Experimental Characterization of Clad Microstructure and its Correlation with Residual Stresses

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Abstract

The repair of dies and molds used in the automobile industry by laser cladding (LC) is an important and emerging trend in additive manufacturing (AM) today. LC provides an alternative to the traditional deposition techniques which are ad-hoc and imprecise for powder metallurgical steels used in the repair of these components. The current study focuses on understanding the correlation between microstructure and the residual stress developed due to the deposition process. The microstructure was characterized using Electron Backscatter Diffraction (EBSD) analysis and the residual stress was measured using micro focus X-ray diffraction technique. The EBSD study revealed that the relative difference in martensite phase fraction resulted in local grain misorientations. A thermomechanical finite element (FE) model was also developed to predict the magnitude and nature of residual stresses in the component. The FE model calculated the stress field by considering only the thermal strain developed between the clad and substrate layers. The FE model was able to capture the nature of residual stresses in the clad and substrate where the thermomechanical effects dominate. The study revealed the importance of incorporating the effect of metallurgical transformation in FE model to accurately predict the residual stress variation in the substrate region.

Keywords: Laser cladding; repair; EBSD; X-ray diffraction; thermomechanical finite element model

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1. Introduction

The localized damage of molds and dies used in hot and cold working industry due to cyclic thermomechanical loading is a matter of serious concern [1-3]. Over the years, it has been observed that repairing these dies and molds with Crucible Particle Metallurgy (CPM) steels can potentially address the existing difficulty of excessive localized damage during operation [1, 4]. CPM steels are a special class of steels which have high weight percentage of vanadium and more uniform distribution of finer size carbides. Thus, the carbide segregation can be avoided which results in excellent combination of toughness, hardness and wear resistance as compared with conventional ingot cast tool steels [5]. Traditional repair techniques, such as thermal spraying, are ad-hoc and imprecise for these CPM steels. Moreover, the inherent issues with traditional repair techniques can lead to thermal damage and distortion of the finished component [3]. In addition to this, the dies and molds have complex 3-D shapes and they call for a very precise contoured deposition so as to avoid high tensile residual stresses. Therefore, a precise and focused thermal energy transfer process is required for the repair of these components. In this regard, a laser-based deposition technology, such as laser cladding, characterized by localized heating and rapid fusion of materials, is a promising technique.

Laser Cladding (LC) or Laser Engineered Net Shaping (LENS) are defined as Directed Energy Deposition processes, according to ASTM F42 standard [6], in which multiple layers of clad are deposited over a substrate (see Figure 1(a)). A strong interfacial bond with minimum dilution between the material layers is a pre-requisite of the process [7]. This is because clad dilution, which in generally is considered as contamination of deposited layer with the substrate material, can alter the mechanical and metallurgical properties of the clad. Moreover, laser cladding generates a relatively narrow dilution and heat affected zone (HAZ) [8, 9]. Several physical phenomena influence the quality and integrity of the final cladded component. These are the melt pool morphology, microstructure evolution and residual stress generation [3, 4, 10-12]. Characterization of microstructure of the clad, dilution, heat affected zone and substrate has been extensively reported in literature. However, these studies have been mainly restricted to Tungsten Carbide-Cobalt powder [13], Stellite 12 [14], Stellite 6 and Tungsten Carbide [15-17]. In addition to the above microstructural analysis of various metal matrix composite (MMC) such as metallic tool steel M2, Stellite 21, NiCrBSi-alloy and Inconel 625 [18] and selective laser melting (SLM) [19] has also been reported. These studies have reported phase and elemental investigation, using Energy dispersive scattering (EDS) and X-ray diffraction analysis along with micro-hardness analysis.

