Prediction and measurement of residual stresses and distortions in fibre laser welded Ti-6Al-4V considering phase transformation

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Abstract

Residual stresses and distortions due to time dependent and localised heating imposed during fibre laser welding a 2.0 mm thick titanium alloy Ti-6Al-4V sheet were studied. Sequentially coupled thermo-metallurgical-mechanical simulations were performed to predict welding induced residual stresses and distortion in the fibre laser weld sample, and validated using an experimental database including weld pool geometry and temperature fields. Residual stress measurements were taken using X-ray and neutron diffraction techniques and distortion measurements were recorded using a coordinate measuring machine (CMM). The influence of thermally driven non-isothermal diffusional and diffusionless solid state phase transformations on welding residual stresses and distortions were considered in the numerical model. An internal state variables approach was used to represent the transformed volume fraction of different microstructural phases as a function of cooling rate and peak temperature, and the volumetric change due to temperature variations and phase transformations were calculated. In addition, post weld heat treatment (PWHT) as a method for reducing residual stresses was examined.

Key words

Residual stress; Ti-6Al-4V; Fibre laser welding; Numerical simulation; Phase transformation; Neutron diffraction

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1. Introduction

Fibre laser welding has the advantage of producing less distortion and residual stress than conventional fusion welding processes due to its lower overall heat input. Nevertheless, some residual stresses are formed which can have either positive or negative effects on integrity, fracture toughness, load capacity, stress corrosion resistance, fatigue life and fatigue crack initiation and propagation of the welded component under cyclic loading [1]. Tensile residual stresses are generally detrimental since they lead to brittle failure or accelerated crack growth near the weld region and increase the rate of damage by fatigue, whereas, compressive residual stresses can improve fatigue life by suppressing crack growth along the weld but may also lead to buckling [2]. Distortion can also pose serious problems since the shape of the final component is affected. The main distortion mode in welded thin sheets is out-of-plane distortion caused by angular change and cambering along the weld centreline.

A good understanding of the welding process and information about residual stresses and distortions in welded components are of great interests for quality control and improvement of structural performance of integral structures so that in service failures can be avoided [3]. It is therefore, important to investigate the effect of residual stress and distortion on the structural performance and mechanical properties of the welded joints such as the tensile, fracture and fatigue behaviour and reduce them to acceptable levels by using optimised welding parameters, joint geometry and well characterised welding procedures [3]. Determination of residual stresses and distortions by experimental measurements is complex, expensive, time consuming and requires significant amount of resources. Finite element modelling can be used as a tool for welding process optimisation and prediction of residual stress and distortions so that the use of post weld stress relieving procedures can be minimised. It is much easier to produce structures without distortion than to reduce it after welding. The methods of controlling welding distortions involve selection of appropriate restraint conditions such as supporting material and fixtures [4]. Similarly, while it is possible to relieve residual stresses in heat treatable alloys by post weld heat treatment (PWHT), it is not practical in the case of large structural applications to perform a PWHT on the entire structure due to difficulties in super saturated solutionising the material at high temperatures and then quenching without considerable deformations.

Titanium alloy, Ti-6Al-4V, is one of the most commonly used titanium alloys. It has properties which make it ideal for high performance aircraft applications such as high strength to weight ratio and good mechanical properties, where structural strength is important and the relatively high material cost can be justified. To date, very little has been reported on the weldability of Ti-6Al-4V alloy using high power fibre lasers and so the process is far from being optimised. Also, research on welding residual stresses in laser welded Ti-6Al-4V considering solid-state phase transformation is very limited [5,6]. In addition, in a lot of published work, residual stresses calculated from numerical welding simulations were only validated using simple experimental methods such as destructive hole drilling or non-destructive X-ray diffraction techniques.

In the present work, an advanced numerical model to accurately simulate residual stresses and distortions in fibre laser welded and post weld heat treated Ti-6Al-4V sheet considering both non-isothermal diffusional and diffusionless solid state phase transformations was developed. The effectiveness of the numerical model was verified via experimental measurements using X-ray and neutron diffraction techniques to measure residual stresses, a coordinate measuring machine (CMM) to measure distortions as well as weld pool geometry and temperature fields measurements. Non-destructive X-ray and neutron diffraction techniques were used to measure residual stresses. The purpose of using these techniques to measure welding residual stresses on small scale components was to experimentally validate the numerical model so that its outputs are representative for the real welded structures, and to analyse the influence of welding on the magnitude and distribution of residual stresses. It is therefore, necessary to make the weld model predictions as accurate and realistic as possible so that largely conservative assumptions such as simple yield strength level residual stress profiles defined in BS 7910, R6 and FITNET can be reduced, and more efficiently meet the in-service operating requirements and ensure structural integrity of a welded component.

Comparison of the numerical and experimental results suggested that the developed numerical model can be effectively used to estimate welding residual stresses and distortions in the fibre laser welded Ti-6Al-4V sheet. Based on these results, the influence of solid-state phase transformations on the residual stresses and distortions was studied.

2. Experimental Procedures

2.1. Materials

The material considered in this investigation was a 2.0 mm thick mill-annealed titanium alloy Ti-6Al-4V (Grade 5) sheet with chemical composition as shown in Table 1.

| Table 1 Chemical composition of Ti-6Al-4V Grade 5 (Wt. %) |
|-----------------|-----------------|-----------------|-----------------|-----------------|
| Ti              | Al              | V               | Fe              | O               |
| Balance         | 5.5-6.76        | 3.5-4.5         | 0.25            | 0.2             |

2
Literature values were used for the temperature dependent thermo-physical material properties of Ti-6Al-4V as shown in Figure 1. The solidus temperature of Ti-6Al-4V ($T_{\text{solidus}}$) was chosen to be equal to 1878 K, β transus temperature ($T_{\beta}$) equal to 1248 K, liquidus temperature ($T_{\text{liquidus}}$) equal to 1928 K and boiling point ($T_{b}$) equal to 3315 K. The latent heat effect associated with the release or absorption of energy upon solidification or melting as a result of phase transformation was considered and so the latent heat of fusion ($\Delta h_{\text{fus}}$) was chosen to be equal to 286 kJ/kg and the latent heat of evaporation ($\Delta h_{\text{evap}}$) equal to 9830 kJ/kg [7,8].

The temperature dependent mechanical properties of Ti-6Al-4V were determined by uniaxial tensile testing Ti-6Al-4V specimens at temperatures ranging from 20°C to 1000°C under a 10⁻³ torr vacuum condition and a constant strain rate of 0.001 s⁻¹ using a Gleeble 3800 thermo-mechanical simulator.

Figure 1 Temperture dependent thermo-physical [9,10] and thermo-mechanical material properties of Ti-6Al-4V used in the finite element model

2.2. Fibre laser welding

A 5 kW continuous wave (CW) ytterbium fibre laser system YLS-5000 from IPG Photonics was used in TEM₀₁ mode. The beam diameter at focus was 630 μm. The wavelength of fibre laser was 1070 nm, the beam quality factor, $M^2$ was around 7.3, the divergence half angle of the focused beam was 12.5 mrad and the Rayleigh length for the multimode beam, scaled with the $M^2$ factor was around 22.6 mm. The focal length of the focusing lens was 300 mm, and the diameter of the focusing lens was 50 mm. The focal length of the collimator lens was 100 mm and the diameter of the collimator lens was 50 mm. A beam parameter product (BPP) of less than 2.5 mm mrad was formed. All Ti-6Al-4V welding trials were autogenous. The optimum welding parameters as listed in Table 2 were chosen based on the work by Ahn et al. [11].

