Object-Oriented Finite Element and Inverse Analysis to Determine Elastic-Plastic Properties of an Arc-Sprayed Composite Coating

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Abstract:

The characterization of thermal sprayed coatings is often limited to microstructural analysis to evaluate the coatings morphology. Indentation is commonly used to determine the mechanical properties of different kinds of engineering materials. However, due to the complex structure of thermal sprayed coatings few results have been obtained so far. In this paper instrumented micro-indentation and meshing in the OOF2 program was combined with a inverse analysis to determine elastic-plastic properties of an arc-sprayed FeCNiBSi-(W/Ti)C Coating.

Keywords: OOF2, Inverse analysis, Arc-spray, Composite coating

1 Introduction

Microstructures of thermally sprayed coatings are complex assembling pores, cracks and different material phases. Few researchers have therefore made an attempt to simulate the correlation between a thermal spray microstructure and mechanical properties of these coatings [1]. The determination of the mechanical properties of thermal sprayed coatings is quite complicated, and often contradictory properties are reported. Non-destructive experimental procedures have been increasingly used to determine the mechanical properties of materials. Instrumented indentation tests have been used to measure the depth of penetration of an indenter into a test piece. The results of such tests can be used not only to obtain and to interpret the hardness of the material but also to provide information related to near surface mechanical properties and the deformation behavior of bulk solids and coating.
Instrumented indentation technique emerges as an attractive technique for measuring the mechanical properties of materials of small volume, and it is convenient, quick, and inherently simple without extensive effort of sample preparation in comparison with conventional tensile or compression experiments [1-4]. An instrumented indentation test (IIT) can, unlike a tensile test, characterize local properties. This test has been employed in numerous works to investigate the elastic and plastic properties of materials [5-10].

Object-Oriented Finite element analysis (OOF2) has recently been shown as an effective tool for evaluating thermo-mechanical material behavior, because of its capability to incorporate the inherent material microstructure as an input to the model. The complexity of a thermal sprayed microstructure makes it difficult to model and simulate by classical analytical or numerical techniques and thus it is appropriate to this approach. In this paper instrumented micro-indentation and meshing in the Object Oriented Finite Element 2 (OOF2) program was combined with a nonlinear finite element analysis to determine elastic-plastic properties of an arc sprayed composite coating. To generate a FE-mesh from such an image, the software OOF2, from the United States National Institute of Standards and Technology (NIST), is used. This software was developed to investigate the behavior of microstructures. OOF2 takes a non-reductionist approach to build a data structure on the digitized image of the microstructure whereby it gets connected to the associated material properties. Three elastic-plastic parameters (modulus Young’s E, yield stress $\sigma_y$ and work hardening exponent n) are extracted, in a non-linear optimization approach, fully integrated with FE analysis, using results from a single indentation curve. The iteration procedure of optimization is based on the MATLAB® nonlinear least-squares method, where a result file is created to automatically update the plastic material properties of a power-law material in the ABAQUS® input file and then run ABAQUS® to obtain a loading- unloading curve, which is then compared to an experimental data curve.

## 2 Experimental Procedure

### 2.1 Coating materials

The coatings were sprayed on grit blasted and cleaned carbon steel substrate cylindrical form with 25 mm in diameter and 5mm in thickness applying a voltage of 30 V, a current of 220 A, and air pressure of 6 bar with a spraying distance of 140 mm.

### 2.2 Electric arc spraying (EAS)

The specimens were spray-coated using ARCSPRAY 234-Metallization to achieve a coating thickness of approximately 460 μm. The spraying parameters are 100 A arc current, 36 arc voltage, 0.38 MPa air pressure and 140 mm spray distance.

### 2.3 Microstructural study

The samples were transversally sectioned using a metallographic cut-off machine, mounted in cold epoxy resin, polished with grit papers (roughness’s ranging from 400 to 1200), and polished with 1μm alumina particles to reveal the coating microstructures. The microstructure of the as-sprayed and annealed coatings was observed using optical microscopy (OM).
JEOL JSM6360 scanning electron microscope (SEM), energy dispersive X-ray spectroscopy (EDS) are also used to characterize the structures and composition of the coatings. Percentage of porosity was evaluated from SEM micrograph of the cross-section using image analysis with ImageJ program.