Apart from microstructural analysis, the residual stress in the finished components is of immense importance. This is evident from the fact that tensile residual stresses in the clad layer or clad-substrate interface region can lead to accelerated fatigue failure [1, 3]. The importance of metallurgical transformation of metallic alloys on residual stress can be understood from the fact that in metallic alloys liquid-solid transformation, formation of second phase particles and displacive transformations occur. Limited work has been reported in literature to investigate the effect of process parameters on residual stresses being developed in the laser cladded components using X-ray and synchrotron diffraction techniques [20]. Neutron diffraction [21] for Cobalt-chromium alloys. However, comprehensive residual stress characterization and modelling for CPM steels has not been reported in the literature. Therefore, it is important to understand the causes for evolution of residual stresses in a laser cladded component and their relationship with microstructural transformation for CPM steels. Accordingly, this study is aimed at correlating the effect of metallurgical transformation such as phase evolution and associated grain misorientation on the residual stress developed during laser cladding of H13 tool steels using CPM 9V steel powders.

In addition to experimental characterization, it is desirable to develop Finite element (FE) models to predict the clad quality as a function of process parameters and identify the optimal cladding conditions. This is because FE model is an appropriate tool to estimate the temperature distribution, and characterize the clad quality, which includes clad dilution, HAZ, microstructure evolution and residual stress field. As LC is a temperature driven melting and solidification process [9], the residual stress primarily develops due to differential thermal expansion and subsequent contraction between the clad and substrate layers [4]. Various transient stress analysis for non-powder metallurgical material systems, such as titanium alloy [22], stellite on austenitic stainless steel AISI 304 [23] and monel on Ni-based alloys [24] have been presented in literature. In addition to these, thermal analysis to investigate the effect of surface tension on the melt pool in laser cladding of CPM steels [12] has also been reported. Pal et al. [25] has reported 3D dislocation density based thermomechanical finite element analysis for SLM. FE
model for residual stress analysis on LC using particulate MMC has been reported in literature by Plati et al. [26]. However, the studies reported in literature lack a comprehensive analysis of thermal and mechanical interaction for powder injection mode of laser cladding for CPM steels.

Consequently, in this work the residual stress predicted from a thermomechanical finite element model is compared with the residual stress measured using X-ray diffraction. Element birth technique has been used to simulate powder injection laser cladding of CPM 9V over H13 tool steel. The heat load addition is simulated by writing a user-defined subroutine DFLUX in ABAQUS®. The residual stress due to thermal expansion is calculated by defining the mechanical material model in user sub-routine UMAT in ABAQUS®. Note that the thermomechanical model predicts the stress field developed in the component purely due to differential thermal expansion and subsequent contraction between the clad and substrate layer. In addition to the thermomechanical analysis, the influence of microstructural transformation on grain size distribution and grain misorientation is analyzed. Furthermore, a correlation is drawn between the microstructure and the grain misorientation with the experimental and predicted residual stresses to understand the role metallurgical transformations on the residual stress evolution.

2. Experimental description

The experiments were carried out at Monash Centre for Additive Manufacturing (MCAM), Monash University, using a 4kW; continuous-wave CO2 disk laser (make: Trumpf TruLaser cell 7040). The system is equipped with full CNC controlled 5-axis motion stage and twin powder feeder system using argon as the carrier gas. Argon was also used as shielding gas, to prevent oxidation of the powder. A schematic of the laser cladding setup is shown in Figure 1(a). As particle, metallurgical vanadium carbide steels such as CPM 9V, are extensively used for repair of damaged or worn out dies made up of H13 tool steels [27, 33], so, the substrate considered for the current study is H13 tool steel and clad material is vanadium carbide steel, CPM 9V. Chemical composition of H13 tool steel and CPM 9V is provided in Table 1. Single tracks of clad material were deposited and a metallograph of the cross section of the clad and substrate is shown in Figure 1(b).