Table 2 Welding parameters used to perform fibre laser welding experiments on butt welded Ti-6Al-4V sheet

<table>
<thead>
<tr>
<th>Material</th>
<th>Thickness (mm)</th>
<th>Weld type</th>
<th>Laser power (kW)</th>
<th>Welding speed (m/min)</th>
<th>Focal position (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ti-6Al-4V</td>
<td>2.0</td>
<td>Butt</td>
<td>2.1</td>
<td>2.1</td>
<td>+4</td>
</tr>
</tbody>
</table>
2.3. Distortion measurement

Angular distortion and cambering out-of-plane displacements in the welded sheet were measured using a Nikon LK G-90C coordinate measuring machine (CMM) along three lines in both longitudinal and transverse directions to the weld centreline with 10 mm spacing between points.

2.4. Residual stress measurement

The lattice spacings were calculated using Bragg’s Law by measuring the scattering angle, \(2\theta\) with the instrument. Elastic strains were determined using the stress free lattice spacing, \(d_0\) and the corresponding diffraction angle, \(\theta_0\). The elastic strain was calculated using Equation 1 [12]. The determined strain is an average elastic lattice strain over a sampled gauge volume defined by slits and formed by the intersection of the incident and diffracted beams [13].

\[
\varepsilon_{hkl} = \frac{d_{hkl} - d_{0,hkl}}{d_{0,hkl}} = \frac{\sin\theta_{0,hkl}}{\sin\theta_{hkl}} - 1 
\]  

The orthogonal stresses (assumed to be the principal stresses) were calculated from the linear elastic properties of the material and the measured residual elastic strain in the relevant directions as shown in Equation 2.

\[
\sigma_i = \frac{E_{hkl}}{(1 + \nu_{hkl})(1 - 2\nu_{hkl})} \left[ (1 - \nu_{hkl})\varepsilon_{ij}^{hkl} + \nu_{hkl} \left( \varepsilon_i^{hkl} + \varepsilon_j^{hkl} \right) \right] 
\]  

where \(E_{hkl}\) and \(\nu_{hkl}\) are the elastic modulus and Poisson’s ratio, respectively of a specific crystallographic plane. The diffraction peak specific elastic constants for texture free materials are listed in Table 3.

| \(hkl\) specific E and \(\nu\) of titanium [14] |
|----------------|----------------|----------------|----------------|----------------|
| \(E_{hkl}\) (GPa) | 121 | 110 | 113 | 110 |
| \(\nu_{hkl}\) | 0.31 | 0.33 | 0.32 | 0.33 |

The reflections weakly affected by residual intergranular stresses are recommended for measuring the lattice strain. The measured lattice spacings can also be affected by changes in chemical composition, phase transformations and the presence of texture due to reorientation of grains.

In a reactor based diffractometer such as the E3 used in this investigation, a continuous monochromatic single wavelength neutron beam is produced from a polychromatic neutron beam by using a monochromator [15]. Since the incident wavelength of the diffracting neutrons is known, the lattice spacings of a specimen can be determined by measuring changes in the peak diffraction angle of a single diffraction peak as shown in Figure 2.

![Figure 2 Diffraction spectrum of fibre laser welded Ti-6Al-4V from reactor based diffractometer E3](image)

Measurements were taken at around 30 points across the sheet’s mid thickness (1 mm) and mid length at 1 to 2 mm intervals near the weld and increasing increment size away from the weld as shown by the measurement positions in Figure 3. The small increments near the weld was necessary to capture the large stress gradients in the weld region. It was expected that the distribution is symmetric around the weld centreline so it was valid to assume symmetry in the planes parallel and transverse to the welding direction and also assume that the values measured along the longitudinal
and transverse directions are the principal stresses.

Figure 3 Residual stress measurement positions for butt welded Ti-6Al-4V sheet

For X-ray diffraction measurements, a diffractometer with the X-ray tube operating at 20 kV and 4 mA target current was used. The longitudinal and transversal residual stresses distributions were measured at a depth of 30 μm from the top surface of the samples and perpendicular to the welding direction. The area of single XRD analysis was 1 mm².

Neutron diffraction measurements were made using the E3 continuous reactor source at HZB. A gauge volume of $2 \times 2 \times 2 \text{mm}^3$ was used to measure longitudinal strains parallel to the welding direction, whereas, a $2 \times 19.3 \times 2 \text{mm}^3$ matchstick shape gauge volume in the transverse and normal directions assuming small changes in the welding direction. Measurements in the Ti-6Al-4V specimens were proven problematic as very weak diffraction patterns were observed in certain orientations. While three peaks {103}, {112} and {201} were visible in the transverse direction, the {103} peak was not observed in the longitudinal direction and the {201} peak was very weak in the normal direction. The likely cause of this phenomenon was texture in the weld material created during the solidification phase of the welding procedure which is frequently observed in hexagonal close packed (HCP) materials like titanium.

3. Numerical Simulation

3.1. Finite element model geometry and mesh

Table 4 shows the details about the finite element model mesh including the number of nodes and elements, element type used for thermal and mechanical analyses.

Table 4 Mesh details for butt welded and T-joint fillet welded plates

<table>
<thead>
<tr>
<th>Thermal</th>
<th>Mechanical</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nodes</td>
<td>Elements</td>
</tr>
<tr>
<td>527693</td>
<td>115800</td>
</tr>
</tbody>
</table>

In the thermal analysis, 2nd order 3D 20 node quadratic diffusive heat transfer brick hexahedron elements (DC3D20) were employed. In the mechanical analysis, 1st order 3D 8 node linear hexahedron reduced integration elements (C3D8R) were used. In order to transfer the nodal temperature data from the thermal results file that was generated during the thermal analysis to the mechanical model for the mechanical analysis, the same finite element mesh was used as shown in Figure 8 with the same number of elements but different element types. Convergence studies on mesh density were conducted prior to this investigation [1] to ensure that a sufficiently refined mesh is used to yield accurate simulation results and to examine the solution’s sensitivity to element type and boundary conditions, the details of which are shown in Table 4 and Figure 8, with the smallest element size of $0.5 \times 0.5 \times 0.5 \text{mm}^3$. The mesh converged when further mesh refinement produced a negligible change in the solution. It was found that a model with 115,800 elements for butt welds is more than sufficient to accurately represent stress values in the weld region. A very fine mesh density was required in the weld region due to the small diameter of the moving heat source which traverses along the weld at specific time steps and the resulting high temperature and stress gradients in the fusion zone and the heat affected zones. The element size increased progressively with increasing distance from the weld centreline. Figure 4 shows mesh refinement for two different element sizes, 1-2 mesh transition. At least three to four stages of mesh refinement were used by partitioning and transforming the mesh to create a user controlled refined mesh so that the computation time can be minimised and still be able to achieve accurate results.
3.2. Thermal analysis

A 3D conical heat source model with a Gaussian power density distribution radially and a linear distribution axially was used as it produces accurate results for deep penetration laser beam welds [1].

