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In-situ Measurements of Stress During Thermal Shock in Clad Pressure Vessel Steel Using Synchrotron X-ray Diffraction^{*}

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Abstract

Thermal shocks are an important incident in operation of a pressure vessel which can have a significant impact on the structural integrity of the vessel. Often experiments that consider the state of the vessel before and after the thermal shock are used to evaluate the effects of the thermal shock. The studies can be complemented by time-resolved numerical simulations, which may be validated against the final state of the vessel obtained experimentally, to infer the transient response of the material. The transient response is important as the material experiences the highest level of stress in a short period which can induce catastrophic failure. This paper reports time-resolved experimental quantification of strain in reactor pressure vessel material during thermal shock measured by in-situ synchrotron diffraction. Specimens were extracted from a plate of nuclear pressure vessel steel with a nickel alloy cladding deposited by overlay welding. The specimens, with and without cracks, were subjected to thermal loading by heating then rapidly quenching the cladding in cold water. Strains were measured during thermal loading at a point near the crack tip from which the stress state around the crack tip was calculated and compared with a transient finite element model of the experiment. It was found that the peak near-tip stress occurred within the first second after the onset of rapid cooling. It was demonstrated from experimental measurements that the peak stress intensity factor occurred during thermal shock, rather than under steady conditions before or after the thermal shock. It was shown that although the finite element simulation predicts the steady state condition of the material after thermal shock, its transient response depends significantly on a number of inputs with high uncertainty, making its time-resolved results unreliable for high-fidelity integrity assessments.

Keywords : Thermal shock, cladding, synchrotron X-ray diffraction, thermal stress, fracture.

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1 Introduction

The reactor pressure vessel (RPV) is a major component of a pressurised water reactor, where its design must maintain structural integrity under the most severe possible loads [1]. Some of the most severe loads that an RPV experiences occurs under fault or emergency mitigation conditions which results in the temperature of the primary coolant to fall rapidly. This causes the internal surface of the vessel to cool rapidly whilst the bulk of the material remains at high temperature. The resulting thermal mismatch gives high tensile stresses near the inner wall of the vessel, a scenario called thermal shock [2]. Basic elastic analyses predict tensile stresses of the order of 600 MPa at the inner wall during thermal shock, well over its yield stress and ultimate tensile strength of alloys typically used in this application [3]. There are a number of stresses that act on the RPV during the thermal shock including: stress from internal pressure, and residual stresses created from the process of applying the corrosion resistant cladding [4–7] The dependence of both the pressure and residual stress on the temperature during thermal shock makes calculation of the transient stress development which an RPV endures prohibitively complex.

Thermal shock could pose a risk to the structural integrity of an RPV if the combined stresses from different sources are high enough to initiate propagation of pre-existing defects. Numerical and analytical methods have reached sufficient sophistication to predict stresses and fracture parameters during a thermal shock event [2,8–11]. Experimental work, however, has focussed on observing fracture events by post-mortem characterisation, following failure by thermal shock [12,13]. Few experimental studies exist, as thermal shock experiments are costly and difficult to carry out safely. This paper presents an experiment in which stresses are measured by high speed X-ray diffraction during thermal shock, for the first time. The time-resolved measurements enable direct validation of time-resolved numerical analysis. This work considers thermal shock without internal pressure, that is only residual and thermal stresses, due to constraints imposed by local health and safety rules.

Seven specimens were extracted from a plate of a low alloy ferritic steel clad with nickel alloy, and surface cracks (through-cladding) were machined into four of them. The specimens were subjected to thermal shock using a bespoke apparatus which enabled in-situ measurement of stress by synchrotron X-ray diffraction. Stress was measured at a single point close to the crack tip at an acquisition rate of 30 Hz. Additionally, the stress around the crack tip was mapped under steady-state conditions before and after thermal shock, both at room temperature and at high temperature representing steady operating conditions in an RPV. A finite element model of the experiment was constructed with the aim of validating the experimental results and using it as a benchmark for more general thermal shock analyses.

