J-C) constitutive equation [59] was employed.

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4 190 In the J-C model, the relationship between von Mises flow stress (σ_{eq}), yield strength, hardening,
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7 191 and temperature softening is defined as:

$$10 \quad \sigma_{eq} = \left[A + B(\bar{\epsilon}^{pl})^N \right] \left[1 + C \ln \left(\frac{\dot{\bar{\epsilon}}^{pl}}{\dot{\bar{\epsilon}}_o^{pl}} \right) \right] \left[1 - \left(\frac{T - T_{ref}}{T_{melt} - T_{ref}} \right)^M \right], \quad (1)$$

14 193 where A is the yield strength, B is the strain-hardening modulus, $\bar{\epsilon}^{pl}$ is the equivalent plastic
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17 194 strain, C is the strain rate hardening coefficient, $\dot{\bar{\epsilon}}^{pl}$ is the equivalent plastic strain rate, $\dot{\bar{\epsilon}}_o^{pl}$ is
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20 195 the reference strain rate, T is the temperature at operating condition, T_{ref} is the reference
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23 196 temperature, T_{melt} is the melting temperature, and N and M are strain the hardening exponent and
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28 198 Based on the equivalent plastic strain ($\Delta \epsilon^{pl}$), a damage parameter (D) was defined in the J-C
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31 199 damage model as:

$$33 \quad D = \sum \frac{\Delta \epsilon^{pl}}{\epsilon_f^{pl}}, \quad (2)$$

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38 201 where ϵ_f^{pl} is equivalent plastic strain at failure, which was defined as:

$$40 \quad \epsilon_f^{pl} = \left[D_1 + D_2 \exp \left(D_3 \left(\frac{\sigma_m}{\sigma_{eq}} \right) \right) \right] \left[1 + D_4 \ln \left(\frac{\dot{\bar{\epsilon}}^{pl}}{\dot{\bar{\epsilon}}_o^{pl}} \right) \right] \left[1 + \frac{T - T_{ref}}{T_{melt} - T_{ref}} \right], \quad (3)$$

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45 203 where D_1 to D_5 are material constants and σ_m is the mean stress.

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49 204 In the J-C damage model, element removal occurs when the strain in the element exceeds the
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51 205 failure strain, which is when $D = 1$. At this stage, material stiffness decreases. This element
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54 206 removal leads to material loss on the surface that is under the sliding indenter. This modelling
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56 207 approach was also used in impact [59, 60] and erosion [61, 62] processes.

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208 The Johnson-Holmquist (JH-2) constitutive model, which is based on the elastic-viscoplastic
209 approach, was used to simulate the response of WC particles to deformation. This model is mainly
210 used to simulate deformation in brittle materials (e.g., SiC [64], B₄C [65], and AlN [66]). In this
211 model, the strength of the reinforcing particles is assumed to vary with changing pressure, strain
212 rate, and tensile strength. Initially, elastic deformation is considered in the material. In this region,
213 the stress-state is described based on the elastic material properties and equation of state. The
214 relationship between pressure on the material and density ρ can be calculated based on the current
215 material deformation as follows [66, 67]:

$$P = K_1\mu + K_2\mu^2 + K_3\mu^3 \quad \text{if } \mu \geq 0 \text{ and} \tag{4}$$

$$P = K_1\mu \quad \text{if } \mu \leq 0, \tag{5}$$

where $\mu = \rho / \rho_0$, ρ is the material density, ρ_0 is a reference density, and K_1 , K_2 , and K_3 are constants (K_1 is the initial bulk modulus).

An increment in damage leads to material bulking, meaning that a larger volume is occupied by the fractured material compared with the intact condition. This leads to an increase in local pressure in a constrained material. Initially, the bulking pressure is zero for an undamaged material, and this bulking pressure can be calculated at the next time increment as [64, 65]:

$$\Delta P_{t+\Delta t} = -K_1\mu_{t+\Delta t} + \left[(K_1\mu_{t+\Delta t} + \Delta P_t)^2 + 2\beta K_1\Delta U \right]^{1/2}, \tag{6}$$

where β is the fraction of elastic energy loss converted to potential hydrostatic energy and ΔU is energy loss due to increased bulking pressure, which is defined as [65–68]:

$$\Delta U = U(D) - U(D_{n+1}) \text{ and} \tag{7}$$

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$$228 \quad U(D) = \frac{\sigma}{6G}, \quad (8)$$

229 where G is the elastic shear modulus.

230 In the JH-2 model, under compressive loading, the damage accumulates progressively with plastic
231 deformation. A damage parameter, ranging from 0 to 1, is employed to track this damage
232 accumulation, and this serves to degrade the overall strength in the material. The strength of the
233 material is expressed in terms of the normalized von Mises equivalent stress as [66]:

$$234 \quad \sigma^* = \sigma_i^* - D(\sigma_i^* - \sigma_f^*), \quad (9)$$

235 where D is the damage parameter, and σ_i^* and σ_f^* are the normalized intact and fractured
236 equivalent stresses, respectively. These normalized equivalent stresses (σ^* , σ_i^* , and σ_f^*) have the
237 general form of $\sigma^* = \sigma / \sigma_{HEL}$. In this definition, σ is the actual von Mises stress and σ_{HEL} is the
238 equivalent stress at the Hugoniot elastic limit (HEL).

239 In the JH-2 model, the normalized intact and fractured stresses can be expressed as a function of
240 pressure and strain rate as follows:

$$241 \quad \sigma_i^* = A(P^* + T^*)^N (1 + C \ln \dot{\epsilon}^*) \text{ and} \quad (10)$$

$$242 \quad \sigma_f^* = B(P^*)^M (1 + C \ln \dot{\epsilon}^*), \quad (11)$$

243 where A, B, C, M , and N are material constants, and P^* and T^* are the normalized pressure and
244 normalized maximum tensile hydrostatic pressure, respectively, which can be defined as:

$$245 \quad P^* = P / P_{HEL} \text{ and} \quad (12)$$

$$T^* = T / P_{HEL}, \quad (13)$$

where P_{HEL} is the pressure at the HEL and T is the maximum tensile pressure that a material can withstand.

To determine P_{HEL} and σ_{HEL} , HEL experimental data is required. HEL, which comprises of the pressure and deviatoric components, represents the point at which the shock wave exceeds the elastic limit of the material and is presented as a one-dimensional shock wave [66]. The HEL is defined by [65, 68]:

$$HEL = P_{HEL} + \frac{2}{3} \sigma_{HEL}. \quad (14)$$

Using Eq. (14), the value of P_{HEL} and σ_{HEL} were determined using the procedure described in several studies that implemented the JH-2 model [64, 65, 68]. The volumetric strain at HEL is determined using the following equation [66]:

$$HEL = K_1 \mu_{HEL} + K_2 \mu_{HEL}^2 + K_3 \mu_{HEL}^3 + \frac{4}{3} G \frac{\mu_{HEL}}{1 + \mu_{HEL}}. \quad (15)$$

The data presented in Moxnes, et al. [70] was employed to find the volumetric strain (μ_{HEL}) at HEL, and then this value was used in Eq. (4) to find P_{HEL} . Then, σ_{HEL} was determined using Eq. (14).

The damage evolution and fracture term of the model is similar to those in the J-C model described in Eq. (2). However, the fracture strain definition is different in this model and is given as:

$$\varepsilon_f^{pl} = D_1 (P^* + T^*)^{D_2}, \quad (16)$$

264 where D_1 and D_2 are material constants.

265 All material parameters used in J-C and JH-2 models were listed in Table 1 along with other
 266 material properties and constants for Ni and WC. The Ni properties were obtained from Ghelichi,
 267 *et al.* [71], and WC properties were obtained from Moxnes, *et al.* [70] and Holmquist, *et al.* [72].

269 **Table 1** Ni and WC properties and constants used in J-C and JH-2 constitutive models.

Material properties/parameters	Ni [71]	WC [69, 71]
A	163 [MPa]	0.9899
B	648 [MPa]	0.67
C	0.06	0
E	200 [GPa]	N/A
M	1.44	0.0322
N	0.33	0.0322
$\dot{\bar{\epsilon}}_o^{pl}$	1	1
ρ_o	8900 [kg/m ³]	14560 [kg/m ³]
ν	0.31	N/A
D_1	0.54	0.005
D_2	4.89	1
D_3	3.03	N/A
D_4	0.014	N/A
D_5	1.12	N/A

G	N/A	219 [GPa]
HEL	N/A	6.566 [GPa]
lDamage	N/A	0
K_1	N/A	362 [GPa]
K_2	N/A	694 [GPa]
K_3	N/A	0

2.4. Element Size and Model Validation

The FE model developed in this study needs to be independent of the number of elements and validated with experimental data. To perform validation, the results of this study were compared with the experimental study of Ul-Hamid, *et al.* [52] for the scratch testing of a low-porosity and fine-grained Ni material. This data set in this published study was the best validation case and aligned well with the low-porosity Nickel material that existed in our simulations. To reduce the computation time, the mesh independence test was conducted with increasing element size from 2,200 elements (element size of 60 μm) to 50,400 elements (element size of 5 μm). Choosing an optimum number of elements was important to reduce the computational time while keeping the results independent of the number of elements. The load on the indenter was considered to be 10 N, and the material undergoing the scratch was Ni with the material properties listed in Table 1. The average von Mises stress measured in the middle of the groove created by the scratch, and the scratch depth along the scratch length were calculated for different elements sizes and shown in Fig. 3. It was found that the average stress was independent of the element size when the number of elements was greater than 20,000 (element size of 10 μm), as shown in Fig. 3 (a). Similarly,

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the scratch depth did not significantly change when the number of elements was greater than 20,000, as depicted in Fig. 3(b). Thus, the minimum of 20,000 elements was chosen in this study to keep the results independent of the number of elements, while promoting computational efficiencies.

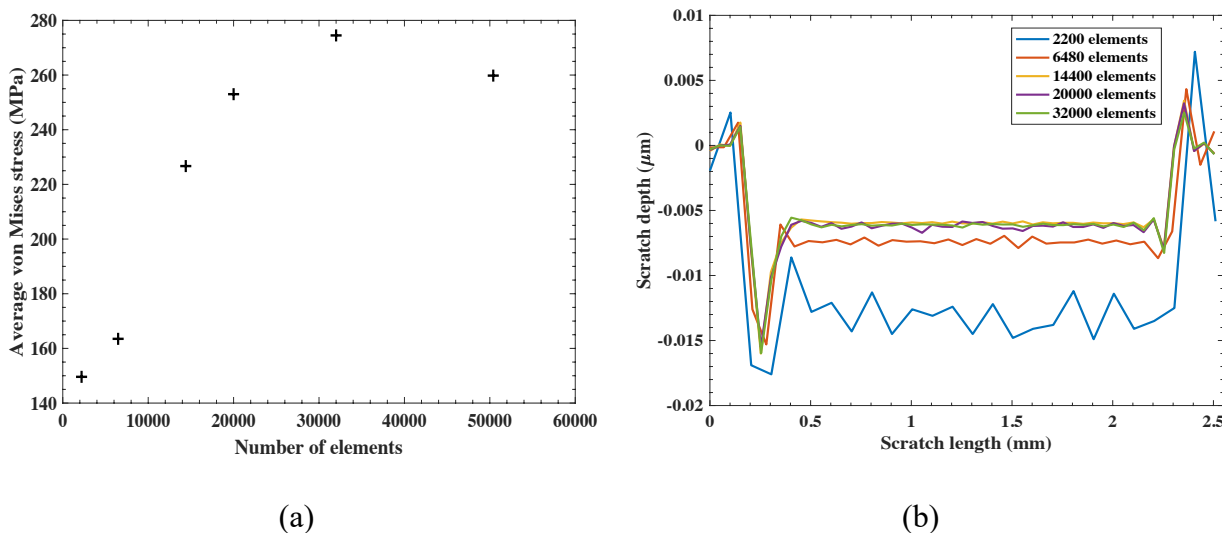


Fig. 3 Number of elements vs. (a) average von Mises stress and (b) scratch depth.

2.5. Artificial Neural Network Approach

Developing a model to predict the material removal requires a computerized numerical system to model the complex and nonlinear relationship between the operating parameters and the output. In these simulations, the operating parameters were considered to be scratch load, particle volume fraction, and particle size. To correlate the operating parameters considered in this study with the wear volume, artificial neural networks (ANNs) were employed. The artificial neural network, which has been widely employed across a variety of science and engineering disciplines [73–77]

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299 has the capability to model the behaviour of linear and nonlinear systems, which have a high degree
300 of complexity [47].