2.4 Depth-sensing indentation test

To explore the feasibility and robustness of the optimization algorithm in real-life applications, it is appropriate to consider an experimental load–displacement curve test to extract the material properties. In this case, experimental load–displacement curves of arc sprayed AISI 316 coating used in this study are based on microindenter Z2.5 with a Vickers tip. A Zwick/Roell equipment, with a resolution of ±0.01% in force and 0.02 μm in displacement, was used. The experiment was displacement controlled with an indentation velocity of 8.3μm/s. When the maximum available depth was reached, the indenter was held for 15 seconds, and then moved back with the same velocity. A Vickers indenter with a maximum load of 5 N was used. The load-displacement curve was recorded continuously and elastic modulus determined from the unloading curve according to the Oliver and Pharr method.

3 FEA Model

The plastic properties of the coatings were determined by solving the inverse problem using a two-dimensional finite element analysis (FEA) model. For this purpose, the determined elastic modulus was given as input in the FEA model with a stress-strain curve first assumed as an initial constitutive relation for the coating. A load-displacement curve was then predicted using the model. The predicted load-displacement curve was then compared to the experimental load-displacement curve, and the constitutive curve was iteratively modified until a best fit was reached. In this study, the finite element simulations were performed using the commercial finite element code ABAQUS®. Contacts between indenters and composite coating are modeled. The methodology to create such a model is based on three independent steps (Fig. 1). In the first step, a digital microstructure cross section is made. In the second step, this image is imported into the object-oriented finite element program OOF2 and a mesh constructed. The last step considers development of a nonlinear elastic-plastic simulation model of micro-indentation in the finite element software ABAQUS®.

Two models of the approach are provided: one simulation with uniform mesh (FE model) and another with mesh constructed from real micrographs (OOF2 model). The substrate was not included in the FEA model. The OOF2 model is utilized to study the effect of porosity on the relationship between indentation load and displacement.

3.1 The OOF2 Model

The OOF2 model was created from an image of a microstructure cross-section determined with an SEM. The digital image of the cross-section, consisting of 304 x 291 pixels, was imported into the program OOF2; an object oriented finite element program. A typical cross-section is shown in Figure1. The dark areas represent pores and micro-cracks, while the light areas correspond to the Fe-rich phase material.
3.2 Indentation model

Instrumented indentation was performed using the finite element software ABAQUS®. The overall objective with the FEA model is to predict the elastic-plastic material behavior, namely, stress-strain relationship based on load-displacement relationships determined through indentation, that is, through inverse analysis.

For the two models FE and OOF, the sample was modeled using a two-dimensional axisymmetric mesh. The four-sided pyramid indenter Vickers was substituted by an axisymmetric cone with a semi-angle of 68°. At the edge tip of the indenter, a spherical rounding with a radius of 5µm was constructed because of the fact that no real indenter can be ideally sharp. For the first model, the specimen is modeled as an axisymmetric geometry with four-node axisymmetric quadrilateral continuum elements with reduced integration (CAX4R).

The specimen was meshed with a total of 1818 axisymmetric elements. A fine mesh density was used around the area of contact indenter-coating, this density becomes coarser as the one moves away from this zone (Fig. 2). The surface-to-surface contact constraint was established between the rigid indenter and top surface of the specimen. The impenetrability condition was imposed between the “master surface” indenter and the “slave surface” specimen. Mathematically, the contact problem is equivalent to constrained optimization, which can be solved using the Lagrange multiplier method. The boundary conditions were specified in the following way. First, along the horizontal bottom line of the sample, the bottom surface of the specimen is fixed in the y-direction. Then, the left side is fixed in the x-direction. The simulation is carried out in two distinct steps, a loading step and unloading steps. In the first step, the measured displacement was given as initial condition in the FEA; a total indenter displacement of 6.513µm is imposed. During the loading step, the rigid cone indenter moves downwards along the z-direction and penetrates the foundation up to the maximum specified depth. In the second step, the indenter then taken back to the initial position. The contact between the indenter and the material is assumed to be perfect and without friction.

The mesh created in OOF2 is written in Abaqus format. The specimen is modeled as an axisymmetric geometry with four-node axisymmetric quadrilateral continuum elements with reduced integration (CAX4R) and three-node axisymmetric quadrilateral (CAX3).
3.3 Material model

The elastic behavior is modeled by the elastic modulus. The plastic behavior of the materials used in the numerical simulations was modeled considering that the stress and plastic strain, a power law strain hardening curve has been used. The stress–strain relationship \[\sigma - \varepsilon\] is assumed to be:

\[
\sigma = \begin{cases} 
E\varepsilon & \text{for } \sigma \leq \sigma_y \\
K\varepsilon^n & \text{for } \sigma > \sigma_y 
\end{cases}
\]  
(1)

where \(K\) is a strength coefficient. Considering continuity at the initial yield point,

\[
\sigma_y = E\varepsilon = K\varepsilon^n
\]  
(2)

such that

\[
K = E^n\sigma_y^{3-n}
\]  
(3)