The conical heat source has a maximum heat flux at the top surface and a minimum on the bottom surface as expressed in Equation 3.

\[ q_r(r,z) = q_0 e^{-\left(\frac{r}{r_0}\right)^2} \]

where \( r_0 \) is the radius of the heat source at a specific height \( z \), \( q_0 \) is the maximum volumetric power density and \( r \) is the current radius of the interior point, which according Equation 4 is:

\[ r = \left[ \left( x - x_e \right)^2 + \left( y - y_e \right)^2 + v t \right]^{\frac{1}{2}} \]

The distribution parameter, \( r_0 \), decreases linearly from the top to the bottom of the conic region as shown in Equation 5.

\[ r_0(z) = r_e - (r_e - r_i) \frac{z_e - z}{z_e - z_i} \]

where \( z_e \) is the top surface and \( z_i \) is the bottom surface of the cone region. The maximum volumetric power density can be obtained by integrating the volumetric heat flux, \( Q \) over the body and rearranging it to the total heat input as shown in Equation 6.

\[ Q = \int \int \int q_0 e^3 \frac{3r^2}{r_e^3} r dr d \theta dh \]

\[ q_0 = \frac{9 \eta Q e^3}{\pi (e^3 - 1)(z_e - z_i)(r_e^2 + r_e r_i + r_i^2)} \]

where \( H = z_e - z_i \), and \( h = z - z_i \), \( e \) is the base of the natural logarithm and \( \eta \) is the heat source efficiency. Heat source efficiency or energy transfer efficiency is defined as the ratio of the energy absorbed by the irradiated materials to the laser power output. The energy transfer efficiency used in the thermal model simulation was in the range of 75-80\% after calibration with experimental thermocouple measurement of welding transient temperatures.

Prediction of the weld pool size and shape requires calculation of the weld pool dynamics by solving a full solution of Navier-Stokes equations and energy equations. However, due to the complexity of the physics of the welding process, a simplified solution was used based solely on the heat equation, where the heat source was simulated instead by prescribing volumetric heat flux input to the weld model. The heat equation derived from Fourier’s law and conservation of energy can be expressed as shown in Equation 7 and is used to solve the transient temperature field \( T \) in time \( t \) and space \( (x, y, z) \):

\[ \rho C_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial x} (k \frac{\partial T}{\partial x}) + \frac{\partial}{\partial y} (k \frac{\partial T}{\partial y}) + \frac{\partial}{\partial z} (k \frac{\partial T}{\partial z}) + \dot{Q}_V \]

where \( T \) is the temperature, \( \rho \) is the density, \( C_p \) is the specific heat, \( k \) is the thermal conductivity and \( \dot{Q}_V \) is the
volumetric heat flux in W/m$^3$. In order to solve the heat equation, the thermal conductivity, density and specific heat must be specified. For a material which undergoes phase transformations, latent heats of phase transformation and microstructural evolution must also be considered.

The thermal analysis consisted of two stages. The first stage involved applying a volumetric heat flux to realise the welding process and in the second stage, the heat source was removed to let the workpiece cool down to steady state condition. Representation of the heat source with complex geometries was done using the ABAQUS user subroutine DFLUX programmed in FORTRAN. The DFLUX subroutine calculated the position of the heat source with respect to time, welding speed and nodal coordinates, and the volumetric heat flux at each integration point as a function of the heat source power, and the radius and depth of the affected area [16]. It was important to model the heat source accurately in order to predict welding residual stresses and distortions correctly. Calibration of the heat source such as the peak temperature, shape and dimensions of the weld pool was performed by adjusting welding process parameters and heat source parameters for each weld FE model to fit the experimentally observed macrograph of a weld cross-section showing the FZ and the HAZ boundaries through thickness. The calculated temperature fields after matching the macrograph were then evaluated against thermocouple measurements of the transient temperature fields captured during real welding experiments at corresponding locations for further calibrations.

Thermocouples were directly mounted on the surface of the workpiece at various locations across the weld path. Around four to five locations transverse to the weld were recorded using K-type thermocouples. It was difficult to place the thermocouple very close to the weld without exceeding temperatures above the limit of the thermocouple so the temperature histories were measured a small distance away from the FZ, in the HAZ and a few points further away.

Initial and ambient temperatures of the FE model at the beginning for all simulations were set to 20°C. Thermal boundary conditions were set to model heat transfer due to convection in air, radiation from the surface of the workpiece to ambient air according to the Stefan-Boltzmann relation and conduction from the workpiece to the mild steel support as shown in Figure 5 for butt welded and T-joint fillet welded plates. Heat transfer coefficients were adjusted in order to calculate the similar temperature fields as those measured experimentally using thermocouples.

![Figure 5 Thermal boundary conditions for butt welded plates and T-joint fillet welded plates showing heat loss due to convection in air, radiation from the surface of the workpiece and conduction between workpiece and the support](image)

Equation 8 and Equation 9 define heat loss due to surface convection and radiation, respectively, as boundary conditions.

$$ q_{\text{conv}} = h_{\text{conv}}(T - T_0) $$

$$ q_{\text{rad}} = \varepsilon\sigma[(T - T_{\text{abs}})^4 - (T_0 - T_{\text{abs}})^4] $$

where $T$ is the current temperature, $T_0$ is the ambient temperature, $T_{\text{abs}}$ is the absolute zero temperature, $\varepsilon$ is the emissivity or the ability to emit thermal radiation and $\sigma$ is the Stefan-Boltzmann constant ($5.68 \times 10^{-8}$ J/K$^4$m$^2$s$^{-1}$). The calibrated values used for the heat transfer coefficients and radiation constants were $h = 10$ W/Km and $\varepsilon = 0.4$.

### 3.3. Mechanical analysis

Mechanical analysis was performed to investigate the effect of thermal expansion and contraction due to welding on the macroscopic residual stresses and distortions using the nodal temperature data imported from the thermal analysis as a predefined field. The mechanical response of the material was calculated using infinitesimal strain theory as shown in Equation 10 assuming elastic-plastic behaviour with an isotropic hardening law.

$$ \epsilon_{ij}^{\text{total}} = \epsilon_{ij}^{\text{p}} + \epsilon_{ij}^{\text{th}} + \epsilon_{ij}^{\text{tr}} + \epsilon_{ij}^{\text{ct}} + \epsilon_{ij}^{\text{rp}} + \epsilon_{ij}^{\text{ep}} $$

$$ \epsilon_{ij}^{\text{th}} = \Delta T \sum_{i=1}^{n} a_i[T(t)] f_i(t + \Delta t) + \sum_{i=1}^{n} \epsilon_v^{\text{tr}}[T(t)] \Delta f_i(t + \Delta t) $$

7
where $\varepsilon_{ij}^{Total}$ is the total strain, $\varepsilon_{ij}^e$ is the elastic strain, $\varepsilon_{ij}^p$ is the plastic strain, $\varepsilon_{ij}^{th}$ is the thermal strain, $\varepsilon_{ij}^{vp}$ is the volume change strain, $\varepsilon_{ij}^c$ is the creep strain, $\varepsilon_{ij}^{tp}$ is the viscoplastic strain, $\varepsilon_{ij}^{tp}$ is the transformation plasticity strain, $\alpha_i$ is the thermal expansion, $f_i$ is the phase fraction of phase $i$ and $n$ is the number of existing phases in the phase mixture. The total strain was composed of the above strain components. It was assumed that the strain caused by creep, viscoplasticity and trip components are negligible and therefore, not included in the calculations. Since the viscoplastic effects were ignored, the yield stress was assumed to be independent of the strain rate and dependent upon plastic strain and temperature. In the case where a material undergoes phase transformation, the resulting volume changes during the phase transformations and the phase dependent thermal expansions can be calculated and then added to the thermal strain component (caused by temperature changes) as a numerical modification to the coefficient of linear thermal expansion.