301 In this study, the ANN model was developed based on the biological neural network [78]. The
302 biological neural network included small units called neurons receiving electrochemical signals
303 via synapses. The synapses modify the weight of the received signal during learning. In biology,
304 the brain consists of subsystems, and each subsystem consists of a group of neurons [78].
305 Similarly, the ANN model acts as a brain with subsystems and neurons, which represent ANN
306 layers and neurons, respectively. These neurons link input data to output using synaptic weights.

307 Among many types of ANNs, a multilayer perceptron network (MLP) is more common and has
308 been used previously in nonlinear problems (e.g., corrosion [79], erosion [80]). MLP generally
309 consists of an input layer, hidden layers, and an output layer, as shown in Fig. 4. According to
310 other investigators, one hidden layer is usually sufficient to predict the actual output with
311 acceptable accuracy [80, 81]. The number of neurons in the hidden layer is determined by a trial
312 and error approach based on the mean square criterion [83]. In an ANN model, each input is
313 weighed between 0 and 1. The closer the weight to 1, the more significant the input is. The sum
314 of all of the signals' weights consists of the net value of the neurons. Each neuron is also set to a
315 number that corresponds to a threshold over which the neuron will transfer the signal to another
316 neuron. This signal transfer happens if the net value exceeds the neuron threshold. Thus, the
317 generalized knowledge gained in the training process is memorized in terms of the weight of the
318 signals [83, 84].

319 In MLP, the data is split into training data and test data. Training is the act of continuously
320 adjusting the signal weights until they reach appropriate values that allow the network to closely
321 predict the actual output. The accuracy of the network depends on the weights of these signals.

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322 The training data creates a set of training patterns (x_p, t_p) where p represents the pattern number,
 323 x_p and t_p are the input vector pattern and the desired output for the p^{th} training pattern. The input
 324 to the j^{th} hidden neuron, $net_p(j)$, is defined as [86]:

$$net_p(j) = \sum_{k=1}^{N+1} W_{hi}(k, j)x_p(k) \quad 1 \leq j \leq N_h, \quad (17)$$

326 where $W_{hi}(k, j)$ is the weights connecting the k^{th} input to the j^{th} hidden neuron and subscript k is
 327 used to show N input neurons.

328 The output activation for the p^{th} training pattern ($O_p(j)$) is expressed as:

$$O_p(j) = f(net_p(j)). \quad (18)$$

330 The sigmoid function is typically chosen as the nonlinear activation function as [83]:

$$f(net_p(j)) = \frac{1}{1 + e^{-net_p(j)}}. \quad (19)$$

332 The overall performance of MLP is calculated by the mean square error (MSE) as follows:

$$E = \frac{1}{N_v} \sum_{p=1}^{N_v} E_p = \frac{1}{N_v} \sum_{p=1}^{N_v} \sum_{i=1}^M [t_p(i) - y_p(i)]^2, \quad (20)$$

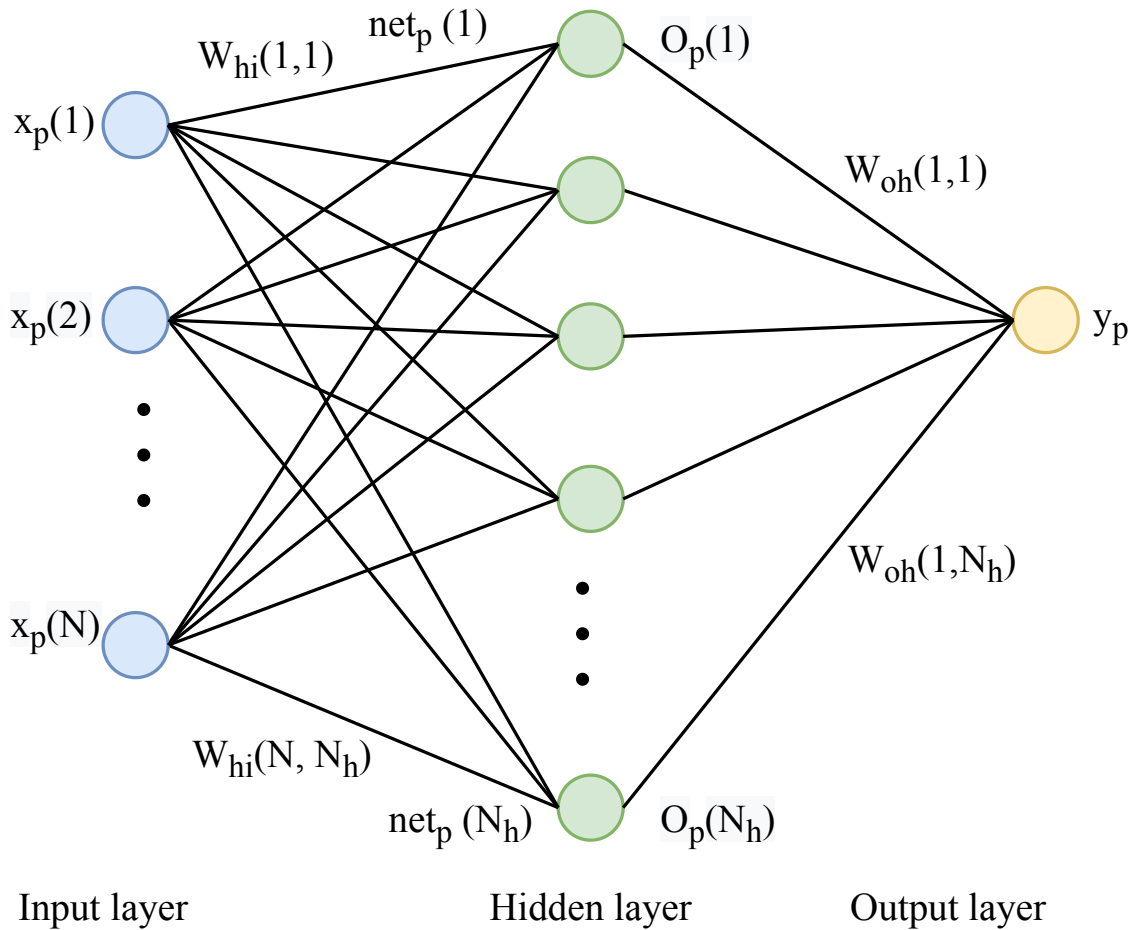
334 where, N_v is the number of training patterns, the i^{th} output for the p^{th} training pattern can be
 335 defined as:

$$y_p(i) = \sum_{k=1}^{N+1} W_{hi}(k, j) \cdot x_p(k) + \sum_{j=1}^{N_h} W_{oh}(i, j) \cdot O_p(j), \quad (21)$$

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337 where $W_{hi}(k, j)$ denotes the weights from input to output neurons and $W_{oh}(i, j)$ the weights from
338 hidden to output neurons.

339 In this study, $i = M = 1$, the ANN model had just one output, which was the volume loss, and the
340 input layer consisted of WC particle volume fraction, size, and scratch load. The ANN model was
341 developed to correlate these inputs and output using a Matlab[®] code.



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343 **Fig. 4** Topology of an artificial neural network.
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3. Results and Discussion

Initially, a scratch test was simulated under progressive load increasing from 0.1 to 30 N to validate the FE scratch model, and the result was compared with the experimental result obtained in the study by Ul-Hamid, *et al.* [52], as shown in Fig 5. Simulating the scratch test under progressive load facilitated examination of the validity of the FE model. As expected, the scratch depth increased with increasing the load in both experiment and simulation. Although the uncertainty of the study by Ul-Hamid, *et al.* [52] was not given, the scratch depth result obtained using the FE scratch model showed a good agreement with the experimental result in Fig. 5.

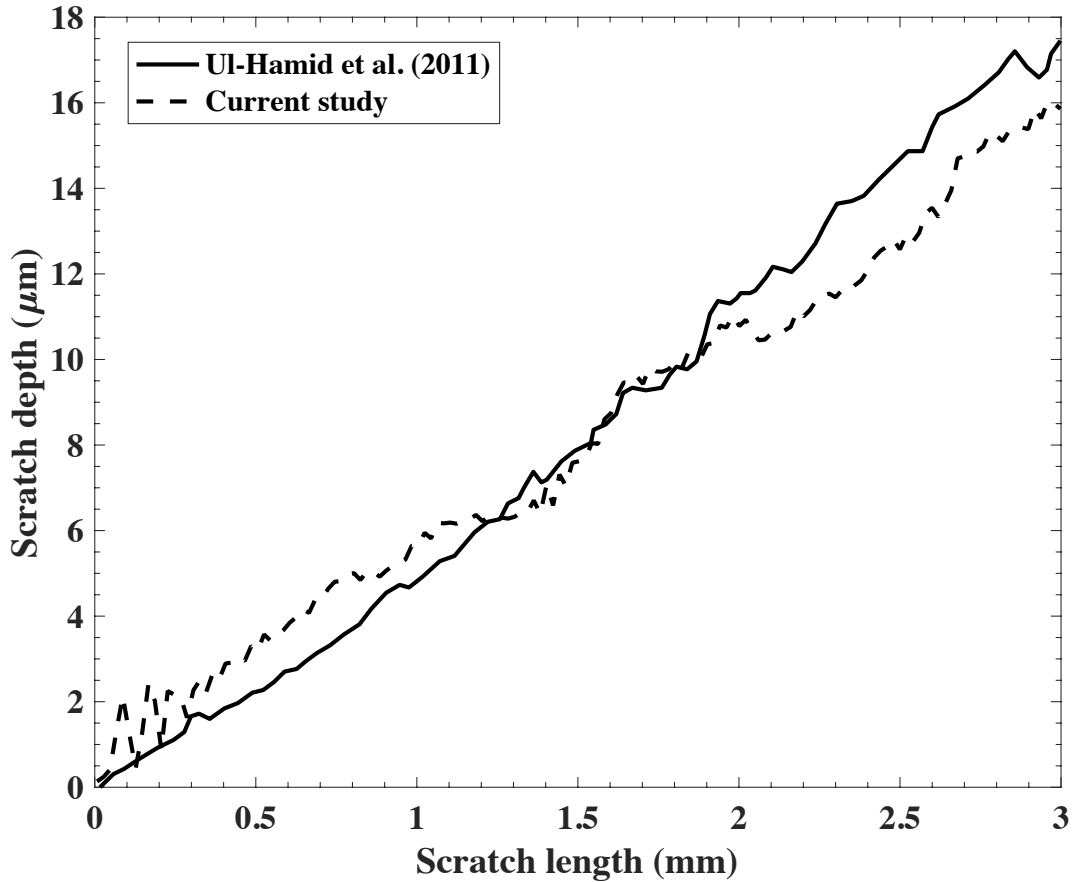


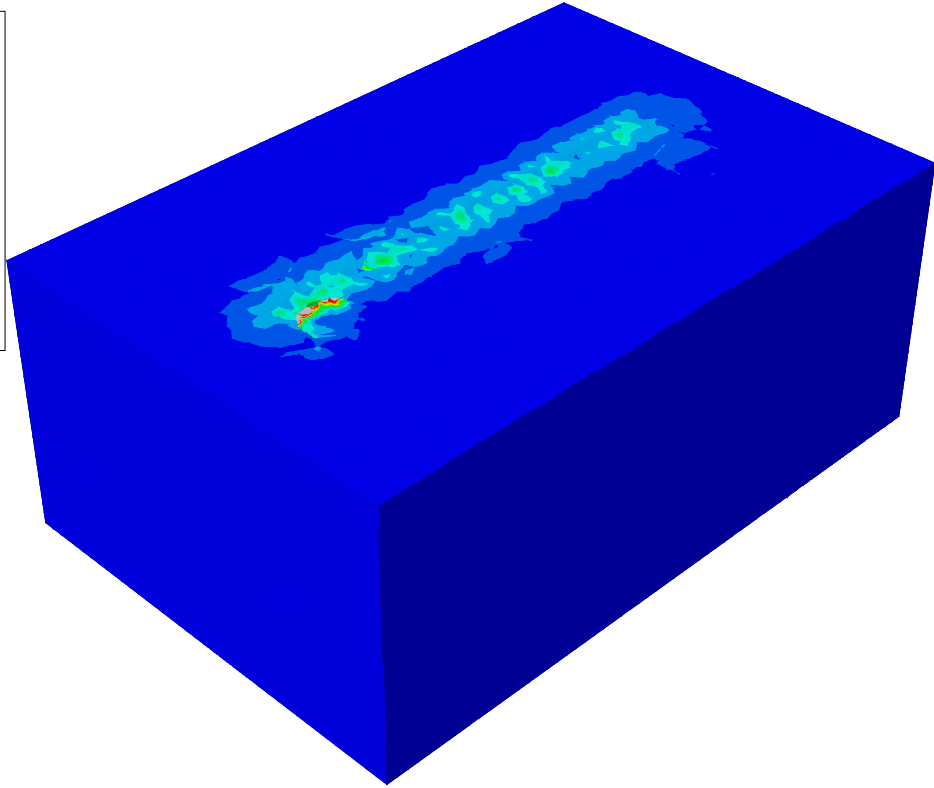
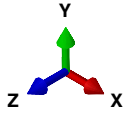
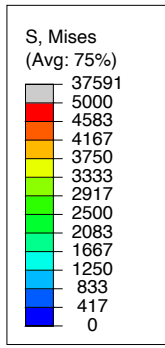
Fig. 5 The scratch length vs. scratch depth comparison between the present model and UI-Hamid, *et al.* experimental study [52].