2 Experiment

2.1 Materials and specimens

Seven specimens were extracted from a clad plate provided by Wood in which the parent material is SA508 Grade 4N and the cladding of Alloy 82. The cladding is a weld-overlay

deposited by gas metal arc welding details followed by post-weld heat treatment [14,15], and the cladding machined back so that the surface is flat. The clad plate was previously subjected to a programme of steady state room temperature residual stress measurements, results of which are reported elsewhere in detail [5] thus only described briefly in the Results section. The specimens were extracted using wire electrical discharge machining to reduce the machining residual stresses.

The geometry of the specimens is shown in Figure 1. The nominal thickness of the cladding determined by visual inspection was 7 mm as is shown in Figure 1 (a). The specimens were relatively thin at only 2 mm thick to enable sufficient X-ray transmission (see next section on X-ray diffraction). Out of 7 specimens, 4 specimens contained a through-crack of length, a , at their mid length, which represents a through-cladding surface defect. Two specimens were crack-free. Two specimens contained 7.4 mm long cracks, terminating in the parent just beyond the interface with the cladding. Two specimens contained 10 mm long cracks, terminating well beyond the interface in the parent. Cracks were machined from the surface of the cladding using electrical discharge machining with a 0.1 mm diameter wire. It was stipulated that no fatigue pre-cracking was required as the crack opening displacement at fracture for this material was much larger than the notch diameter created by the wire electro-discharge machining [16]. One final specimen was manufactured with a comb feature to relieve stresses in the material for measurement of stress-free diffraction parameters. The comb feature is illustrated in Figure 1(b).

(a)

(b)

Figure 1 Overview of the specimens tests (a) specimen geometry (b) stress free d_0 specimen (c) dimensions of the area mapped during steady state X-ray diffraction (d) position of the thermocouples in a cracked simple (T1 – T5). All numerical dimension values are in mm.

Figure 2 Experimental setup: the bespoke thermal shock apparatus on 112 diffraction stage (b) stress free sample (c) different mapped areas

2.2 Synchrotron X-ray diffraction

When a crystalline material is exposed to a monochromatic X-ray beam, the beam is diffracted if Bragg's law is satisfied:

$$2d^{hkl} \sin \theta^{hkl} = \lambda \quad (1)$$

where d^{hkl} is the spacing between the hkl lattice planes, θ^{hkl} is the diffraction angle, and λ is the wavelength of the incident X-ray beam. The X-ray diffraction data from a single measurement in a metal, which has a large number of randomly orientated grains, comprises a number of X-ray cones each corresponding to the hkl lattice plane families that satisfy the Bragg's law. The intersection of the cones on the X-ray detector is the concentric Debye-Scherrer rings in which

the distance of each point on the ring from its centre has a direct relationship with the lattice spacing. The analysis of the rings before and after loading reveals the elastic stress components as detailed in [17]. In this work, a single ring was used for analysis, corresponding to the $\{110\}$ plane in the ferritic steel. The ring was divided into 36 segments (i.e. every $\varphi = 10^\circ$), and the diffraction spectrum was integrated across each segment. The diffraction vector, Q_φ^{110} , in each segment was calculated by fitting to a Gaussian function using the pyXe Python package [18]. The peak position is related to the spacing between lattice planes via Equation (2):

$$Q_\varphi^{hkl} = \frac{2\pi}{d_\varphi^{hkl}} \quad (2)$$

where d_φ^{hkl} is the lattice spacing, which is related to the diffraction angle via Bragg's law in Equation (1). The lattice strain, $\varepsilon_\varphi^{hkl}$, was therefore calculated using Equation (3):

$$\varepsilon_\varphi^{hkl} = \frac{d_\varphi^{hkl} - d_0^{hkl}}{d_0^{hkl}} = \frac{Q_0^{hkl}}{Q_\varphi^{hkl}} - 1 \quad (3)$$

where d_0^{hkl} is the stress-free lattice spacing and Q_0^{hkl} is the corresponding stress-free peak position. Q_0^{hkl} was measured in the specimen, which was manufactured with a stress-free reference comb as shown in Figure 1(b). Measurements of Q_0^{hkl} were made at different angles (φ), different positions (x_2), and different temperatures between 20°C and 450°C . The temperature of the reference specimen was adjusted using the heating arrangement in the thermal shock apparatus, which is described later in this paper.