The welding thermal cycle is non-isothermal meaning that the use of isothermal elastoplastic data to define strain hardening during cooling at lower temperatures can be problematic. To solve this problem, an annealing step was modelled by setting the equivalent plastic strain to zero above the specified annealing temperature so that the effect of prior hardening is lost. If the temperature at a material point falls below the annealing temperature, then it can work hardening again.

The boundary conditions were set to simulate the actual welding fixtures (clamp) used during welding experiments as displayed in Figure 6. It is common practice to use fixtures to reduce welding distortions. However, distortion control is a difficult task because the welding fixtures strongly affect the residual stresses and distortions induced during welding due to the complexity of the welding process so they should be designed carefully. The amount of restraint determines the magnitude of residual stress fields and distortions. Removal of the welding fixtures after cooling to room temperature partially releases the locked-in stresses or elastic strains by causing the workpiece to deform.

![Figure 6 Restraint conditions introduced to the FE model for mechanical analysis](image)

### 3.4. Solid state phase transformations

Welds consist of a complex heterogeneous microstructure within a small volume due to very steep temperature gradients during welding. Solid state phase transformation may occur during cooling and the associated volume change and phase specific material properties can have a significant influence on welding residual stresses and distortions. In many weld models, the influence of phase transformation is neglected. Few researchers studied the kinetics of phase transformations in Ti-6Al-4V but were mostly case specific because they are known to vary with the chemical composition, the temperature history and the initial phase morphology prior to transformations. Shah et al. [17,18] initially modelled analytically various phase transformations during a welding thermal cycle using modified Rosenthal equations in the heat affected zone in terms of heat input and plate thickness. Malinov et al. [19,20] studied the phase transformation kinetics under isothermal condition using resistivity technique and continuous cooling conditions using differential scanning calorimetry at different cooling rates using the Johnson Mehl Avrami and Kolmogorov (JMAK) equation [21–23] and the additivity rule to determine the fraction of $\beta$ transformed to $\alpha$. Ahmed and Rack [24] studied the effects of cooling rate from above the beta transus on phase transformation during cooling and determined that martensitic formation forms at high cooling rates above 410 K/s, while Gil Mur et al. [25] studied the decomposition of martensite into $\alpha$ and $\beta$ during tempering heat treatment and observed fully martensitic structure at much lower rates. Kelly and Kampe [26,27], Crespo et al. [28] and Murgau et al. [29] modelled microstructural evolution in Ti-6Al-4V during a laser metal deposition process and Fan et al. [30] numerically investigated the effect of phase transformations on laser forming of Ti–6Al–4V using JMA kinetic parameters for isothermal transformation from Malinov et al. [19] but without applying additivity principles to diffusion controlled transformation. Elmer et al. [7] measured experimentally using the synchrotron X-ray diffraction technique the transformation kinetics during gas tungsten arc welding (GTAW) of Ti-6Al-4V. Longuet et al. [31] developed a general multiphase model for Ti-6Al-4V and applied it to direct laser fabrication and laser welding processes.

It is known that transformation induced volumetric strains in steels are caused by phase work hardening due to
differences between the specific volumes and thermal expansion coefficients of phases, and promote reorientation of new phases [32]. This is not the case with pure titanium, because the specific volumes of α and β unit cells are similar. This means that there is almost no change in crystallographic orientation during α to β allotropic transformation and therefore, the phase work hardening effect is not significant and only small internal stresses are produced. In the case of Ti-6Al-4V, the transformation occurs over a temperature range rather than at a particular point during heating due to the presence of a small fraction of β phase in the initial base metal microstructure. As a result, the transformation proceeds from α + β to β where the β phase volume increases by diffusional migration of the α/β interface [32]. Therefore, the volume effect of transformations in Ti-6Al-4V was modelled by taking into account changes of specific volumes of different phases determined from the lattice parameters of these phases. The linear coefficients of thermal expansion for α and β phases as a function of temperature were obtained from JMatPro [33] as shown in Figure 7 in order to account for internal stresses caused by the differences in the coefficients in calculations.

![Linear coefficient of thermal expansion and unit cell volume for each phase, and transformation induced volumetric strains as a function of temperature](image)

Figure 7 Linear coefficient of thermal expansion and unit cell volume for each phase, and transformation induced volumetric strains as a function of temperature [33,34]

The unit cell volume for each phase was determined from the real time in-situ synchrotron X-ray diffraction measurements of the lattice parameters of the α and β phases during heating of Ti-6Al-4V by Elmer et al. [34]. The lattice parameters were measured from the bcc {110} reflection for β phase and hcp {101} reflection for α phase and the volume of α phase was calculated using $a^3\cos 60^\circ$ assuming $c/a = 1.5963$ and $a^3$ for β phase as shown in Figure 7. The volumetric strains during phase transformation due to the differences in unit cell volumes between these two phases was therefore calculated by multiplying the volume fraction of each phase in the microstructure by its respective unit cell volume as a function of temperature during welding.

In this investigation, ABAQUS user defined subroutines (FORTRAN) were developed based on time temperature transformation (TTT) diagrams to include the effect of solid state phase transformations in Ti-6Al-4V during welding. The transformed volume fraction of different microstructural phases was calculated in the thermal analysis as internal state variables using ABAQUS user defined subroutine USDFLD as a function of cooling rate and peak temperature, and the volumetric change due to temperature variations and also phase transformations were calculated in the mechanical analysis using ABAQUS user defined subroutine UEXPAN by mimicking the thermal strain due to thermal expansion.

During the heating stage, Ti-6Al-4V undergoes a rapid allotropic diffusion controlled transformation from β to α phase which involves nucleation and growth of β and dissolution of α by movement of the α/β interface due to the transport of beta stabiliser across the interface [32]. The volume fraction of β reaches 100% above the beta transus temperature and remains stable up to the melting temperature. Since β is an intragranular phase, it is difficult to evaluate its volume fraction accurately. As Equation 11 shows, it was assumed that β growth increases by the equivalent amounts of α dissolution and that the transformed β reaches its equilibrium fraction instantaneously during heating and follows the beta equilibrium curve in Figure 8. A simplified single α phase was assumed to avoid differentiating variants of phase morphologies such as globular, Widmanstätten (or Thomson pattern), basket weave and grain boundary α phases. As Equation 12 shows, a single α phase was calculated by subtraction of the current β phase fraction from the equilibrium β phase fraction.

$$f_\beta(t_1,T_i) = f_\beta^{eq}(T_1)$$

$$\Delta f_\beta = -\Delta f_\alpha = f_\beta^{eq}(T_1) - f_\beta(t_0,T_0)$$

Figure 8 shows the equilibrium fraction of α and β phases determined from various models in the literature. A similar trend can be found in all models except for the JMatPro model which predicts the volume fraction of α as 0% and 100%
for \( \beta \) at low temperatures, whereas, other models predict around 10% retained \( \beta \) when cooled to room temperature. Since some \( \beta \) phase was present in the actual base metal microstructure, the Castro model was used in the numerical simulations to predict the equilibrium phase fractions.