3.1. Simulation of Residual Stress and Displacement

The contours of stress and displacement will be presented to illustrate the spatial distribution of deformation in the material following a scratch test. This was done by varying the load (1 N to 9 N), particle size (60 μm to 220 μm), and volume concentrations (10 Vol.% to 50 Vol.%). These were shown to see how mechanisms change and evolve as a function of these internal/external parameters. During sliding of the indenter, the shear force was created on the surface of the material, which caused the uppermost layer of the material to be compressed, as shown in Fig. 6. Depending on the size of this shear force, different material removal mechanisms

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7 367 were the only ones that contributed to the stress distribution (see Fig. 6 (a-I)) and composite
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9 368 hardness and material removal mechanism. The load on the indenter caused the stress is distributed
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12 369 in the substrate and the material is plastically deformed and accumulated on the side of the groove
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14 370 when $\phi = 10$ Vol.% as shown in Fig. 6 (a-II). This is referred to as “microploughing” and this
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17 371 mechanism was also reported by Xiao, *et al.* [87] as the dominant mechanism of material removal
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19 372 at small loads. When increasing the particle volume fraction to 50 Vol.% with the same scratch
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27 375 loading, which resulted in fragmentation and material removal, as shown in Fig. 6 (b-II).
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29 376 Increasing the WC particle volume fraction, which makes the composite brittle [32], may explain
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32 377 this small amount of material removal. In Fig. 6 (b), no clear plastic deformation was observed in
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37 379 matrix. This protective role of the WC particles was also observed in an experimental study by
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39 380 Cao, *et al.* [89].
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42 381 The residual damage in the substrate was investigated to probe potential damage accumulation and
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44 382 micro-fatigue mechanisms [90]. Typically, the stress was stored in both the matrix and particles at
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47 383 the scratch load of 1 N . The load caused the damage parameter represented in Eq. (2) is increased
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50 384 in each element. This parameter illustrated for the WC particles size of 60 and 140 μm in Fig. 7
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52 385 revealed that the damage parameter is relatively small (smaller than 0.5) in all the elements, which
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55 386 means that the reinforcing particles may not be significantly damaged even if the scratch test had
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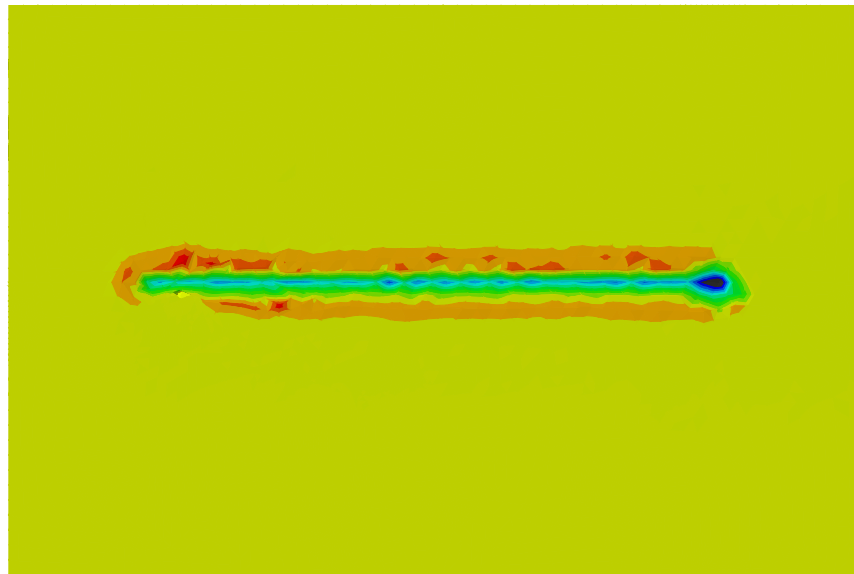
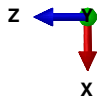
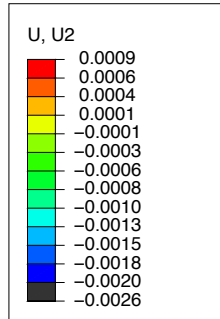


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(a-I)

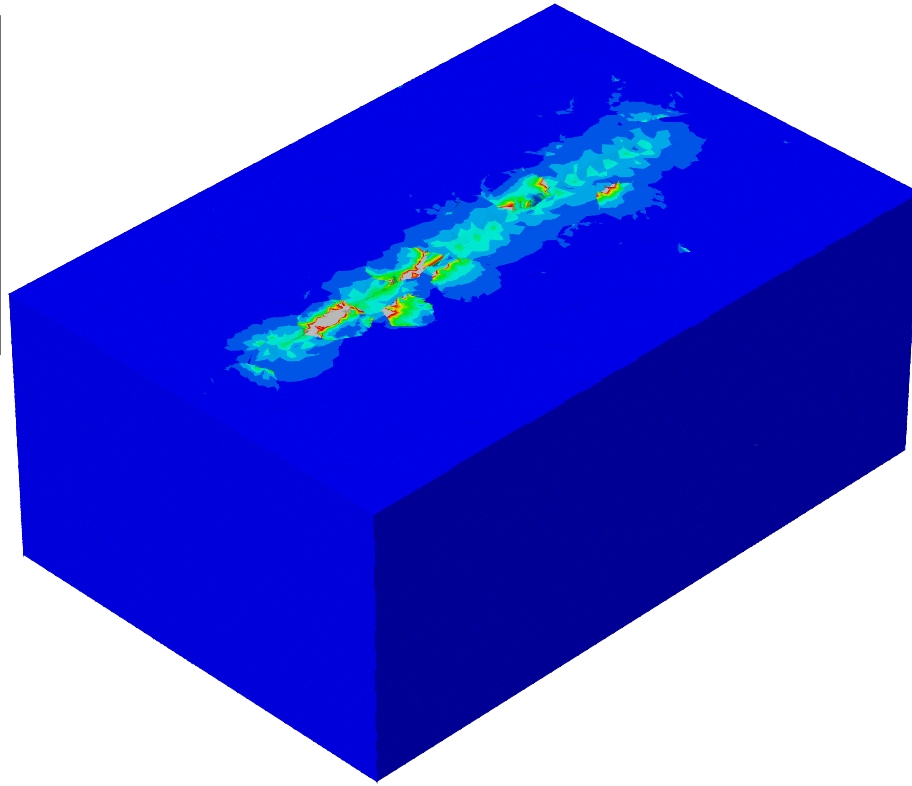
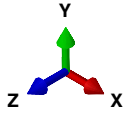
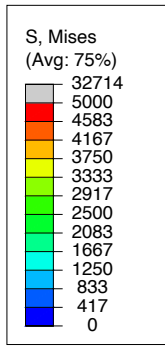
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(a-II)

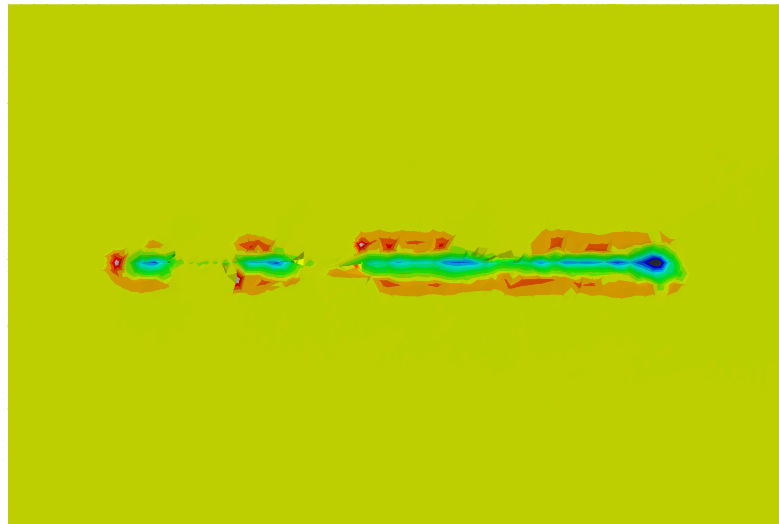
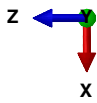
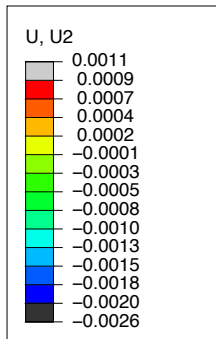
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(b-I)

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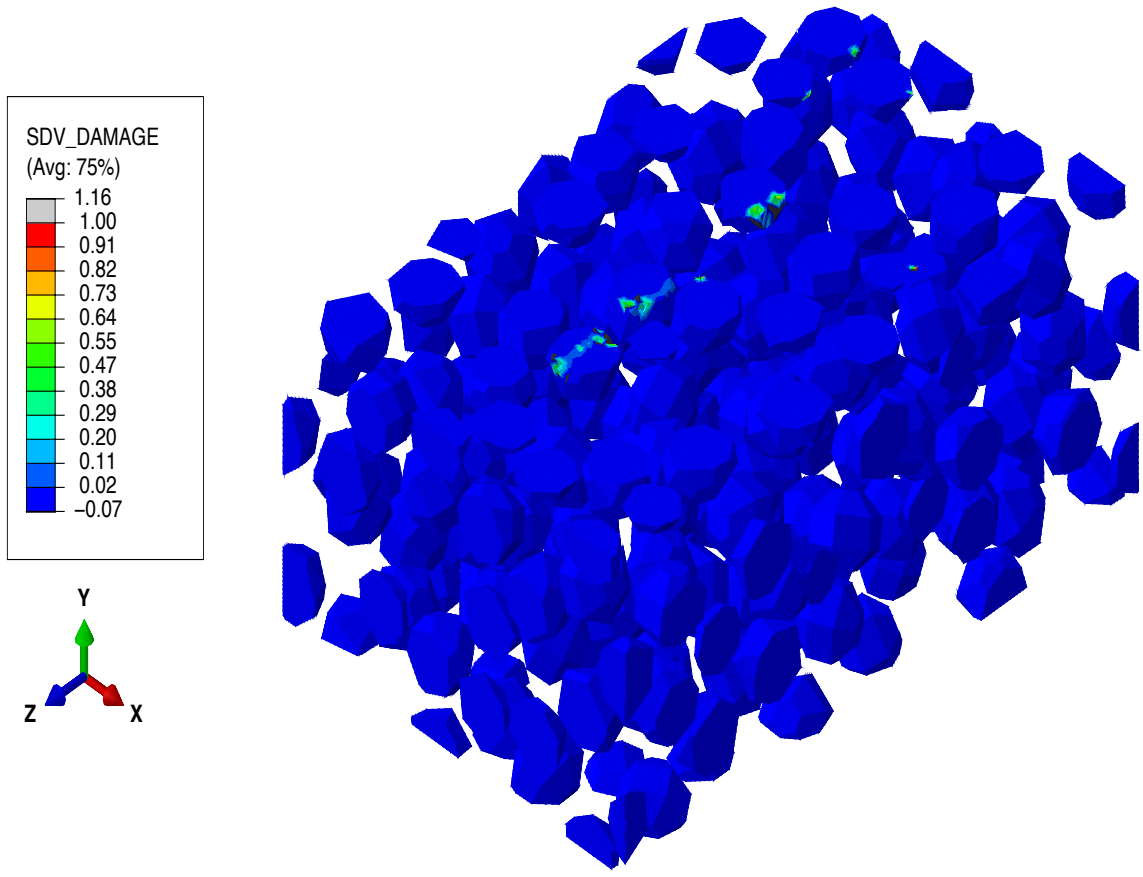