<table>
<thead>
<tr>
<th>Element</th>
<th>C</th>
<th>Si</th>
<th>Cr</th>
<th>Mo</th>
<th>V</th>
<th>Mn</th>
<th>Fe</th>
</tr>
</thead>
</table>
| H13     | 0.4| 1  | 5.25| 1.35| 1  | 0.4| Bal.
| CPM 9V  | 1.9| -  | 5.2| 1.3 | 9.1| -  | Bal. |

The actual dimension of the substrate was 100 mm × 50 mm × 25 mm over which a 100 mm long clad was deposited. A uniform laser heat source was employed with beam diameter of 3 mm and power of 1700 W. The powder particles were spherical in shape with size range of 44-104 µm.

![Fig. 1. (a) Schematic of laser cladding process [12], (b) Cross section of clad layer through microscope](image)
3. Microstructural characterization

Microstructural characterization using Electron backscatter diffraction (EBSD) technique was conducted on a specimen to determine the phase fraction, average grain size distribution and misorientation of grain along the cross section of the specimen. The EBSD scans were obtained at 4 different locations of the specimen where microstructural aspects were expected to vary. The location of the points for microstructural characterization along with the process parameter has been listed out in Figure 2.

![Fig. 2. Location of points for metallurgical characterization and process parameters](image)

The current study is in continuation of the work conducted by the same research group [33]. The specific process parameters (listed out in Figure 2) used in the current study is one representative case aimed at understanding the influence of microstructure evolution on residual stress.

3.1. Phase analysis

Visualization of microstructure of the final laser cladded component was conducted using Image Quality (IQ), Inverse Pole Figure (IPF) and Phase maps constructed from the EBSD data. The IQ, IPF and phase map variations at various locations along the cross section of the laser cladded specimen are shown in Table 2. For EBSD scan a step size of 0.3 µm was used with confidence index (CI) >0.1 and grain tolerance angle of 5°. The CI>0.1 filter was applied to ensure that only correctly indexed points are included in the calculation of phase fractions. The points excluded from the data due to CI filter form a partition. Thus, the partition fraction indicated in the phase maps is total minus the CI partition fraction. Hence, if the phase fractions are added they make up for partition fraction but will not be equal to 1 in case of total fraction.

In EBSD analysis it is very difficult to index the alpha ferrite phase having a grain structure and BCT martensite phase having lath morphology. So, generic FCC and BCC phases have been used to index the phases during the EBSD analysis. From Table 2 it is observed that, very fine equiaxed alpha phase is present in the clad region. On the other hand, in the interface region prior austenitic grains appear with larger grain size, as evident from Table 2. Further, it is observed that in the predominantly prior austenitic grain, lath morphology is present in the interface and substrate regions. The possible reason for evolution of such microstructure along the cross section will be investigated in the following sections.
3.2. Grain size variation

To comprehensively understand the variation of microstructure along the cross section, it is important to analyze the grain size distribution along the cross section. The grain size distributions at different EBSD scan locations are shown in Figure 3(a). It can be observed from Figure 3(a) that very fine grains are present in the clad region. This is also supported by phase analysis in Section 3.1, which shows very fine equiaxed alpha phase present in the clad region. This can be attributed to the fact that; very high cooling rates are present in the clad region due to conduction and convection. However, from Figure 3(a) it can be seen that, the interface region is primarily composed of larger grains in comparison to the substrate regions.
From the grain size distribution at specific locations in the cross section in Figure 3(a), the weighted average grain diameter can be calculated. The variation of average grain diameter along the cross section is shown in Figure 3(b). From Figure 3(b) it can be seen that, the average grain diameter around the interface region is ~79% more than the average grain diameter in the clad region. On the other hand, the average grain diameter in the substrate region ~32% less than the average grain diameter in the interface region. The appearance of comparatively large grains around the interface hints at possible lower cooling rates in the substrate layer between the interface and melt depth, during solidification. To understand this behaviour further investigation will be conducted using a finite element model in Section 5.