Figure 8 Modelled equilibrium phase fraction of \( \alpha \) and \( \beta \) phases as a function of temperature [29,33,35,36]

During the cooling stage, the cooling rate determines the transformation kinetics and the resultant phases formed. For slow cooling rates less than around 20 K/s at temperatures below the beta transus, the \( \beta \) decomposes into \( \alpha \) via a nucleation and diffusion controlled reaction [24,29,37]. The diffusive transformation of the \( \beta \) phase into the \( \alpha \) phase which occurs at a constant temperature can described using the Johnson Mehl Avrami and Kolmogorov (JMAK) law [21–23] as shown in Equation 13.

\[
f_\alpha(t, T) = \left[ 1 - \exp\left(-k_{\beta \rightarrow \alpha}(T)t^n_{\beta \rightarrow \alpha}\right) \right] f_\alpha^{eq}(T)
\]  

(13)

where is \( f_\alpha \) the fraction of the \( \alpha \) phase at time \( t \), \( f_\alpha^{eq} \) is the equilibrium fraction of the \( \alpha \) phase, and \( k_{\beta \rightarrow \alpha} \) and \( n_{\beta \rightarrow \alpha} \) are the temperature dependent and independent JMAK parameters that define the kinetics of the \( \beta \) to \( \alpha \) transformation, determined from available time temperature transformation (TTT) start and end curves from the literature for this transformation [38] as shown in Figure 9. As it can be seen from Figure 9, there are considerable variations in the TTT curves [20,26,29,39] so the derived JMAK parameters depend on the selection of TTT curves.

Figure 9 Time temperature transformation (TTT) diagrams from the literature determined experimentally and calculated using JMatPro [19,20,29,40]

The JMAK parameters, \( k_{\beta \rightarrow \alpha} \) and \( n_{\beta \rightarrow \alpha} = 2.5 \) used in this investigation were based on the TTT diagram for Ti-6Al-4V in Kelly [40] obtained by fitting the modelled JMatPro TTT curves as shown in Figure 10.
The JMAK models for both dissolution, and nucleation and growth of $\alpha$ phase are based on kinetic parameters derived for isothermal transformation. In order to extend the application of the isothermal models to non-isothermal phase transformations during welding, Scheil’s additivity rule was used [41]. The additivity rule approximates an arbitrary continuous temperature variation, in this case the total time to reach a specific stage of transformation, as a sum of small incremental isothermal time steps connected by instantaneous temperature change [29,39,42]. The phase fractions at any time and temperature steps depend on the values from the previous steps and can be expressed as shown in Equation 14.

$$\int_0^t \frac{dt}{f_f(T)} = 1$$

where $t_f(T)$ is the isothermal time to stage $f$ and $t$ is the time to $f$ for a non-isothermal reaction. The modified JMAK equation is shown in Equation 15.

$$f_a(t, T) = \left[ 1 - \exp\left( -k_{\beta-a}(T_1)(t_0^* + t_1 - t_0)n_{\beta-a}(T_1) \right) \right] \left( f_\beta(t_0, T_0) + f_\alpha(t_0, T_0) \right) \left( f_a^{eq}(T_1) \right)$$

where $t_0^*$ is a fictive time required to reach $f_a(t_0, T_0)$ during an isothermal transformation at temperature $T_1$, $f_a^{eq}$ is the equilibrium fraction of the $\alpha$ phase, which represents the fraction of the $\alpha$ phase. The expression for the fictive time is given in Equation 16.

$$t_0^* = \left[ \frac{1}{k_{\beta-a}(T_1) \ln \left( \frac{f_a^{eq}(T_1)}{f_\alpha(T_1) - f_\alpha(t_0, T_0)} \right) n_{\beta-a}(T_1)} \right]$$

Very fast cooling from above the beta transus transforms $\beta$ into another form of $\alpha$ phase, a thin needle like acicular martensite $\alpha'$, that is different from the equilibrium $\alpha$, with high residual stresses due to relatively larger differences in the crystallographic orientation of adjacent lamella and interfaces with low coincidence [37]. The martensitic transformation is a diffusionless solid state transformation which causes very fast changes in the crystal lattice structure without rearranging the atoms. It can be defined by the Koistenen Marburger (KM) law as shown in Equation 17.

$$f_a(t, T) = \left[ 1 - \exp\left( -k_{\beta-a}(M_s - T) \right) \right] f_\beta(t, T)$$

where $f_a$ is the fraction of $\alpha'$, $f_\beta$ is the fraction of $\beta$ and $k_{\beta-a}$ is the material dependent KM parameter and $M_s$ is the martensite start temperature. Figure 11 shows the equilibrium phase fraction of $\beta$ and the rest consisting of $\alpha'$ as a function of $\gamma$ and $M_s$ determined using the KM equation. The $\gamma$ was chosen to be equal to 0.015 and the $M_s$ equal to 650°C.
Post weld heat treatment (PWHT) is often used to reduce and redistribute the residual stresses that result from welding titanium and titanium alloys [43], without seriously affecting the mechanical properties such as strength or ductility. Stress relief enhances dimensional and structural stability as well as preventing problems such as stress corrosion cracking and loss of compressive yield strength. Titanium alloys have a high yield strength and elastic modulus at room temperature so post weld mechanical treatment such as stretching is less effective than PWHT. As it can be seen from Figure 12, the yield strength of Ti-6Al-4V decreases with increasing temperature due to dislocation activation. By uniformly heating the welded material, the yield limit is reduced and the stress in the material becomes greater than the yield strength at the treatment temperature. The material then plastically deforms by local creep and any residual stresses that exist in the material are reduced to the yield strength at the treatment temperature.

Figure 11 Phase fraction of $\beta$ and $\alpha$ calculated using the Koistenen Marburger model as a function of $M_s$ and $\gamma$

For fast cooling rates greater than 410°C/s, a fully martensitic microstructure is formed and diffusive transformation to $\alpha$ is suppressed according to Ahmed and Rack [24].

$$f_\alpha(t, T) = f_\alpha(t_0, T_0) + \Delta f_\alpha = \left[1 - \exp(-k_\beta \alpha (M_s - T))\right] \left[1 + \exp\left(-k_\beta \alpha (M_s - T)\right)\right]$$

(18)

For moderate cooling rates between 20 and 410°C/s from above the beta transus leads to partial transformation of $\beta$ to grain boundary massive $\alpha_m$ and intragranular martensitic alpha $\alpha'$ adjacent to the prior $\beta$ grain boundary. It was assumed that $\alpha_m$ includes both $\alpha$ and $\alpha'$ and also that both transformations are diffusional and martensitic.

$$f_{\alpha_m}(t, T) = f_{\alpha_m}(t_0, T_0) + \Delta f_{\alpha_m} = \left[1 - \exp(-k_\beta \alpha \alpha_m (M_s - T))\right] \left[1 + \exp\left(-k_\beta \alpha \alpha_m (M_s - T)\right)\right]$$

(19)

where $f_{\alpha_m}$ is the fraction of $\alpha_m$ and $f_\beta^{eq}$ is the equilibrium fraction of $\beta$. In this case, the current equilibrium fraction of $\beta$ is subtracted from the available for the transformation in order to prevent a full transformation to $\alpha'$.