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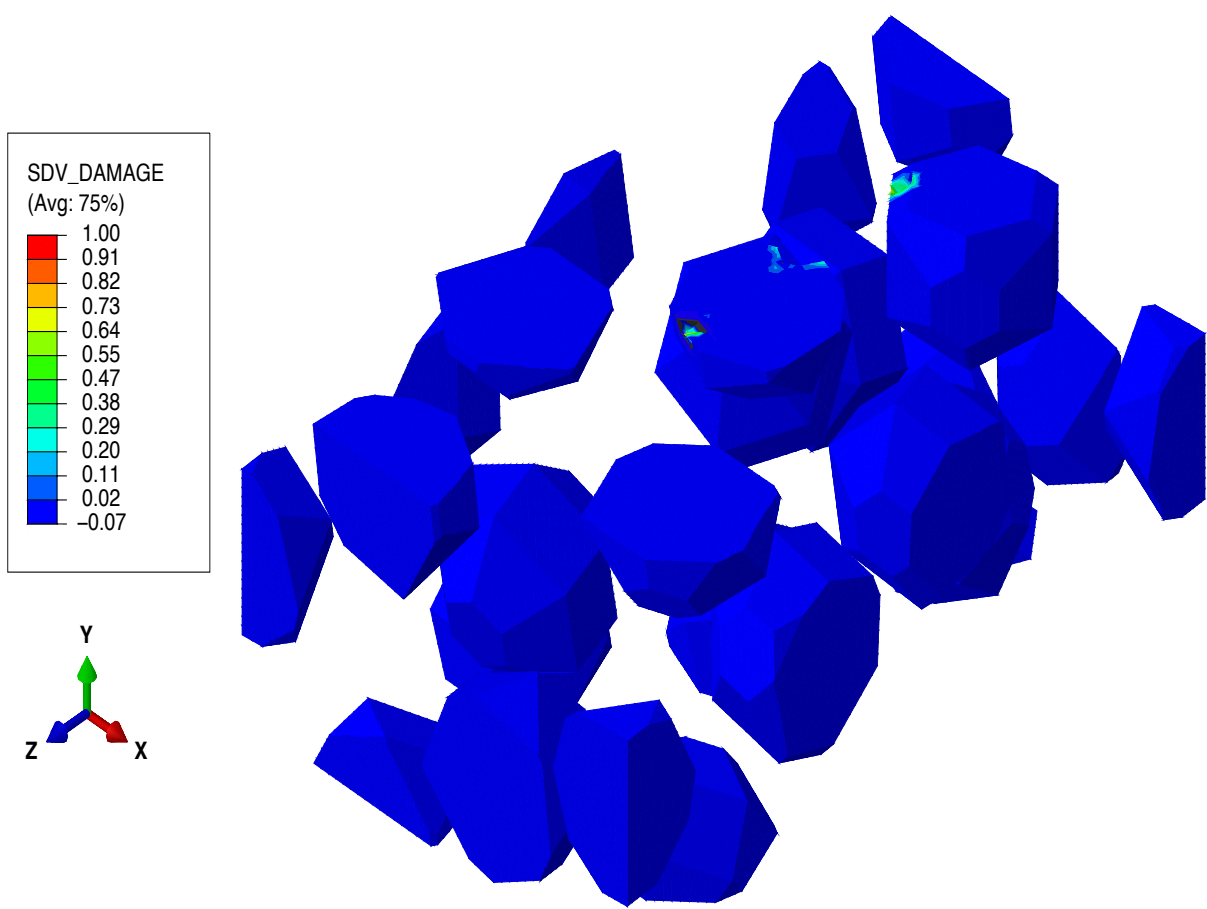
(b-II)

Fig. 6 (I) Residual stress (MPa) and (II) displacement (mm) contours of WC-Ni composite coating with WC particle size of 60 μm and (a) $\phi = 10$ Vol.% and (b) $\phi = 50$ Vol.%, at Load = 1 N.



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(b)

Fig. 7 Damage parameter contour of the composite coating under 1 N scratch load with 50 Vol.% WC particle content and the diameter of (a) 60 μm and (b) 140 μm .

The stress and displacement contours were also evaluated for the volume fraction of 10 Vol.% at 9 N, as shown in Fig. 8 (a). At this load, the stress was less homogeneously distributed at the volume fraction of 10 Vol.% than the case with 50 Vol.% volume fraction. This could be due to the larger mean free path [91] between the carbide particles [24], which caused the particles that were farther from the groove to undergo lower stresses than the same case with 50 Vol.% (See

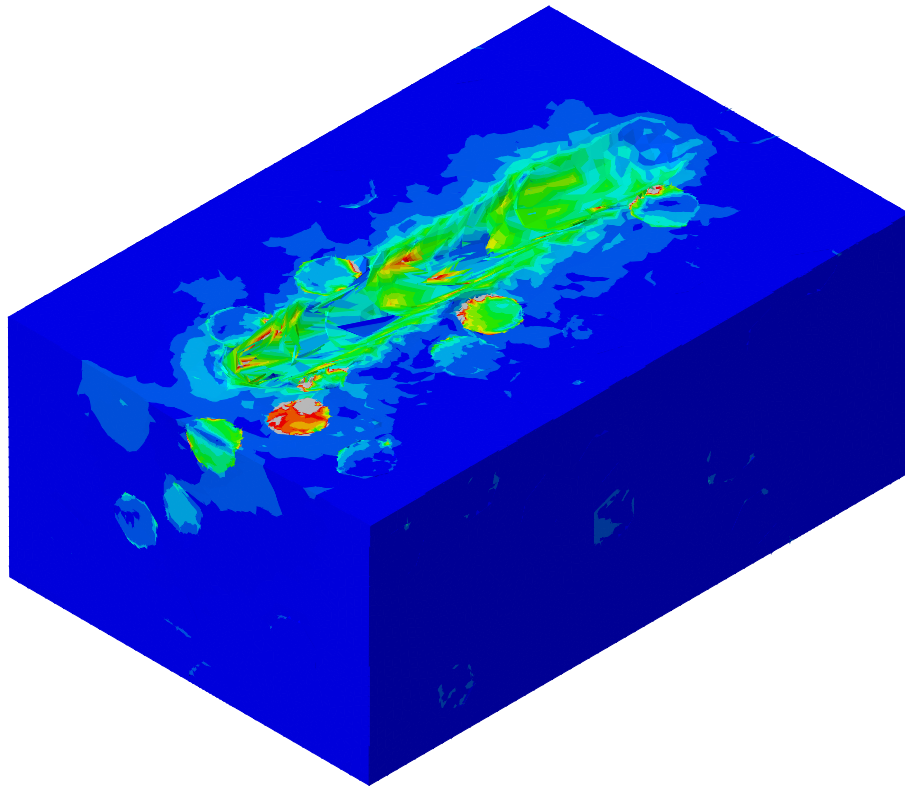
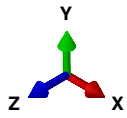
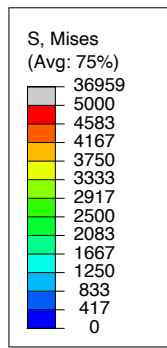
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413 Fig. 8 (a-I, c-I)) and the deformation and damage occur quite freely due to the weak resisting role
414 of the reinforcing particles to deformation (See Fig 8 (a-II)). Increasing the particle size from 60
415 to 140 μm and larger caused the mean free path to become even larger, which caused the plastic
416 deformation to occur in the matrix during sliding even at large volume fractions (i.e., $\phi = 50$ Vol.%
417). In the case of large WC particle reinforcement, the stress simulated in the composite coating
418 with 10 Vol.% WC particles was greatly affected by the behaviour of the matrix with limited WC
419 particle interference, as shown in Fig. 8 (b). By increasing the particle volume fraction to 50
420 Vol.% (see Fig. 8 (c)), the mean free path decreased, which caused the material surrounded by the
421 WC particles to be forced laterally and the vertical flow of the matrix between the WC particles
422 was reduced. Also, the higher volume fraction caused the stress to be distributed more uniformly
423 in the composite coating, as shown in Fig. 8 (c-I). This is because the local load can be more easily
424 transferred to the adjacent particles due to the smaller mean free path. This smaller mean free path
425 caused transfer of stress to the particles and matrix, and the particles located further from the
426 groove experienced larger residual stresses than the case with the same particle size and volume
427 fraction of 10 Vol.%, as illustrated in Fig. 8 (c-I). Also, the composite revealed severe deformation
428 in the areas surrounded by WC particles, as shown in Fig. 8 (c-I). This deformation related to the
429 presence of the WC particles was also observed in a study conducted by Varga, *et al.* [40].

430 Increasing the particle volume fraction affected the material removal mechanism. The material
431 removal mechanism changed from microploughing to microcutting with increasing the particle
432 volume fraction from 10 to 50 Vol.%, as less matrix deformation and accumulation on the side
433 of the groove was observed in Fig. 8 (c-II). Instead, a chip was formed in front of the indenter at
434 the end of sliding. This chip formation in front of the indenter was also observed in the scratch
435 experiment conducted by Tkaya *et al.* [88], where the microcutting mechanism was dominant.

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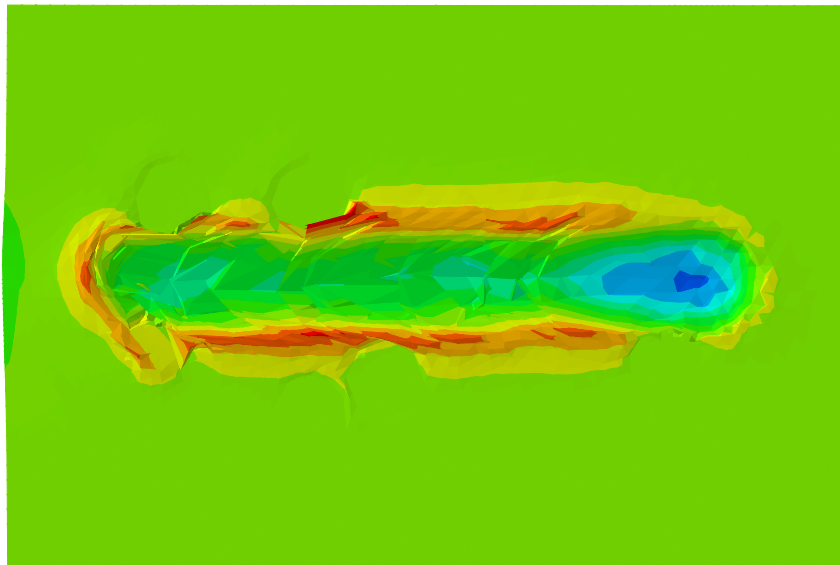
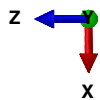
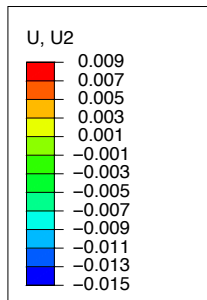
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(a-I)