In ABAQUS® input file, a discrete set of points was required to represent the uniaxial stress–strain data, rather than specifying the work-hardening exponent \(n\). Therefore, the set of plastic strain values varied from 0 to 0.2 with an increment of 0.02 in order to specify the plastic stress–strain data in ABAQUS®. The friction coefficients at the contact between the indenter and the top surface of the bulk material were assumed to be zero; since friction had a negligible effect on the indentation process [12]. The presence of the substrate material was ignored in the analyses, as the indentation depth was shallow enough to regard the influence of the substrate material.

Application of inverse analysis in indentation problem

There are four material parameters, namely \(E, \sigma_y, n\) and \(\nu\), to be defined for an elastic–plastic material. For simplicity, the value of Poisson’s ratio (\(\nu\)) of the composite is assumed to be 0.3. A number of optimization techniques have been used in several works [13-16] to determine material properties from indentation load–displacement curves tests. In this study, a non-linear optimization technique is devised within MATLAB®, which provides an excellent interface to FE codes such as ABAQUS®. The inverse analysis based on Levenberg–Marquardt (LM) method is used to estimate two material properties. The LM method is described extensively in [17] and its use within the context of this work is illustrated by the flow chart shown in Figure 3.
Essentially, it processes the experimental data and attempts to obtain the best estimates for unknown state variables based on least-squares method. The inverse analysis is based on the minimization of a cost functional measuring the discrepancy between the measured data and the one computed from the direct problem model. The expression of this cost functional for the indentation test can be expressed as in Eq. (4).

\[ J(U) = \frac{1}{2} \sum_{i=1}^{N} \left[ F_{i}^{\text{comp}}(U) - F_{i}^{\text{meas}} \right]^2 \]  

(4)

Where \( F_{i}^{\text{comp}}(U) \) and \( F_{i}^{\text{meas}} \) are respectively the reaction forces on the indenter obtained from measurement and computation of the direct problem. \( U \) is a vector that contains the unknown parameters, \( U^T = [E, \sigma_y, n] \), and \( N \) is the number of measurements.

Fig. 3: Flow chart of the optimization algorithm used to determine the mechanical properties

4 Results and discussion
4.1 Experimental results

Metallographic Investigation

X-ray energy dispersive spectroscopic (EDS) and SEM observations of the coating microstructure studies revealed the presence of porosity and oxides, it can be seen that all coatings consisted of lamellas built up from composite splats, unmolten particles. The carbides are also bounded with these Fe-rich phases. The exposed Fe-rich surfaces however were in contact with oxygen at high temperature, resulting in surface oxide layers around the particles, which became incorporated into the coatings, see Figure 4.(a). The oxide layers can be clearly seen as dark gray layers between the lamellae and porosity as black spots (Figure 4.(b)). The volume fraction of porosity of the coating is the order to 8%.
The EDS analysis of the coating in Figure 5 exhibits the dissolution of W, Ni and Cr in Fe-rich phases. The interface between the coating and substrate is compact with no voids or delamination detected.
**Micromechanical properties of the coatings**

The depth-sensing indentation measurements are used to determine the hardness and the Young’s modulus. The Oliver-Pharr method [18] was used to determine the elastic modulus. The reduced modulus is related to the specimen modulus through:

\[
\frac{1}{E_{IT}} = \left(1 - \nu_i^2\right) \frac{E_i}{E_s} + \left(1 - \nu_i^2\right) \\quad (5)
\]

Where \( E \) and \( \nu \) are the Young’s modulus and the Poisson’s ratio, respectively, of the specimen (s) and of the indenter (i). Table 1 shows the ten reduced E-moduli calculated from the indentation experiments.

<table>
<thead>
<tr>
<th>Properties</th>
<th>( H_{IT} ) N/mm²</th>
<th>( E_{IT} ) kN/mm²</th>
<th>( d_h ) µm</th>
<th>( d_v ) µm</th>
<th>HV</th>
</tr>
</thead>
<tbody>
<tr>
<td>Results</td>
<td>4846±38</td>
<td>78,41±52</td>
<td>39.44 ± 1.4</td>
<td>40.68± 0.9</td>
<td>577.76 ± 06</td>
</tr>
</tbody>
</table>

Two experimental indentation curves, corresponding to maximum and minimum values of determined E-modulus are shown in Figure 6. The Two curves coincide at the beginning but deviate at the high force points, this may be due to micro-cracks, which could be created progressively under the indenter when the load increases. Also, probably for the same reason, the penetration depth of the indenter increases with porosity.