Post weld heat treatment (PWHT) involves heating the as-welded sheet at 600°C for 6 hours. Heating and soaking at the treatment temperature
for a long time induces a partial recovery of the \( \alpha \) and \( \beta \) phases from the massive \( \alpha_m \) and martensitic \( \alpha' \) phases via a diffusional process. It is then followed by the decomposition of the transformed \( \beta \) into \( \alpha \) during cooling to room temperature via a nucleation and diffusion controlled reaction until the equilibrium \( \beta \) phase fraction is reached. The final microstructure then mainly consists of \( \alpha_m \) and \( \alpha \), and a very small equilibrium fraction of \( \beta \).

4. Results and Discussion

4.1. Simulated thermal histories and weld seam geometry

The temperature distribution when half way through welding the Ti-6Al-4V workpiece is shown in Figure 13. The FE model shows a fine mesh in and around the weld, where the temperature gradient is very steep and confined to a narrow region around the heat source at the location of keyhole formation. The maximum temperature at the keyhole can reach close to the boiling point of the material. The elongated temperature distribution in the welding direction is caused by the high power density and low heat input characteristics of the moving fibre laser. The welding heat quickly dissipates behind the heat source towards the lower temperature outer edges of the sheet due to very high welding speed and elevated thermal conductivity values of the material at higher temperatures. It can be seen that the regions in white which are above the liquidus temperature of 1650°C completely penetrate through the thickness of the sheet, indicating a full penetration mode welding.

Figure 13 Temperature contours obtained from thermal analysis when half way through welding Ti-6Al-4V

Calibration of the welding temperature fields involved matching the simulated weld pool geometry to the experimental macrograph of polished and chemically etched weld transverse cross-section. In the FE model, the FZ width was determined by the temperature contour above the liquidus temperature of 1650°C and the HAZ width was determined by the temperature contour between the liquidus and the solidus temperature of 1600°C. It was difficult to precisely match the HAZ width due to the very narrow gap between the liquidus and the solidus but still a good agreement was made. Figure 14 shows the simulated and experimental FZ side by side and it shows that the experimental fusion boundary and penetration depth are in good accordance with the simulated fusion boundary isotherm. The experimentally measured weld seam had a top width of 2.80 mm and bottom width of 2.35 mm. Small reinforcement and excessive penetration as observed in the actual macrograph were not modelled as they were assumed to have negligible influence on residual stresses and distortions. The heat source after calibration had a laser power of 3 kW, heating efficiency of 80%, welding speed of 3 m/min, \( r_e \) equal to 0.4 mm and \( r_i \) equal to 0.3 mm.

Figure 14 Comparison of weld transverse cross-section geometry through thickness between the calibrated temperature distribution from the FE thermal model and the source experimental macrograph juxtaposed

Further calibration on the welding temperature fields involved matching the simulated curves to the temperature history recorded at various thermocouple positions by changing the thermal boundary conditions such as thermal convection and radiation to the surroundings and conduction to the worktop. Figure 15 shows that the experimental and simulated time-temperature curves match well in terms of heating rate, peak temperature and cooling rate. The heating and cooling
rates were determined by calculating the difference between the initial and current temperature values divided by the fixed time step. As the temperature reached significantly higher than the maximum operating temperature of the thermocouple in the FZ, the closest measurement was taken at a distance of 3 mm away from the weld centre line and a few more further away. It can be seen that the calibrated simulated curves are in excellent agreement with the experimental curves after several iterations. The cooling rate at distances greater than 4 mm away from the weld centre line showed significantly reduced peak temperature while still reasonably maintaining similar heating and cooling rates compared to those closer to the weld. This means that the area affected by the welding heat source mostly is within less than 5 mm. It was decided that the thermal FE model experimentally validated through transient temperature and weld pool measurements became accurate enough to transfer the nodal temperature histories for mechanical analysis.

![Figure 15](image.png)

Figure 15 Numerically calculated thermal histories calibrated using thermocouple measurements at various distances from the weld centre line

4.2. Simulated residual stresses and out of plane displacements

Welding induces highly inhomogeneous stresses which may be as high as the yield strength of the material in the weld as well as considerable distortions. Figure 16 and Figure 17 show the magnitude and distributions of residual stresses after cooling and with clamping fixtures removed. The maximum longitudinal stress reached is approximately in the range between 750 and 780 MPa, comparable to the yield strength of around 900 MPa at room temperature.

![Figure 16](image.png)

Figure 16 Residual stress distributions a) across the entire width of the workpiece in all three principal directions, near the weld in b) transverse (11), longitudinal (22), and normal directions with and without phase transformation

Figure 16 shows the transverse, longitudinal and normal stresses from the weld cross-section at the end of cooling and relaxation, where the transverse stress (S11) is perpendicular to the welding direction and the longitudinal stress (S22) is along the welding direction, and the normal stress (S33) is out of plane. The longitudinal stress was found to be the maximum in and near the weld region in tension with a weakly compressive stress field in the rest of the workpiece far from the weld. The transverse and normal stresses were at their maximum and were tensile in nature in the FZ, compressive near the weld and almost stress free further away from the weld. All three principal stresses were symmetrical due to symmetry across the weld centre line.
Figure 17 Residual stress distributions in three principal stress directions after welding, over the weld transverse cross-section (20 mm wide) and the top surface, with and without phase transformation

Figure 16 and Figure 17 also show that introducing the phase transformation effect to the numerical weld model only had a small influence on the resultant magnitude and distribution of residual stresses around the weld at the end of the welding process but a more noticeable difference was observed with sheet distortions. The peak magnitude of longitudinal stress was found to be 50 MPa greater in the phase transformation model with a steeper stress gradient across the weld width with more variations in and near the FZ and the HAZ than in the model without phase transformation which remained almost constant in and near the FZ, while maintaining almost the same trend in RS distribution. Similarly, the calculated transverse and normal stress magnitudes were again larger with phase transformation but only by a very small amount.

Figure 18 and Figure 19 show the magnitude of cambering and angular out of plane distortions. The out of plane displacement is symmetrical about the weld centre line and is close to zero at the weld start and end positions, and the greatest on the outer edges at the mid-length of the specimen. Simulated angular displacements were slightly greater than the experimental results from CMM measurements, whereas, simulated cambering displacements were predicted smaller close to the edge of the sheet and larger towards the centre.