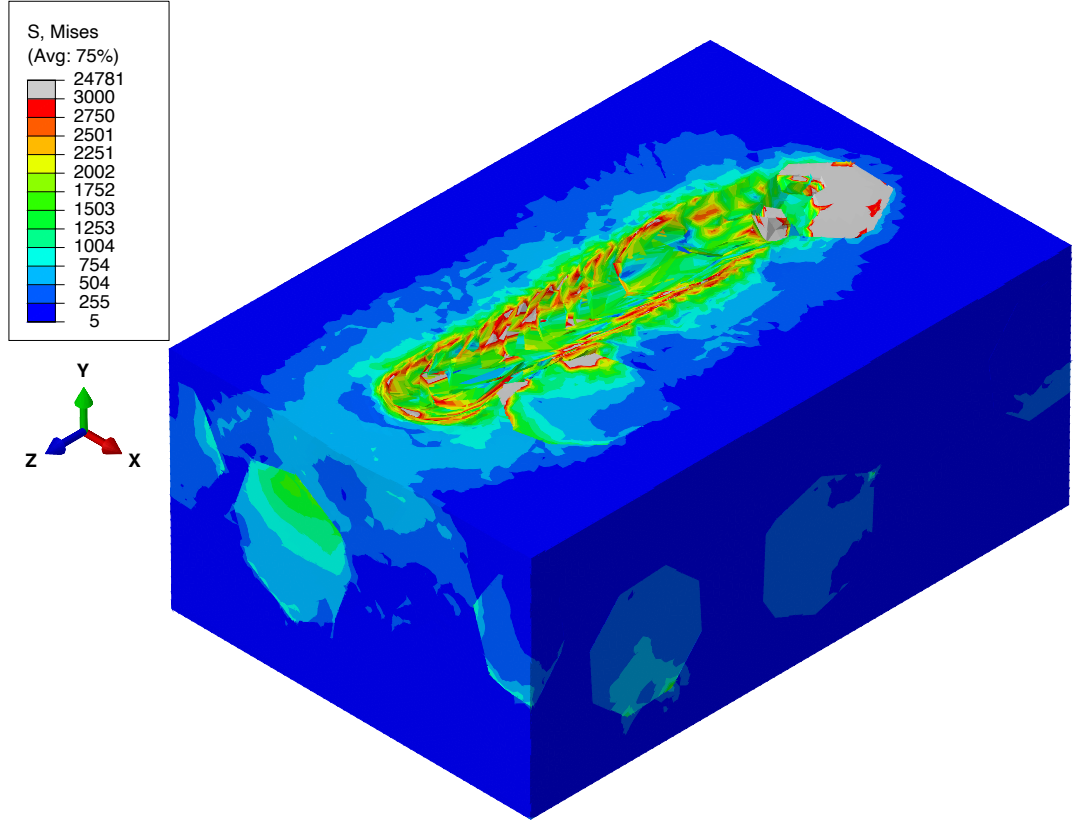


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(a-II)

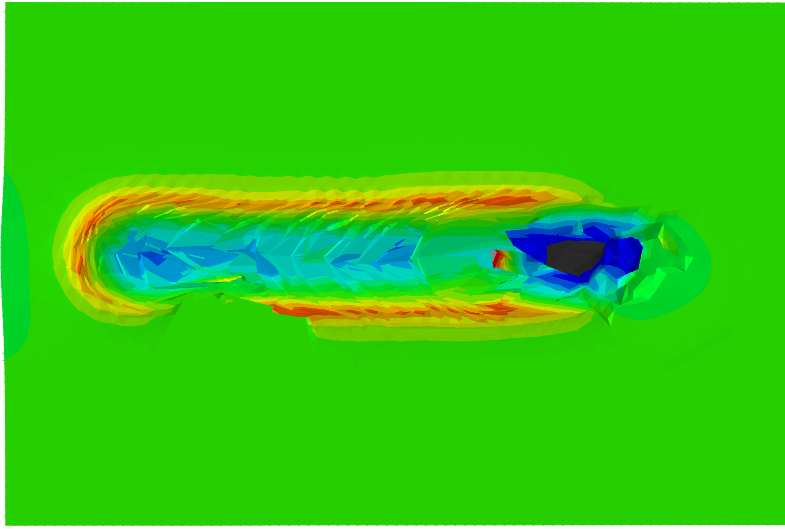
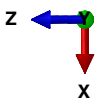
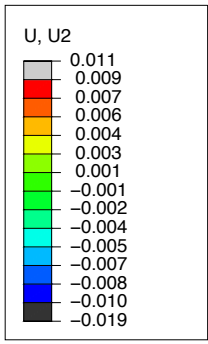


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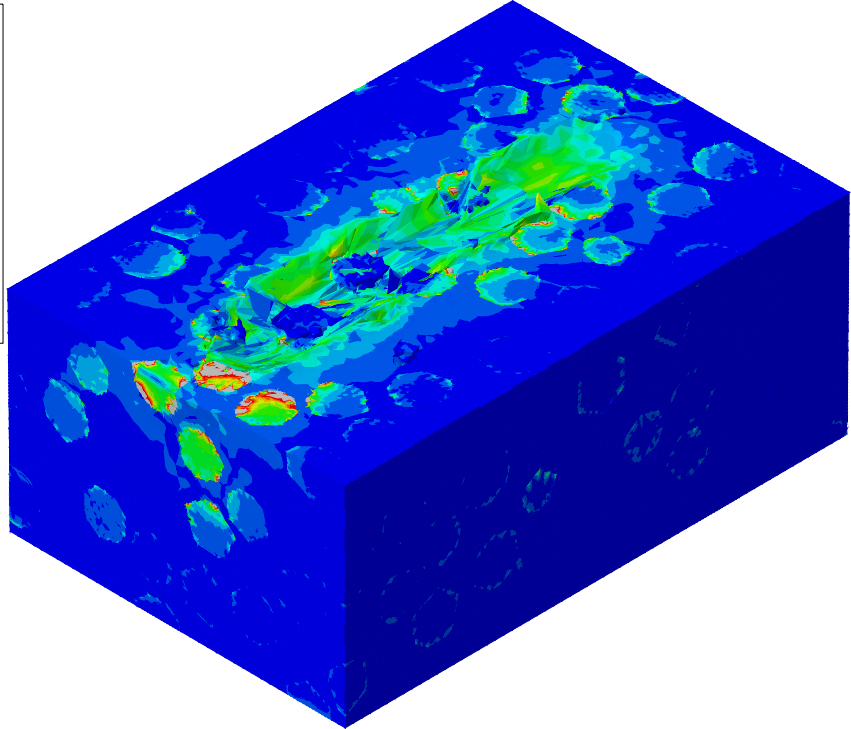
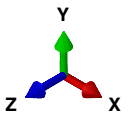
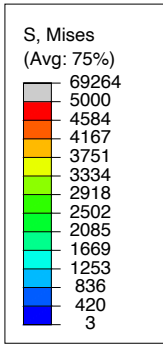
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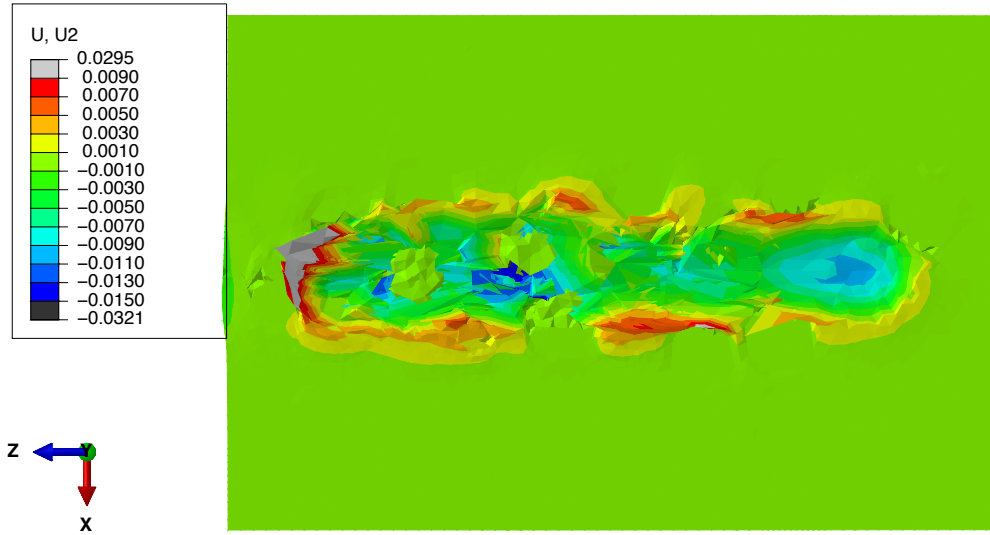
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(b-II)



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(c-I)



(c-II)

Fig. 8 (I) Residual stress (MPa) and (II) displacement (mm) contours of WC-Ni composite coating at (a)

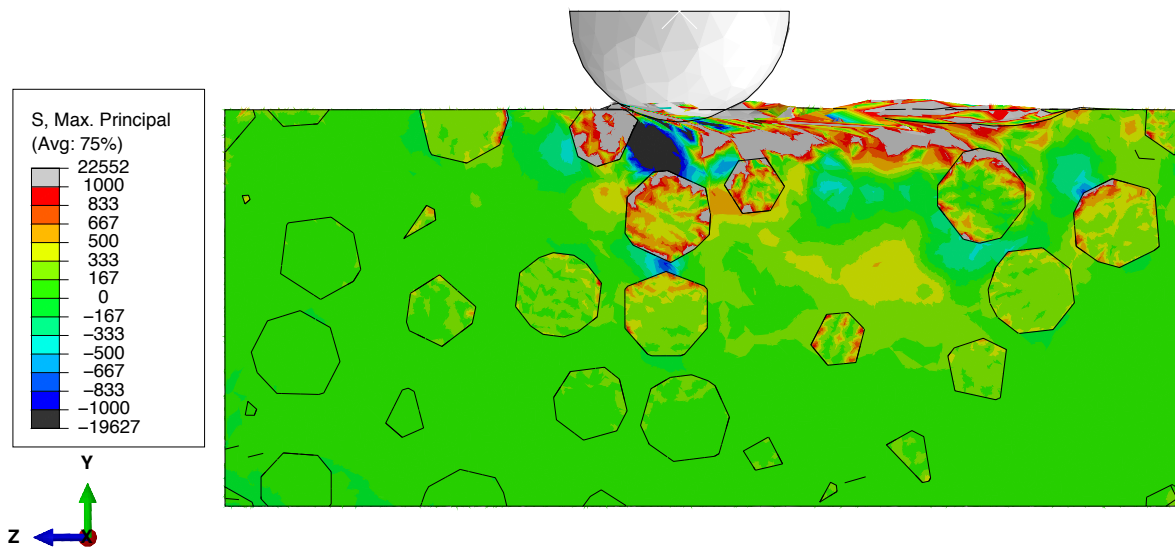
$d_p = 60 \mu\text{m}$, $\phi = 10 \text{ Vol.}\%$, Load = 9 N , (b) $d_p = 140 \mu\text{m}$, $\phi = 10 \text{ Vol.}\%$, Load = 9 N ,
and (c) $d_p = 60 \mu\text{m}$, $\phi = 50 \text{ Vol.}\%$, Load = 9 N .

3.2. Maximum Principal Stress Distribution

To better understand the effects of the WC particles on the scratch resistance of the composite coating and strengthening mechanisms of the composite, the evolution of the maximum principal stress field was determined in the cross-section of the composite along the z -axis for three different particles sizes (i.e., 60 , 140 , and 220 μm). The results are shown in Fig. 9. The stress in the particles was much larger than those in the matrix, which revealed that a larger load was carried by the particles and highlighted the load-carrying role of the particles in the composite [92]. The stress was more homogeneously dispersed in the smaller particles than in those that were larger (see Fig. 9). This facilitated transfer of the stresses to adjacent particles and led to uniform stress

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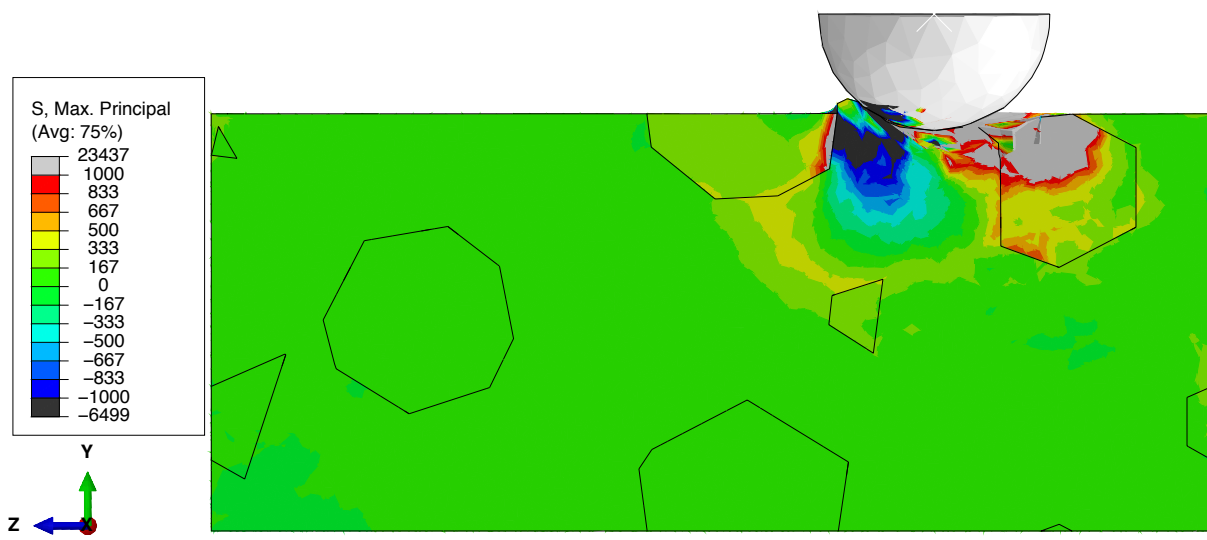
465 distribution in the composite. This stress distribution could be in the form of compression stress,
466 which happened in front of the indenter, and tensile stress, which happened behind the indenter,
467 as shown in Fig. 9. Stress concentration was also observed at the interface of the matrix and the
468 particles, which has been reported to be due to the mechanical properties mismatch between the
469 matrix and particles [24]. This high concentration of stress at the interface may have caused
470 initiation of fractures within the particle and, eventually, material removal.