3.3. Kernel average misorientation

In laser cladding, thermal processing of the component results in the development of local strains in the material. As opposed to macroscopic strains, these local strains are inhomogeneous in nature due to the presence of dislocations. These dislocations result in local misorientation inside the individual grains. Thus, these local strains can be visualized with the help of Kernel Average Misorientation (KAM) [31]. For a given point the average misorientation of that point with all its neighbours is calculated such that misorientations exceeding some tolerance value (Maximum misorientation) are excluded from the averaging calculation. In KAM mode, the misorientation between a grain at the centre of the kernel and all points at the perimeter of the kernel are measured. The local misorientation value assigned to the centre point is the average of these misorientations. For the present study, KAM is calculated for 1st nearest neighbours as shown in Figure 4.

\[
KAM\ value\ at\ A, \Delta \theta_A = \frac{1}{6} \left( \sum_{i=1}^{6} \Delta \theta_{iA} \right)
\]

Fig. 4. Schematic for KAM value calculation from 1st nearest neighbor points

The KAM value distributions at different EBSD scan locations are shown in Figure 5(a). As observed from Figure 5(a), the number fraction of grains with small misorientation (< 0.5°) in the clad is ~55 % more than those at the interface and substrate regions. Conversely, the number fraction of grains in the clad, with medium
misorientation (0.5°< KAM <1.8°) is ~58% less than that in the substrate regions. However, the grains with medium misorientation in the interface region lie within 0.5° to ~2.3° with the number fraction of grains in the interface region comparable to those in the substrate regions.

Fig. 5. (a) KAM value distribution at different EBSD scan locations; (b) Variation of KAM average number along cross section

To quantify the local average misorientation at a specific location in the cross section, the KAM average number can be calculated. Note that the KAM average number is the weighted average of the KAM value calculated from the KAM value distribution at specific locations in the cross section in Figure 5(a). The variation of KAM average number along the cross section is shown in Figure 5(b). Form Figure 5(b) it can be seen that, the KAM average number around the interface region is ~22% more than the KAM average number in the clad region. On the other hand, the KAM average number in the substrate region is ~16% less than the KAM average number in the interface region. Thus, it can be inferred that relatively more local misorientation is present in the interface region. The lower local misorientation in the clad region in comparison to that in the interface and substrate regions can be attributed to the fact that very fine equiaxed grains are present in the clad, as evident from Table 2. While the variation of KAM average number in the interface and substrate region can be attributed to the variation in martensite volume fraction. Note that the transformation from austenite to martensite strongly increases the dislocations density in the structure [32], which is reflected in the KAM value. This will be analysed in Section 5 to draw a correlation between local misorientation and residual stress.

4. Modelling and characterization of residual stress

4.1. Physical description

The schematic for powder injection laser cladding is shown in Figure 1(a). To calculate the residual stress field, a coupled thermomechanical finite element model of laser cladding was developed. The coupled thermomechanical model solves for temperature and displacement simultaneously to calculate the evolving stress field. The cyclic differential thermal expansion and contraction between the layers of the clad and substrate result in the development of residual stresses in the material. The details of the thermomechanical model are provided in a separate work of the same research group [4, 12]. However, the governing equations and boundary conditions along with the details of the numerical formulation are provided in the following sections.

4.2. Governing equations and boundary conditions

In a coupled thermomechanical finite element analysis of laser cladding the values of nodal temperatures obtained after thermal analysis of uniformly moving heat laser source are used as input to calculate the mechanical response, to calculate the residual stresses developed. Transient heat conduction equation for a homogeneous, isotropic material is used as the basic governing equation for thermal analysis, which is given as [34]:

\[
\frac{\partial T}{\partial t} = \nabla \cdot (\kappa \nabla T) + \dot{q}
\]
\[ \rho C_p \left( \frac{\partial T}{\partial t} + U_l \nabla T \right) = \nabla (K \nabla T) + H \]  