Figure 18 Out of plane displacements after cooling down to room temperature and removing fixtures

While both models with or without phase transformations over predicted the angular and cambering out of plane distortions when compared to the experimental measurements obtained using CMM, the simulation results from the model with phase transformation in Figure 19 showed greater differences from the CMM results, than those from the model without phase transformation by around few millimetres. The distribution of the out of plane displacements was therefore, found to be more sensitive than the residual stress distribution to the effect phase transformations. The reason for such a negligible difference between the simulated welding residual stresses from both conditions, as mentioned above, was most likely due to well matched dimensions of $\alpha$ and $\beta$ unit cells, meaning that there was no reason for any
alterations of the initial crystallographic orientation during nucleation and dissolution of new phases. Consequently, the level of internal stresses due to phase transformation remained low unlike other materials which exhibit greater differences in the specific volumes between phases and therefore, no significant changes in the welding induced residual stresses were caused by phase transformation in Ti-6Al-4V. In fact, transformation induced volumes changes in titanium alloys are typically one order of magnitude smaller than those of ferrous alloys [32].

Figure 19 Simulated a) cambering and b) angular out of plane displacements with and without phase transformation compared to experimental measurements

Figure 20 and Figure 21 show the simulated graphical and visual representation of the variations in the volume phase fractions of $\alpha$, $\beta$, and $\alpha_m$ during the welding thermal cycle and PWHT, at the weld centre and around the weld, respectively. The initial microstructure consisted of around 0.9 $\alpha$ and 0.1 $\beta$ which are equivalent to equilibrium volume fractions. As the temperature rapidly increases during heating, the $\alpha$ phase fraction quickly drops to 0 and $\beta$ increases up to 1, which in reality should also become 0 above the melting temperature but for simplicity, it is maintained at 1 above the beta transus temperature. When the material starts to cool below the beta transus temperature, depending on the cooling rate, a different microstructure is produced either by diffusion or diffusionless transformation from the $\beta$ phase. At the weld centre where the peak temperatures reached are very high and the cooling rate is fast, a diffusionless martensitic transformation occurs. It was found from the temperature history that the maximum cooling rate was around 400°C/s which is slightly less than the cooling rate of 410°Cs$^{-1}$ needed for fully martensitic transformation. For that reason, the martensite phase fraction does not reach 1 but only up to around 0.9 and the remaining phase fraction consisted of massive alpha, $\alpha_m$ and no $\beta$ after cooling down to room temperature. Increasing the temperature again slowly to 600°C causes partial recovery of $\alpha$ and $\beta$ by decomposition of martensite. The fraction of $\alpha$ increases to around 0.3, $\beta$ to around 0.2 and martensite decreases to around 0.5. Upon uniform cooling to room temperature, the fraction of $\alpha$ further increases by dissolution of $\beta$ until an equilibrium fraction of $\beta$ is reached, while the fraction of martensite remains the same. The final microstructure is now composed of approximately 50% $\alpha$ and 50% martensite and a negligible amount of $\beta$.

Figure 20 Time-temperature history of the phase fractions of $\alpha$, $\beta$ and $\alpha_m$ phases at the weld centre as a function of temperature during a) welding and after b) post weld heat treatment (PWHT) at 600°C for 6 hours
Simulated weld transverse section (20 mm wide) showing the phase fractions of $\alpha$, $\beta$ and $\alpha_m$ phases at different stages of welding and after post weld heat treatment (PWHT) at 600°C for 6 hours.

As Figure 22 a) shows, the Ti-6Al-4V weld microstructure can be divided into base metal (BM), heat affected zone (HAZ) and fusion zone (FZ). The BM consists of equiaxed $\alpha$ and intergranular $\beta$ distributed at the elongated $\alpha$ grain boundaries. The HAZ consists of acicular martensitic $\alpha'$ phase, acicular $\alpha$, primary $\alpha$ and intergranular $\beta$. Figure 22 b) shows that the FZ consists of fine acicular $\alpha'$ with coarse columnar prior $\beta$ grain boundaries.

Figure 22 Microstructure of fibre laser welded Ti–6Al–4V a) obtained from transverse cross-section and b) in the fusion zone at 200 x magnification

Figure 23 and Figure 24 show a reduced peak tensile longitudinal stress in the welding direction after applying PWHT from around 750 MPa before to 450 MPa after, so almost 40% reduction was achieved with PWHT. The magnitude of longitudinal stress after PWHT was similar to the value of its yield strength at 600°C at a very slow strain rate of 0.001 s$^{-1}$ as shown in Figure 12, as a result of slow and uniform heating and cooling during PWHT. Almost no change occurred outside the weld region and constantly remained close to stress free state. The transverse and normal stresses already had negligible magnitudes in the as welded condition but still they were further reduced after PWHT. However, the contributions from these two components when compared to the longitudinal stress on the final residual stress states were insignificant.
a) RS distributions across a) the entire width of the workpiece in principal directions and b) around the weld, c) angular and d) cambering out of plane distortions before and after PWHT compared to CMM values (without PWHT)

Figure 23 also illustrates the evolution of out of plane displacements after PWHT. Under carefully controlled heat treatment at the correct heating and cooling rate, treatment temperature and soaking time, reduction in residual stresses was achieved by release of locked-in stresses. However, PWHT also resulted in greater distortions, with a small increase in the maximum angular distortion by around 0.5 mm, compared to the CMM measurement points obtained from a sample without PWHT as well as the simulated values before applying the PWHT step.

Figure 24 Longitudinal stress distribution in the welding direction viewed from the top surface and close up weld transverse cross-section (20 mm wide) with or without post weld heat treatment (PWHT) as well as either taking into account the effect of phase transformation or not.
4.3. Experimental measurement of residual stresses via X-ray and neutron diffraction techniques

Surface residual stress measurements were performed using a low energy X-ray diffraction (XRD) technique on the top surface of the butt welded Ti-6Al-4V sheet at a depth of around 10 μm from the surface. Figure 25 shows the bi-axial residual stresses, transverse and longitudinal to the welding direction, measured using the XRD and obtained from FE models either with or without phase transformations. It was assumed that the residual stress distributions are symmetrical about the weld centre line and therefore, only one half of the sheet was measured. Both the measured and simulated transverse residual stresses were found to be within the maximum range of ±100 MPa, which when compared to the yield strength of 1100 MPa were very small.

The FE predictions were in good agreement with the experimental measurements. The predicted stress distributions showed large variations only up to around 4 mm away from the weld centre line and then level off close to zero. The magnitude of tensile and compressive stresses around the weld were predicted to be much greater in the model with phase transformations compared to the model without phase transformations which only showed around ±20 MPa variations at most. The measured stress distribution showed greater stress magnitudes than the model without phase transformations but smaller than the model with phase transformations within the weld. The experimental measurements showed slightly more compressive stresses away from the weld than the predicted stresses but the differences were small. It was therefore concluded that the stresses in the transverse direction were relatively small in this thin sheet.