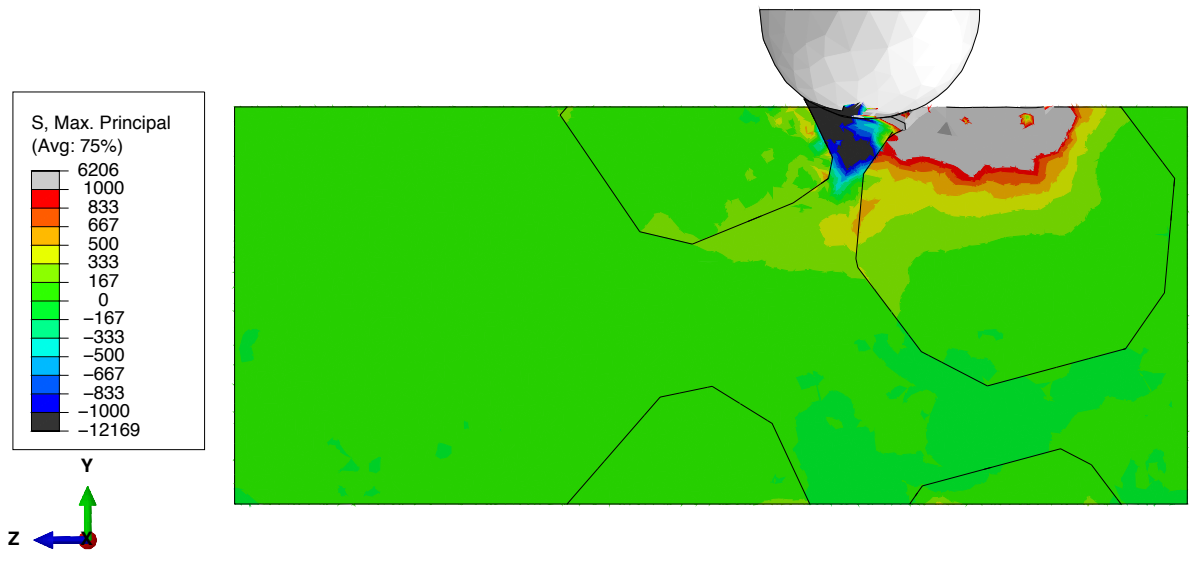
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(b)



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Fig. 9 Maximum principal stress (MPa) contour of WC-Ni composite coating undergoing a load of 9 N with 50 Vol.% particles and particle size of (a) 60 μm (b) 140 μm, and (c) 220 μm.

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3.3. Scratch Characterization and Mechanical Behaviour

To analyze the effect of WC particle size and volume fraction on the scratch depth, the scratch load was held at 5 N, and the residual scratch depth of the composite coatings and the Ni substrate, with no reinforcing particles, was obtained over the geometry, as shown in Fig. 10. Regardless of the size and the volume fraction of the WC particles, the scratch depth was reduced when adding WC particles. This reduction of scratch depth was not monotonic along the scratch length due to the presence of the WC particles, particularly when the WC particle's volume fraction was 30 Vol.% and higher and the particle size was 140 μm and larger. The reinforcing particles impeded penetration of the indenter into the MMC coating. This was the reason for this non-monotonic reduction of the residual scratch depth, which was previously reported in studies by Hu, *et al.* [44, 45].

During sliding of the indenter over the composite coating, the scratch load induced material removal and wear, resulting in worn volume loss. The worn volume loss of the Ni substrate with no reinforcement increased from nearly 300 μm³ to 4.5×10⁵ μm³ by increasing the scratch load from 1 N to 9 N, as shown in Fig. 11. At a scratch load of 1 N, the material from the Ni substrate with no reinforcing particles was removed mainly after plastic deformation, and the worn volume was negligible, as shown in Fig. 11 (a). This negligible material removal with a scratch load of 1 N was also reported in a study by Xiao, *et al.* [87]. By increasing the scratch load, the material that was removed increased considerably (See Fig. 11 (b)-(c)) due to the domination of the microcutting mechanism during material removal at higher loads [87].

At a scratch load of 1 N (See Fig. 11 (a)), the role of the microfatigue mechanism on material removal, was more pronounced at small loads. The worn volume loss was slightly reduced with

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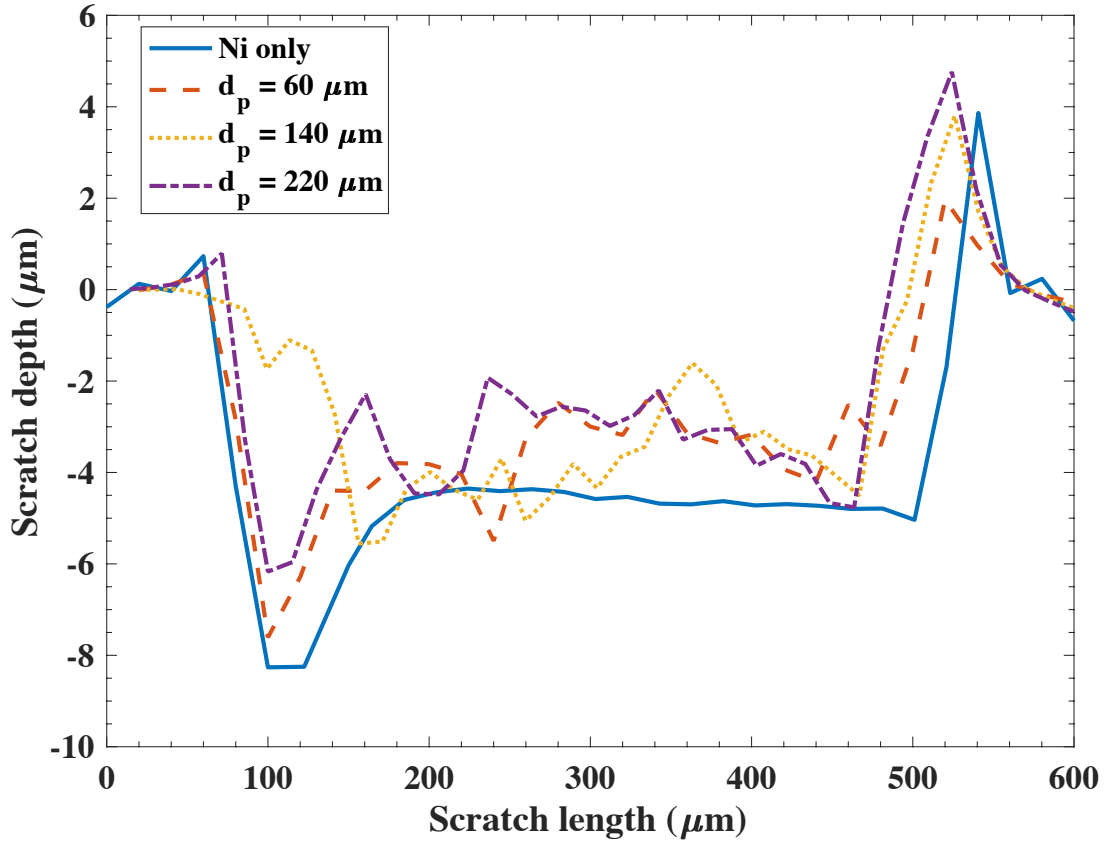
503 adding 10 Vol.% of WC particles regardless of the size of WC particles. Also, increasing the
504 volume fraction and size of the particles showed an adverse effect on the worn volume. Generally,
505 understanding the effect of WC particle volume fraction on material removal and loss might be
506 difficult at small loads with a single asperity scratch test. With the interaction of one abrasive
507 particle, the stress was mostly stored in the element, and the damage parameter remained smaller
508 than 1. This means that multiple cycles are required to clearly demonstrate the role of reinforcing
509 particles and damage on the composite and their effect on microfatigue [32].

510 At a scratch load of 5 N (see Fig. 11(b)), the WC particles improved the wear resistance of the
511 composite compared to the Ni substrate with no WC particle reinforcement. The material
512 resistance varied with changes in the WC particle volume fraction and size due to the competition
513 of two decisive factors, namely hardness of the composite [12, 14, 92] and impeding penetration
514 of the indenter [44, 45]. Larger particles (i.e., 140 and 220 μm) than the indenter impeded indenter
515 penetration into the composite better than the smaller WC particles (i.e., 60 μm), which has been
516 noted elsewhere by Hu, *et al.* [46], as shown in Fig. 10. As a result, the volume worn by the
517 indenter was reduced when the particle's diameter was 140 and 220 μm , as shown in Fig. 11 (b).

518 As noted by Alzouma, *et al.* [17], the larger volume fraction of the WC particles protected the
519 matrix from plastic deformation. With increasing the particle volume fraction, the composite
520 became more brittle [46], which promoted the microcutting mechanism of material removal, with
521 the microfracturing of the WC particles [32]. Thus, with increasing the WC particle volume
522 fraction, the bulk hardness may increase with a tradeoff in toughness. This indicated that a critical
523 WC particle volume fraction exists at which the worn volume is minimum [17, 45], and this is
524 likely related to the competition of hardness and the impeding reinforcing particle effect mentioned
525 earlier (Fig. 11 (b)).

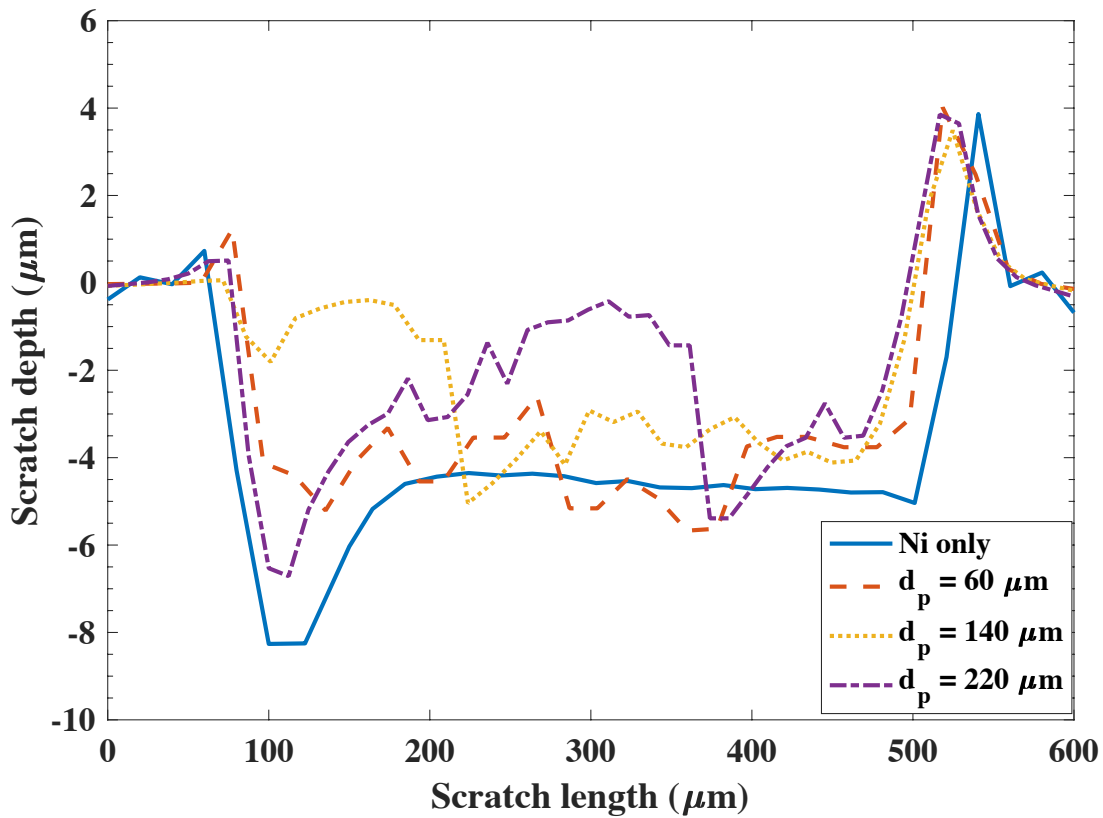
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526 The effects of larger loads on the mechanisms involved in material removal were analyzed by
527 increasing the normal load to 9 N. By increasing the scratch load, the impeding penetration of
528 the indenter due to the larger WC particles was less pronounced, particularly at $\phi = 50$ Vol.%, as
529 the worn volume loss was significantly reduced for any concentration of WC particles when the
530 particle size was 60 μm , as shown in Fig. 11 (c). At this time, the particle fracture played a
531 significant role in damage and failure of the composite. The worn volume loss was related to the
532 bulk hardness of the composite, the volume loss decreased with inclusion of smaller WC particles.
533 This reinforcement was reduced due to particle fracture particularly when the particle size was
534 large [94]. The high stress concentration at the edge of large particles was one possible reason for
535 the fracture of brittle particles. Also, the critical volume fraction at which the lowest worn volume
536 loss was observed was dependent on particle size. These changes in the critical volume fraction
537 were also reported elsewhere [17, 45]. This suggests that a strong relationship exists between the
538 scratch load, particle size, and volume fraction, and material loss during loading.