(1)

where \( \rho, C_p, \) and \( K \) refer to density, specific heat and thermal conductivity respectively of material; \( T \) and \( t \) refer to the temperature and time variables respectively. \( H \) is the rate of heat generation per unit volume. The first term on the left side of Eq. (1) depicts the transient nature of the heat transfer process. The second term in right side depicts the convective part of heat due to movement of the laser beam (moving heat source) with velocity \( U_l \). The associated boundary conditions for three-dimensional thermal analysis are as follows. The top of the material is being added at each instant is subjected to a specified heat flux \( \dot{Q} \) due to laser beam irradiation (uniform heat source). The rest of the work piece surfaces open to atmosphere are subjected to convective and radiative heat losses. The above boundary condition is stated mathematically as [34]:

\[ K \frac{\partial T}{\partial n} + h(T - T_0) + \sigma\epsilon(T^4 - T_0^4) - \dot{Q} = 0 \]  

(2)

where \( n \) denotes the direction normal to surface. \( h, \epsilon, \sigma \) and \( T_0 \) refers to surface heat transfer co-efficient, emissivity, Stefan-Boltzmann constant and ambient temperature respectively. The first term represents heat loss due to conduction from the surface whose unit normal is \( n \). The second and third term refers to convection and radiation heat losses from the surface of the work-piece. The uniform heat source is given by [35]:

\[ \dot{Q}_l = Abs. \frac{\dot{Q} \exp(-\pi R_p^2 N(r,l)l)}{\pi r_0^2} \]  

(3)

where \( \dot{Q}_l \) is the attenuated laser power density, \( r_0 \) is the beam radius, \( Abs. \) is the absorptivity of the clad material. In this study a constant absorptivity value of 0.68 has been used [36]. The variation of absorptivity with temperature is beyond the scope of the current work and will be included in future studies. Also, the width of the deposited clad is assumed to be equal to the powder delivery nozzle diameter. The spatial concentration profile of a converged coaxial powder flow can be approximated by a Gaussian distribution [35] and is given by:

\[ N(r, l) = N_{peak}(l) \exp(-2r^2/R_p^2) \]  

(4)

where \( N(r, l) \) is the number of powder particles in a unit volume and is a function of radial distance \( r \) and axial distance \( l \) in an axial-symmetrical coordinate, \( N_{peak} \) is the peak concentration at the center of powder flow (where \( r = 0 \)), and \( R_p \) is the effective radius of the powder stream at axial distance \( l \). Besides these, the following initial and boundary conditions are also satisfied:

\[ T(x, y, 0) = T_0 = T(x, y, \infty) \]  

(5)

At an instant, the total elastic strain \( \varepsilon_{ij}^{e} \), is calculated from the plastic and thermal strain increments given by:

\[ \varepsilon_{ij}^{e} = \varepsilon_{ij}^{e,old} + \left( d\varepsilon_{ij} - d\varepsilon_{ij}^{p} - d\varepsilon_{ij}^{th,a} \right) \]  

(6)

where \( \varepsilon_{ij}^{e} \) is the final (updated) total strain, \( \varepsilon_{ij}^{e,old} \) is the current total strain, \( d\varepsilon_{ij} \) is the total strain increment, \( d\varepsilon_{ij}^{p} \) is the plastic strain increment (mechanical) and \( d\varepsilon_{ij}^{th,a} \) is the final (updated) thermal strain increment. \( d\varepsilon_{ij}^{th,a} \) is the thermal strain increment due to the presence of differential thermal gradient between the clad and substrate. The thermal strain due to presence of differential thermal gradient between the clad and substrate \( \varepsilon_{ij}^{th,a} \) is given by:
where $\alpha$ is coefficient of thermal expansion, $T_{\text{ref}}$ is reference temperature (i.e., starting temperature from which coefficient of thermal expansion is obtained) and $T$ is instantaneous temperature. Therefore, the constitutive relation is given by:

$$d\varepsilon_{ij}^{\text{th},\alpha}(T) = \alpha \, dT + (T - T_{\text{ref}}) \, d\alpha$$

(7)