![Indentation depth vs Indentation load](image)

**Fig. 6:** Experimental results from indentation tests corresponding to maximum and minimum values of the E-modulus.

### 4.2 Simulation results

The Arbitrary values of \( E, \sigma, \) and \( n \), have been chosen as initial values and the optimization algorithm has been used to find the optimized parameter from which the best fit between the experimental and predicted load–displacement loops can be achieved. The objective function is the error in the force-depth curves between the experiment and FEA. The material parameters that lead to the best fitting agreement can be considered to represent the constitutive behavior of the coating.
The simulation result is observed after nine iteration, in this case, the law of mobilized behavior is defined by \( \sigma_y = 1.69 \text{ GPa} \) and \( n=0.38 \). It is worth mentioning that these parameters varied, depending on the position analyzed and the associated experimental data. Experimental and numerical study \([19]\) shows that stress–strain estimated curve can be approximated by Ludwick law (\( \sigma = \sigma_y + K \varepsilon^n \)).

Table 2 shows the comparison between the results of the identification procedures of Hollomon and Ludwig laws. It is worth mentioning that these parameters varied, depending on the position analyzed and the associated experimental data.

Table 2. Results of the identification procedures

<table>
<thead>
<tr>
<th>Ludwik model [19]</th>
<th>Hollomon model</th>
</tr>
</thead>
<tbody>
<tr>
<td>( E (\text{GPa}) ) = ( E_{\exp} )</td>
<td>( E (\text{GPa}) )</td>
</tr>
<tr>
<td>( \sigma_y (\text{MPa}) )</td>
<td>( \sigma_y (\text{MPa}) )</td>
</tr>
<tr>
<td>( m )</td>
<td>( n )</td>
</tr>
<tr>
<td>137.02</td>
<td>1700</td>
</tr>
<tr>
<td>3.08</td>
<td>0.29</td>
</tr>
<tr>
<td>122.04</td>
<td>1691.80</td>
</tr>
<tr>
<td>0.38</td>
<td></td>
</tr>
</tbody>
</table>

The maximum reaction force from FEA is slightly higher than the experimental data. In addition, there are differences between the experimental data and FE solutions at the end of unloading portion and it is expected that the accuracy of the optimization results will be affected by these differences. On the contrary, an analysis based on the OOF mesh, a good agreement between the experimental curve and corresponding predicted curves can be seen (Fig. 7). The optimization results are summarized in Table 3 where the sensitivity of the proposed algorithm is demonstrated by changing three parameters at a time.

Table 3: Three-parameter optimization for FEA and OOFEA

<table>
<thead>
<tr>
<th>FEA</th>
<th>OOFEA</th>
</tr>
</thead>
<tbody>
<tr>
<td>( E (\text{GPa}) )</td>
<td>( \sigma_y (\text{MPa}) )</td>
</tr>
<tr>
<td>122.04</td>
<td>1691.80</td>
</tr>
</tbody>
</table>

It is well known that Vickers hardness HV is about \( 3 \sigma_{0.08} \), which corresponds to about three times of the flow stress at \( \varepsilon=0.08(8\%) \) \([2,20]\). This means that the measured HV can predict one point on the stress and strain curve (the flow stress of \( \sigma_{0.08} \)).
This HV measurement yields the $\sigma_{0.08}$ of 1925.86 MPa. On the contrary, the estimated stress–strain curve with OOFEA gives us $\sigma_{0.08}$ of 1813.55 MPa, showing the good agreement each other. Thus, the present approach for stress–strain behavior estimation is validated by this HV measurement. The material parameters that defined by this analysis represent the behavior of the coating. The equivalent plastic strains and Von-mises stress for the two models are presented in Figure 8.

![FE model](image1.png)

![OOF model](image2.png)

Fig. 8: Simulated Von-mises stress distribution (a) and equivalent plastic strain under the indenter (b)

5 Conclusion

Object-Oriented Finite element analysis (OOF2) has recently been shown as an effective tool for evaluating thermo-mechanical material behaviour. It has a major advantage over classical numerical modelling techniques, since it is a microstructure-based technique. The major drawback with this technique is that it is limited to elasticity and thermal conductivity calculations. The methodology based on the combination of OOF2 and a non-linear finite element analysis to determine elastic-plastic properties of an arc-sprayed FeCNiBSi-(W/Ti)C was shown successful in this study. The combined experimental OOF2 and inverse analysis were shown capable of investigating mechanical material properties for the specific material.

References