The longitudinal stresses in the direction of the weld were found to be significant even very close to the surface according to both simulated and experimental results. The simulated and experimental longitudinal stresses had approximately the same magnitude and distribution, reaching around 70% of the room temperature yield strength in the weld. Peak tensile longitudinal stresses of around 750 MPa were predicted and observed in a very narrow weld region within the first 2 mm from the weld centre which rapidly dropped by more than half at 3 mm and then to below 0 MPa at 4 mm from the weld centre and became weakly compressive over 50 mm from the weld centre. It seems too conservative to assume in this case that yield magnitude residual stresses occur in the weld. Peak residual stresses as high as the yield strength are likely to occur when the thermal contraction strain becomes larger than the yield strain. Often in steels, the thermal strain can reach more than the yield strain and result in yield magnitude residual stresses. However, in the case of Ti-6Al-4V, the thermal strain is not sufficient to cause yield strength magnitude residual stresses due to its high yield strength and low elastic modulus [44]. The predicted longitudinal stresses at the top of the sheet were the maximum at the FZ/HAZ interface and roughly 50 MPa lower at the weld centre. While the same trend was observed in both models, the model with phase transformations predicted slightly lower stress magnitude at the weld centre and higher at the FZ/HAZ interface than the model without phase transformations. On the other hand, the measured peak tensile longitudinal stresses were located at the weld centre and the opposite trend was observed where the stress was approximately 50 MPa lower at the FZ/HAZ interface. Still, overall the FE predictions were in good agreement with the experimental measurements.

Figure 26 shows the residual stress and strain measurements obtained using the neutron diffraction technique compared to the results from numerical simulations. It was uncertain at first which reflection would be the best to use for measurements or the texture that would be expected. The detector was placed to measure several peaks simultaneously including the \{103\}, \{112\} and \{201\} peaks. As the \{103\} peak is recommended in the ISO/TTA 3:2001 standard [45], it was therefore, included on the detector. As it can be seen from Figure 26 strains from all three reflections were measured in the transverse direction. On the other hand, different intensities were produced for different peaks in the longitudinal and normal directions. Measurement of the \{103\} longitudinal strains was found to be problematic due to very weak or the absence of the \{103\} reflection. Similarly, while the \{103\} reflection was present in the normal direction,
the (201) was very weak. The likely cause of such result could be crystallographic texture in the weld metal induced during the solidification process on cooling. Texture can have influence the peak intensity of a given hkl diffraction peak measured in a particular direction due to preferred orientation of certain crystallographic planes along certain macroscopic directions. It causes the measured relative intensities of the peaks from favourable oriented crystallographic planes to be higher than from less favourably oriented ones, and therefore, prevents the observation of one reflection in all the directions for which strain data are required. According to Standford and Bate [46], martensitic transformation in Ti-6Al-4V led to a significant variant selection of α’ (transformation texture) within each prior β grain. In addition, α and β in the parent material during hot rolling developed a strong texture with basal poles aligned with the rolling direction was observed.

![Figure 26](image-url) Residual strain distributions in the a) transverse, b) longitudinal and c) normal directions for different hkl planes; and the resulting residual stress distributions for d) {112}, e) {201} and f) {103} reflections measured experimentally using the neutron diffraction technique.
Another problem when measuring residual stresses in Ti-6Al-4V is caused by the addition of aluminium and vanadium which reduces the average coherent scattering length of Ti-6Al-4V but also increases its incoherent cross-section. As a result, the reflections even in texture free randomly oriented polycrystalline Ti-6Al-4V are weak and only few times larger than the background, making measurements difficult in this material [47]. For these reasons, it was necessary to use more than one reflection to calculate strains. Figure 26 shows that there is some difference between the {103}, {112} and (201) transverse strains. The {112} and (201) peaks agree well with each other whereas, the {103} peak appears to have larger values in the weld which could be due to intergranular strain or different moduli values. The high textured nature of Ti-6Al-4V resulted in lower intensity counts observed during neutron diffraction measurements for certain reflections where one less diffraction peak was observed in the radial and normal directions than the transverse direction. Only the {112} and (201) peaks were detected in the longitudinal direction and there is a difference between the two longitudinal strains. It was found that the same difference of approximately 1000 micro-strain was also detected in the reference comb, meaning that the difference may also be due to intergranular strain.

As it was not possible to measure the normal strain for the (201) reflection and the longitudinal strain for the {103} reflection due to texture (low count), the longitudinal strain data from the (201) reflection was used to calculate stress for the {103} reflection and likewise, the normal strain data from the {103} reflection was used to calculate stress for the (201) reflection. For the stress calculation, the longitudinal (201) peak and the normal {103} peak were chosen above the corresponding {112} peaks because of the possibility of intergranular strains in the {112} reflection. The experimentally determined stresses in the transverse and normal directions are very close to zero for all reflections and the normal stress being zero is what would be expected from a thin sheet. Also, the stresses in both directions agree well with each other, suggesting a uniaxial stress distribution. In terms of the longitudinal stress in the weld, all three reflections show the same stress distribution but slightly difference peak tensile stress magnitude. The highest stress magnitude is given by the (201) reflection of around 700 MPa, followed by the {103} reflection of around 650 MPa and the lowest for the {112} reflection of around 600 MPa.

It was found that some unrelieved macro residual stresses retained in the longitudinal direction of the reference comb specimen so it was not completely stress free as shown in Figure 27. The FE predictions of all three principal stresses are in very good agreement with the residual stresses measured from the {112} reflection, whereas, the measured longitudinal stresses for the (103) and (112) peaks in and around the weld are less than the simulated values by around 100-150 MPa at most because the calculated (103) longitudinal stress is not the true value for the {103} reflection and also the {112} reflection is prone to intergranular stresses. Therefore, it was concluded that the (201) stresses which are in good agreement with the simulation results are the most reliable and prove that the FE predictions are accurate.

5. Conclusions

Fibre laser beam welding of a butt weld in Ti-6Al-4V was investigated with regard to the macroscopic residual stress state and distortion patterns of the structures after welding. The conclusions inferred from the simulation and experimental results of industrial significance are as follows:

The fibre laser welded specimen was characterised by a more pronounced dominance of longitudinal residual stresses...
over transverse and normal residual stresses. The longitudinal residual stresses were very high but not as high as the room temperature yield strength. They were largely tensile in nature only within the FZ or HAZ and tended to be weakly compressive in the rest of the specimen.

The measured residual stresses were dependent on the crystallographic hkl plane from which they were obtained from and the cause of such difference was found to be due to the presence of microscopic stresses. The reflections were weak and only few times larger than the background due its highly incoherent cross-section, thus making neutron diffraction measurements difficult. In addition, texture in the Ti-6Al-4V weld also contributed to lower intensity counts observed during the measurements. As a result, only certain peaks were detected in certain orientations and therefore, different stress values were obtained for different reflections. The best agreement with the numerical results was found with the (201) peak.

The phase transformations only had a small influence on the magnitude and distribution of residual stresses because the level of internal stresses due to phase transformation remained low unlike other materials which exhibit greater differences in the specific volumes between phases.

Post weld heat treatment induced diffusional phase transformations via decomposition of martensite into $\alpha$. It also decreased the magnitude of longitudinal stresses to the yield strength of Ti-6Al-4V at the treatment temperature by releasing the locked-in stresses.

Some differences in distortion values between FE simulations and CMM measurements were observed. The predicted distortions are suspected to be more sensitive to the mechanical boundary conditions defined than the applied welding heat source. Still, fairly good predictions were made by matching the boundary conditions as close as possible to the real set-up.

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