The method for calculating stress and strain tensors from the measured strain, $\varepsilon_\varphi^{hkl}$, is described in detail elsewhere [17]. Briefly, it was assumed for the analysis that the specimen was in a state of plane stress ($\sigma_{33} = 0$). The lattice plane specific components of strain, ε_{11}^{hkl} , ε_{22}^{hkl} , and ε_{12}^{hkl} , were calculated from the measured strains, $\varepsilon_\varphi^{hkl}$, using co-ordinate system transformations. Since diffraction methods measure the lattice spacing and the peak position is not affected by lattice distortion due to shear (i.e. shear strain), the measured strains are elastic only. Attempts have been made to qualitatively measure plastic strain from the diffraction peak width (e.g. see full width half maximum method [19]), however, the beamline used has strong influence on such measurements and requires accurate calibration for every specimen geometry. The short timeframe allocated to the experiment precluded a lengthy calibration, thus limiting our measurements to elastic strains only. The stress tensor was therefore calculated using Hooke's law for plane stress with bulk elastic constants replaced with lattice plane specific values. For example:

$$\sigma_{11} = \frac{E^{hkl}}{(1 - (\nu^{hkl})^2)} (\varepsilon_{11}^{hkl} + \nu^{hkl} \varepsilon_{22}^{hkl}) \quad (4)$$

where E^{hkl} and ν^{hkl} are the lattice plane specific modulus and Poisson's ratio. In this case, only a single lattice plane was used for analysis, corresponding to $\{hkl\} = \{110\}$. Values for E^{110} and ν^{110} were estimated from bulk values, E and ν , using factors given in reference [20] for

ferritic steel. The bulk values used at 20°C were $E = 206$ GPa and $\nu = 0.3$, and the corresponding lattice plane specific values were $E^{110} = 218$ GPa and $\nu = 0.28$. Poisson's ratio was assumed temperature independent whereas the modulus was reduced by 15% from 20°C to 450°C [21]. The small grain size in SA508 Grade 4N steel (2.5 – 6 micrometre) [22] allowed for acquisition of bright enough rings to be analysed using the procedure detailed above while the size of the Nickel cladding (of the order of 1mm) grains were prohibitively large [23] compared with the slit size used (see below). The nickel alloy had an elastic modulus of 172.4 GPa and a yield stress of 310 MPa [24].

The experiment was carried out in Experimental Hutch 1 on Beamline I12 [25] at Diamond Light Source, the UK's national synchrotron facility. A monochromatic X-ray beam was used with an energy of 80.4 keV. Two sets of measurements were made: steady state, when the specimen temperature was maintained either at room temperature or at elevated temperature; and transient, when the specimen was rapidly cooled by subjecting it to thermal shock.

The steady-state measurement area at which the strain field of the cracked specimens was mapped is shown in Figure 1b. A 10×10 mm² region around the crack tip was split into three square sub-regions: coarse, intermediate, and fine seen in Figure 1(b). The spatial resolution of the mapped strain was increased in a fine region near the interface by selecting a smaller slit size for the X-ray beam and gradually decreased in the intermediate and course regions resulting in approximately 900 measurement points for each cracked sample. The measurement parameters used in each region are given in Table 1. In the crack-free specimens, measurements were made along four lines normal to the interface between the cladding and parent (see Figure 1c).