4.3. Numerical formulation

The methodology for predicting the residual stress using user-defined subroutine UMAT in ABAQUS® is illustrated in Figure 6(a). The moving laser heat source is achieved by defining a Uniform moving heat source in DFLUX subroutine in ABAQUS®. Apart from this the injection of powder is numerically achieved using element birth technique in the finite element code. In laser cladding the mechanical and thermal solutions evolve simultaneously, but with a weak coupling between the two solutions. So, an approximate implementation of Newton's method for fully coupled temperature-displacement analysis was considered. Using an implicit time integration scheme in ABAQUS/Standard the temperatures are integrated using a backward-difference scheme, and the nonlinear coupled system is solved using Newton's method. The modified form of Newton's method involves a symmetric Jacobian matrix and is illustrated in the following matrix representation of the coupled equations [37]:

$$
\begin{bmatrix}
K_{uu} & 0 \\
0 & K_{TT}
\end{bmatrix}
\begin{bmatrix}
\Delta u \\
\Delta T
\end{bmatrix} =
\begin{bmatrix}
R_u \\
R_T
\end{bmatrix}
$$

(9)

where $\Delta u$ and $\Delta T$ are the respective corrections to the incremental displacement and temperature, $K_{uu}$ are submatrices of the fully coupled Jacobian matrix, $R_u$ and $R_T$ are the mechanical and thermal residual vectors, respectively. This modified form of Newton's method does not affect solution accuracy since the fully coupled effect is considered through the residual vector at each increment in time [37].

<table>
<thead>
<tr>
<th>Property</th>
<th>H13</th>
<th>CPM 9V</th>
</tr>
</thead>
<tbody>
<tr>
<td>Conductivity (W/m²-K)</td>
<td>30</td>
<td>26.08</td>
</tr>
<tr>
<td>Density (kg/m³)</td>
<td>7800</td>
<td>7455</td>
</tr>
<tr>
<td>Specific heat (J/kg-K)</td>
<td>430</td>
<td>460</td>
</tr>
<tr>
<td>Young's modulus (G Pa)</td>
<td>210</td>
<td>221</td>
</tr>
<tr>
<td>Poisson's ratio</td>
<td>0.3</td>
<td>0.28</td>
</tr>
<tr>
<td>Thermal expansion coefficient (°C)</td>
<td>1.26×10⁻⁵</td>
<td>1.19×10⁻⁵</td>
</tr>
<tr>
<td>Yield stress (MPa)</td>
<td>1900</td>
<td>1900</td>
</tr>
</tbody>
</table>

The total thermal stress including stress due to differential thermal expansions of the clad and the substrate is calculated during each increment using Eq. (6) to (8). User subroutine UMAT is used to define the mechanical constitutive behaviour of a material. Von Mises plasticity criterion was used with linear kinematic hardening to define the material behaviour beyond yield point. User subroutine UMAT provides a platform to interact with the material model developed in ABAQUS® by updating stress value at each integration point. A flowchart showing the various steps in the computational scheme employed in this work is provided in Figure 6(a). First stress values are calculated assuming elastic strains and von Mises stress is defined. The equivalent von Mises stress is then compared with the yield criterion and if the element is actively yielding then flow stress is calculated and the
stresses are updated. The stress based on the trial stress calculated using Hooke’s law and the incremental strain is used to formulate the elasto-plastic constitutive matrix or Jacobian matrix $C_{ijkl}$. The thermo-physical properties of CPM 9V and H13 are provided in Table 3.

For simulation, a half symmetric model with dimension 6 mm × 6 mm × 10 mm was developed. Three-dimensional, 8-node thermally coupled brick; trilinear displacement and temperature element (C3D8T) were used. As the variation of stress around the clad-substrate interface region is critical. So, in the substrate minimum mesh size of 46 µm × 100 µm × 100 µm is used around the interface with progressively increasing mesh towards the bottom. However, in the clad, uniform mesh of 54 µm × 100 µm × 100 µm has been considered along the cross-section of the clad. The total number of nodes and elements was 28644 and 25890, respectively, which was obtained after mesh sensitivity analysis. In the mesh sensitivity analysis, the variation of secondary variable (stress in this case) for different mesh sizes was compared to ensure the computational efficiency of the current model. Figure 6(b) shows the meshed geometry of the finite element model along with the loading and boundary conditions. The various boundary conditions along with the loading conditions are shown in Figure 6(b).