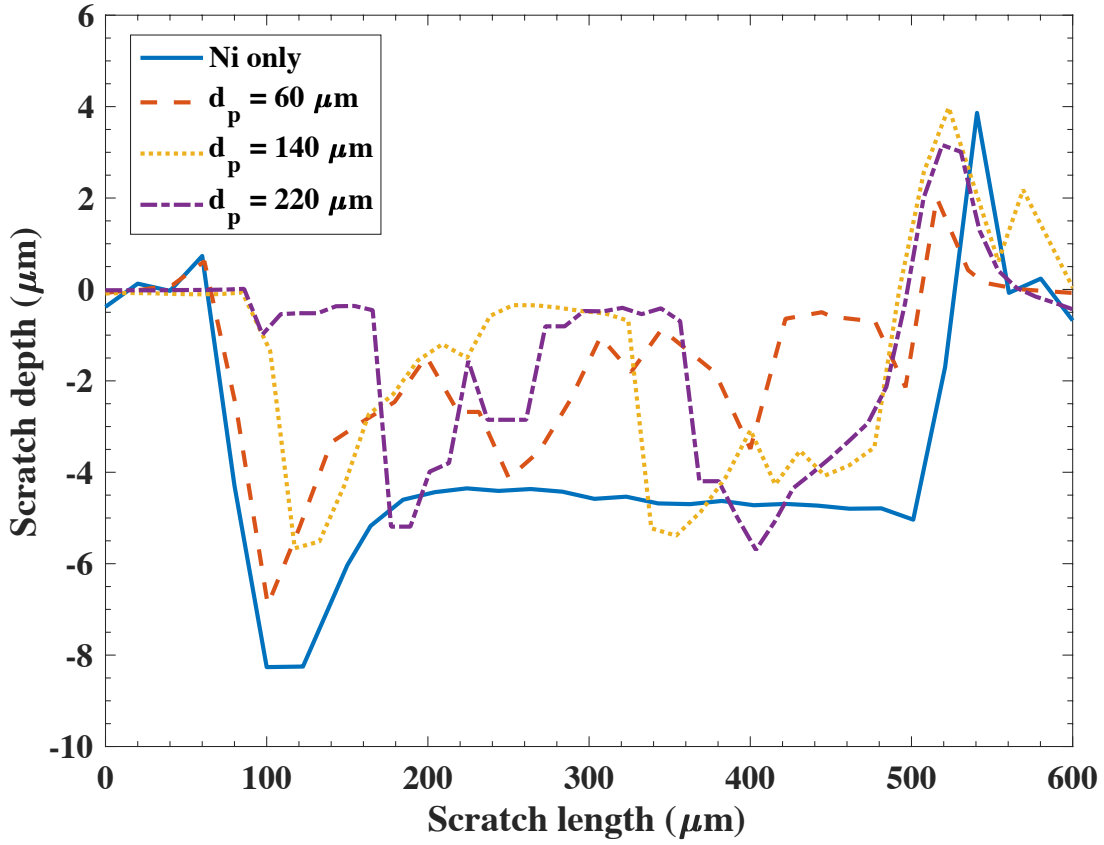


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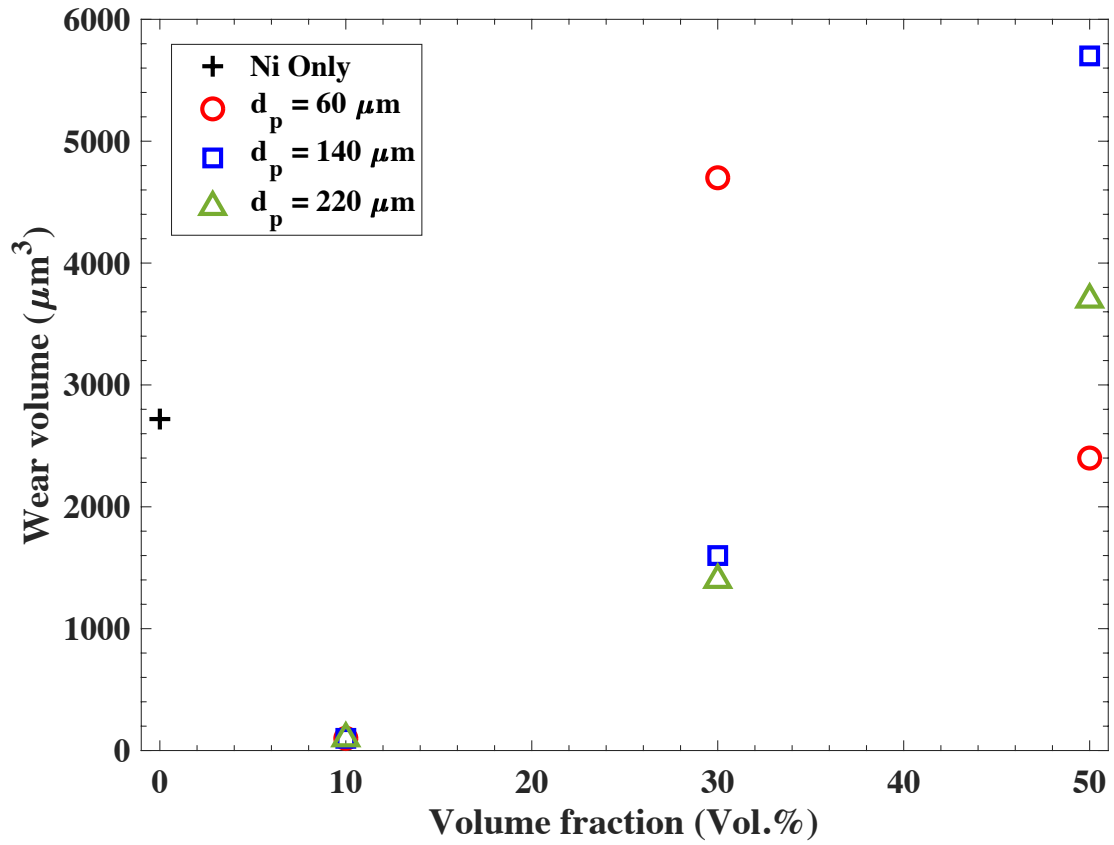


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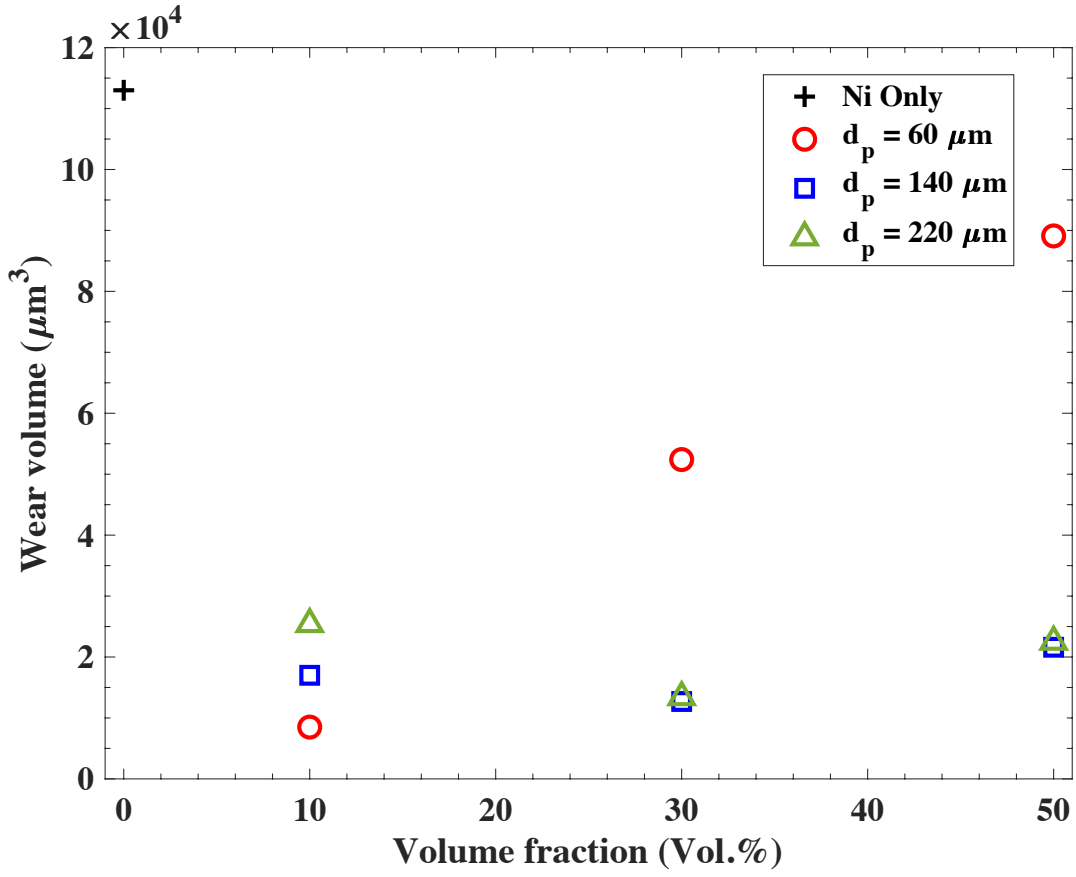


(c)

Fig. 10 Scratch depth vs. scratch length of the Ni and WC-Ni composite coating at the scratch load of 5 N with different WC particle sizes and volume fraction of (a) 10 Vol.%, (b) 30 Vol.%, and (c) 50 Vol.%.