### 4.4. Model validation

Residual stresses in the final laser cladded component develop predominantly due to the presence of relatively high thermal stresses between the layers of the clad and substrate. The thermal stresses develop primarily due to different coefficient of thermal expansions and reference temperatures between the clad and substrate materials [21]. In laser cladding, the substrate is heated up to the melting point, and a molten layer of the clad material is deposited on it. The molten layer of material deposited into the substrate thereafter solidifies and starts shrinking due to thermal contraction, whereas the substrate first expands and later contracts due to the local thermal cycle. This phenomenon of local contraction and expansion leads to the development of residual stresses.

The residual stresses in the clad, interface and substrate region of the laser cladded components were measured using Bruker D8 Discover X-ray diffractor equipped with a 1/4-Circle Eulerian Cradle. The size of the collimator used was 50 µm, with X-ray beam of 50 V and 1000 µA. The detector used was Vantec-500 2D with detector distance 200 mm. For the residual stress measurements, positive and negative tilts of 40° were used. The directions of measurement are shown in Figure 7(a). The comparison between residual stress measured using X-ray diffraction (XRD) and predicted by the thermomechanical model is shown in Figure 7(b). From the XRD analysis it is seen
that, tensile stresses develop in the layer of substrate between the clad-substrate interface and melt depth. During re-solidification, the layer of the substrate between the clad-substrate interface and melt depth has relatively high cooling rate compared to the colder substrate below. As a result, the contraction in this layer is highest. This contraction is restricted by the comparatively colder and bigger substrate underneath, which induces tensile residual stress in the substrate layer between the clad-substrate interface and melt depth. This tensile stress in the substrate layer near the melt depth induces compressive residual stress in the clad layer to maintain force balance [33]. Thus, differential thermal expansion and contraction between the clad and substrate layers induce compressive residual stresses in the clad layer and tensile stress in the substrate near the melt depth.

![Diagram of stress tensor and cross section along the clad deposition direction.](image)

**Fig. 7.** (a) Direction of X-ray diffraction measurements, (b) Comparison of residual stress measured using X-ray diffraction and predicted by thermomechanical model

From Figure 7(b) it is evident that the thermomechanical model can predict residual stress variation in the clad and in the substrate layer near the melt depth, both qualitatively as well as quantitatively with reasonable accuracy. The thermomechanical model predicts compressive residual stress in the clad layer with prediction error of ~26% and tensile residual stress near the melt depth with prediction error of ~29%. Hence, the model is able to capture the nature of residual stresses in the clad and substrate where the thermomechanical effects due to differential thermal expansion and contraction dominate. However, the XRD results (Figure 7(b)) also show the presence of compressive stresses in the substrate region. The occurrence of compressive stress in the substrate region can be attributed to the development of metastable microstructures such as martensite. This aspect will be discussed extensively in the next section.

**5. Correlation of microstructure with residual stress**

This section provides a comprehensive correlation between the metallurgical transformations and the residual stress variation along the cross section of the specimen. To understand the evolution of different grain sizes along the cross section, the variation of average grain diameter and BCC volume fraction is compared with the variation of cooling rate along the cross section in Figure 8. Note that the cooling rate is obtained from the FE model and the BCC volume fraction is obtained from X-ray diffraction (XRD) analysis. This is because; determining the volume fraction of phases using EBSD analysis is dependent on the quality of the Kikuchi bands [38]. The Kikuchi bands are very sensitive to the residual stress in the material which deteriorates the quality of these bands. So, in the present study standard XRD method of phase fraction determination from peak intensities has been used. The FCC ($c_{FCC}$) and BCC volume fractions ($c_{BCC}$) are given by [38]:
\[
\frac{I_{\text{FCC}}}{I_{\text{BCC}}} = \frac{R_{\text{FCC}} c_{\text{FCC}}}{R_{\text{BCC}} c_{\text{BCC}}}
\]

such that, \(c_{\text{FCC}} + c_{\text{BCC}} = 1\)

where, \(I_{\text{FCC}}\) and \(I_{\text{BCC}}\) are the diffracted intensities obtained from 2-theta XRD profile. The parameters \(R_{\text{FCC}}\) and \(R_{\text{BCC}}\) depends on the nature of the phase, Miller indices of plane in crystal lattice \((hkl)\) and Bragg’s diffraction angle \(\theta\) measured from XRD. From Figure 8, it is evident that very high cooling rate is present in the clad layer which results in very fine grains present in the clad region. This fact is also supported by the phase analysis in Section 3.1. However, there is a significant decrease in the cooling rate in the substrate layer between the interface and melt depth. This results in local heat accumulation around the melt depth region during solidification. Thus, comparatively large grains are formed in this region. Furthermore, it is evident from Figure 8 that the BCC volume fraction increases progressively along the cross section. Note that the BCC volume fraction provides a combined measure of both the BCT martensite and BCC ferrite phases.

![Fig. 8. Comparison of cooling rate with average grain diameter and BCC volume fraction](image)

The variation of residual stress (measured using X-ray diffraction and predicted by the thermomechanical model) is compared with the KAM average number and BCC volume fraction in Figure 9. From Figure 9, it is evident that the variation of KAM average number and residual stress follows similar pattern. From Section 3.3 it was concluded that the variation of KAM average number in the interface and substrate regions can be attributed to the variation in martensite volume fraction. Thus, it can be concluded that the variation of KAM average number and BCC volume fraction reflects a variation in the martensite volume fraction in the substrate. This might have affected the residual stresses in the substrate region which is not being captured by a pure thermomechanical model.
As discussed in Section 4.4, the thermomechanical model can predict the residual stress behaviour in the clad and substrate regions where the thermomechanical effects due to differential thermal expansion and contraction dominate. However, in addition to the local thermal stresses developed between the clad and substrate layers, the metallurgical transformation also influence the development of residual stress along the cross section. The deviation in residual stress prediction in the substrate region is primarily because the thermomechanical model considered only the differential expansion and contraction between the clad and the substrate. However, if the metallurgical effects are also included with the thermomechanical analysis, additional strain components due to volumetric dilation and transformation induced plasticity can be included with the thermal strains [36]. The volumetric dilation and transformation induced plasticity strains develop in a material due to crystalline packing rearrangement during displacive transformations from austenite to martensite [39]. Hence inclusion of metallurgical effects with the thermomechanical model is expected to improve the prediction accuracy of compressive residual stress in the substrate region.

6. Conclusions

The current work is focused on a comprehensive metallurgical and mechanical characterization of powder injection laser cladding of CPM 9V on H13 tool steel. In addition to experimental characterization, finite element analysis for prediction of residual stress was also conducted. The following conclusions can be drawn from this work:

- Microstructural analysis of the laser cladded sample reveals distinct lath morphology indicating presence of martensite phase.
- The difference in grain size distribution and local misorientation along the cross section is attributed to the differential cooling rate existing along the cross section.
- The variation of KAM average number and BCC volume fraction has resulted in the variation in martensite volume fraction in the substrate.
- The presence of predominantly compressive residual stress in the substrate region is primarily due to the variation of martensite microstructure as evident from the variation of BCC volume fraction and local misorientation.
- The thermomechanical model can predict residual stress variation along the cross section of the specimen both qualitatively as well as quantitatively with reasonable accuracy. The prediction errors lie within ~26% in the clad and ~29% in the interface region.
• The limitation of the thermomechanical model to predict compressive stress in the substrate region highlights the importance of incorporating the effect of metallurgical transformation in thermomechanical analysis.

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