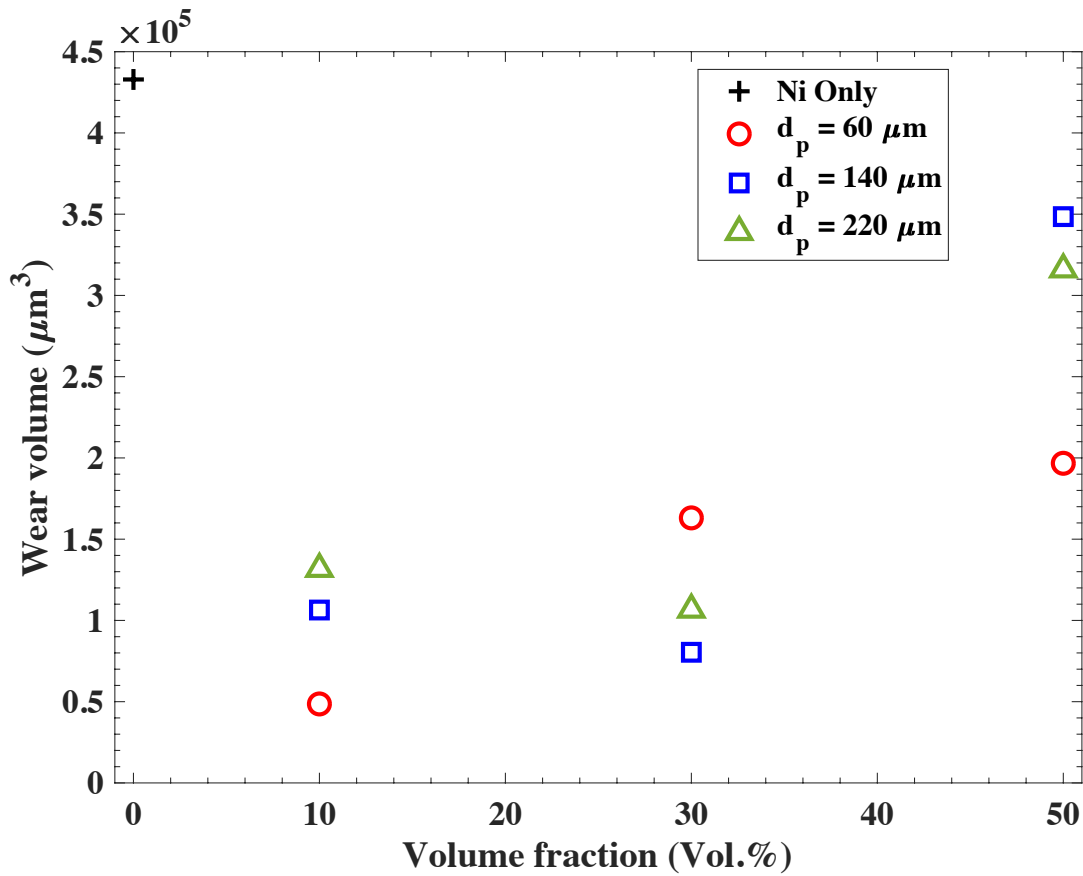


(a)



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(c)

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Fig. 11 Worn volume of all the Ni and the WC-Ni composite coatings with different WC particle size and volume fractions at a normal load of (a) 1 N, (b) 5 N, and (c) 9 N.

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3.4. Predictions from ANN Computation Model

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An ANN model was developed and trained to predict the worn volume of the composite coating by considering different combinations of scratch load, WC particle size, and volume fraction values. The worn volume was shown for all of these combinations in Fig. 11. In addition, mechanical properties for the matrix and particles were varied by 15 % [95] in order to account

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564 for potential variability in the outcomes when generated through this generalized ANN model.
565 Considering this Ni strengthening effect, the worn volume was also obtained for different
566 combinations of the scratch load (1, 5, 9 N), WC particle size (60, 140, and 220 μm), and WC
567 particle volume fraction (10, 30, and 50 Vol.%). The data were randomly categorized into a
568 training set, validation set, and test set. The training and validation sets were employed to train the
569 model for a certain number of neurons in the hidden layer and to optimize the number of neurons
570 in the hidden layer, respectively. For this reason, the model was trained using a hidden layer with
571 1 to 5 neurons, and the root mean square error (RMSE) [96] was calculated for both training and
572 validation sets, as shown in Fig. 12. It was found from the figure that the lowest RMSE can be
573 obtained in both training and validation sets when the number of neurons is set to 3.

574 The hidden layer with 3 neurons was chosen to train the model, and the true versus predicted worn
575 volumes of the training and validation data sets were calculated along with the test data set (see
576 Fig. 13), which was not used to train or optimize the number of neurons. The predicted R^2 [96]
577 was found to be 0.965, which demonstrates the accuracy of the model.

578 Using the proposed ANN model in the industry for evaluating the resistance of the MMC coatings
579 against wear can be beneficial in different aspects. First, reducing the production cost, time-
580 consuming experiments, and the number of expertise to conduct these experiments are some
581 critical benefits of such a model [97]. Second, the proposed model can be used to predict the
582 nonlinear highly complex wear problem of a composite coating with different particle sizes and
583 volume fractions undergoing different normal loads [97, 98].

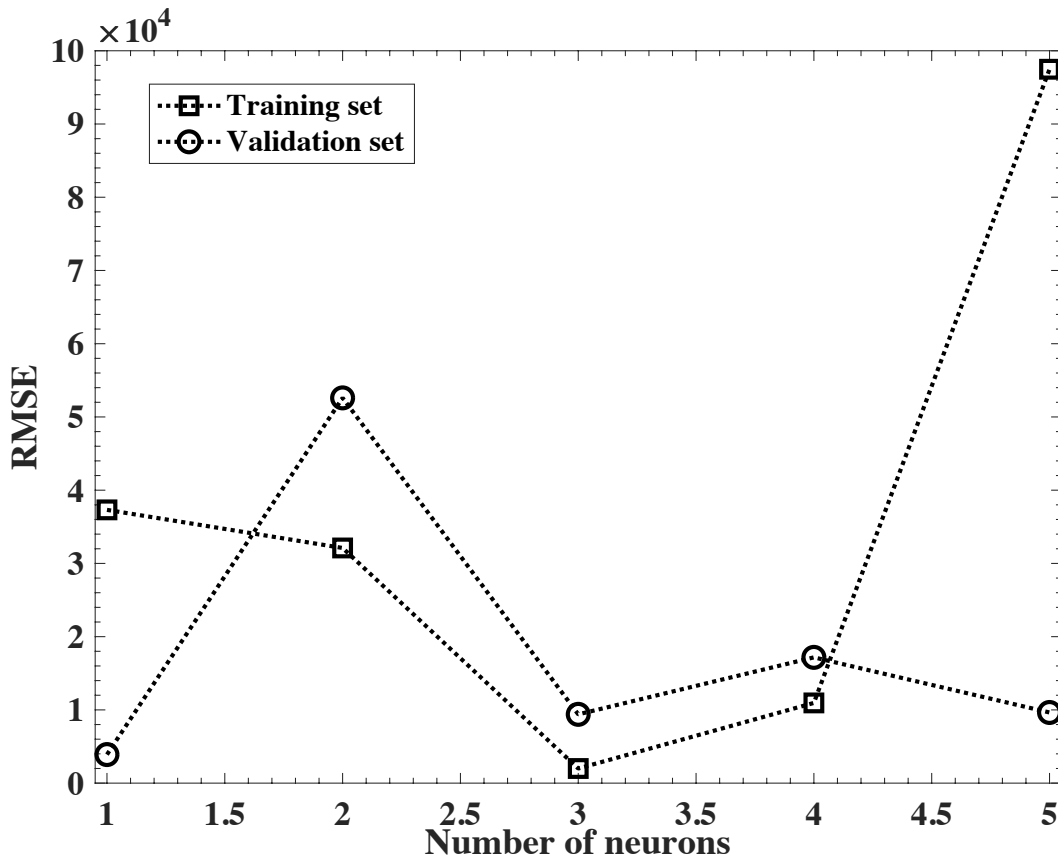


Fig. 12 The number of neurons versus root mean square error for both training and validation data sets.

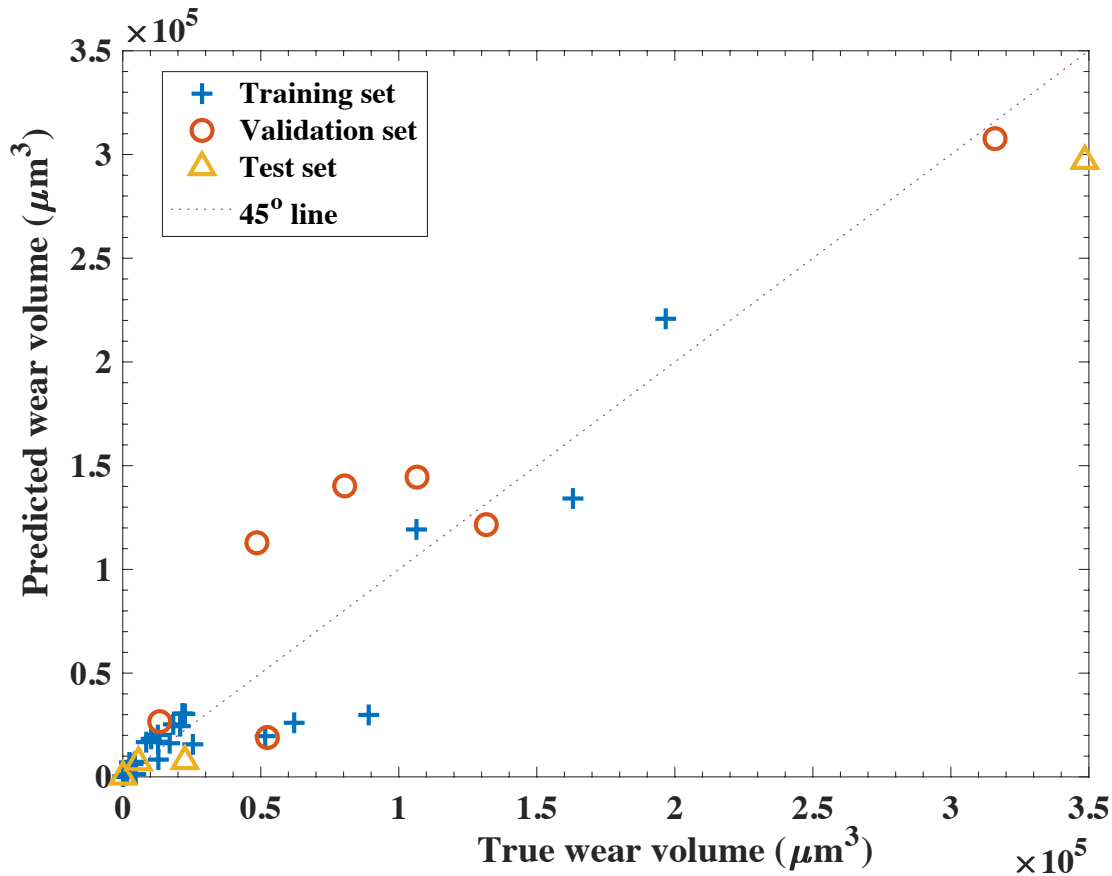


Fig. 13 True wear volume vs. predicted wear volume for all data sets.

4. Conclusions

In this paper, a three-dimensional finite element model was developed to model the scratch test in different WC-Ni composite coatings for ranging WC particle sizes ($60-220 \mu\text{m}^3$) and volume fractions ($10-50 \text{ Vol.}\%$) under different scratch loads ($1-9 \text{ N}$). The indenter size choice was motivated by the sand size observed in the Albertan oil sands. The Johnson-Cook model and Johnson-Holmquist models were employed to simulate the mechanical behaviour of Ni and WC, respectively. The developed model was validated with the experimental data obtained from the literature, and the scratch test was simulated for a substrate made of Ni with no reinforcing

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598 particles. To predict the effects of normal load, WC particles volume fraction and size on the worn
599 volume, the worn volume was calculated for each combination of these parameters, and an ANN
600 model was trained and developed. The mechanisms contributing to the material removal and the
601 influence of different parameters on these mechanisms were evaluated. The effects of the WC
602 particle size and volume fraction on the scratch depth and worn volume of the composite were also
603 analyzed at different scratch loads, and the following main conclusions can be drawn from this
604 study:

- 605 • The microploughing was the dominant mechanism of material removal of the WC-Ni
606 composite with small WC particle volume fraction at low scratch loads as the substrate
607 tended to pile up on the sides along the scratch length. Also, the material removal
608 mechanism changed from microploughing to microcutting with increasing the particle
609 volume fraction to 30 Vol.% and higher.
- 610 • With higher particle volume fraction, the stress was more homogeneously distributed in
611 the case of having smaller WC particles than larger particles, and the stress carrying role
612 of the WC particles in the composite was clearly observed. Also, a large concentration of
613 stress was observed at the interface of the particles and the matrix, which may cause the
614 initiation of material removal. The effect of the particle size and volume fraction on the
615 worn volume varied at different scratch loads due to the relationship that exists between
616 these parameters.
- 617 • With an increase in particle size, the impeding penetration of the indenter was more
618 pronounced. This impeding penetration of the indenter helped reduce the worn volume of
619 the composite.

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- The worn volume predicted by the ANN model was in agreement with the true worn volume, which shows the capability of the ANN model to predict nonlinear and highly complex wear problems.

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Declaration of interests

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests:

Author Agreement Statement

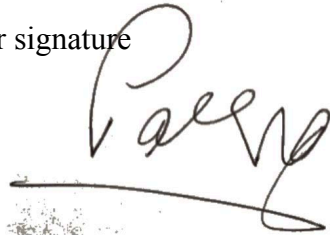
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A handwritten signature in black ink, appearing to read 'P. Allen', with a long horizontal flourish extending to the right.

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