The transient measurements were made during thermal shock at a single point close to the crack tip. The slit size was 200×200 μm^2 and the centre of the measurement point was located 150 μm from the crack tip. A transient measurement was also made in a crack-free specimen, in which case the measurement was made in the same position as for a specimen containing a 10 mm crack. The transient measurements were made at 30 Hz while the steady state measurements had a 1 Hz frequency for each point in the map. This was judged based on the quality of the rings observed on the detector and their signal to noise ratio. Details of error analysis of the strain calculation methodology can be found elsewhere [26]

Table 1 *Geometries of the steady-state X-ray diffraction measurements.*

Specimen type	Region	Length of region (mm)	Slit size equivalent to resolution (μm)
Cracked	Coarse	10	500
Cracked	Intermediate	3	200
Cracked	Fine	1.2	100
Crack-free	Coarse	4.6	500
Crack-free	Fine	5.4	200

2.3 Thermal Shock

An apparatus was designed to subject the specimens to thermal shock whilst allowing simultaneous measurements by synchrotron X-ray diffraction (see Figure 2). The specimen was suspended clad-side-down over a bath of water. The initial water level was set below the bottom of the specimen. An adjacent tank containing extra water and a submerged pump feeding into the bath was implemented. The tank contained just enough water to increase the water level in the bath by 20 mm. Windows were machined in the bath and were sealed with clear polycarbonate to allow the X-ray beam to pass through the specimen and reach the detector. The apparatus imparted thermal shock by the following procedure. The specimen was sandwiched between two 110 V electric strip heaters thus the temperature of the specimen could be adjusted and maintained at steady state using a proportional-integral-derivative controller. For each specimen, the heaters were switched on to raise the temperature of the specimen to a nominal 350°C. Then the heaters are switched off and the pump was switched on simultaneously as the diffracted X-ray beam was being recorded at 30Hz behind the sample. The water level increased until the bottom 5 mm of the specimen was submerged, thereby subjecting it to thermal shock.

It was important that the temperatures in the specimen were known during the diffraction data acquisition because the stress-free lattice spacing used to calculate macroscopic stress varies with temperature. Temperature measurements were made using thermocouples spot-welded directly onto the specimen surface. The thermocouple measurement positions are indicated in Table 2. The temperatures were recorded during thermal shock by a data logger at a sample rate of 1000 Hz.

Table 2 *Co-ordinates of the temperature measurement points. The distance x_2 is shown in Figure 2d.*

Thermocouple ID	x_2 (mm)
T1	0
T2	3.5
T3	7
T4	12
T5	17

The completed tests and successful X-ray diffraction measurements are summarised in Table 3. Steady-state measurements were carried out at room temperature (RT) and elevated temperature (ET). Room temperature was 20°C. For elevated temperature measurements, the temperature at the surface of the cladding (thermocouple T1) was 327°C.

Table 3 *Summary of X-ray diffraction measurements made on each specimen.*

Specimen ID	Crack length, a (mm)	Steady state before thermal shock: RT (20°C)	Steady state before thermal shock: ET (327°C)	Transient during thermal shock	Steady state after thermal shock: RT (20°C)
A	Stress-free reference comb	N/A	N/A	N/A	N/A
B	7.4	✓	✓	✓	✓
C	7.4			✓	
D	0	✓	✓	✓	✓
E	0				✓
F	10	✓	✓	✓	✓
G	10			✓	

3 Finite element modelling

A three dimensional elastic- plastic finite element model was constructed to calculate the near-tip stresses during thermal shock for comparison with the experimental X-ray diffraction measurements. The model was constructed and analysed using the Abaqus 6.14 [27] finite element code. An example of the simulation is shown in Figure 3. The thermal expansion coefficient of the clad and the parent material were selected so that once the model is heated up to 20°C, the difference between the expansion of the clad and the parent induces the same level of residual stress in the as-cladded sample as it was measured at room temperature in previous measurement [5]. A restart file was then written and used in the subsequent stress analysis models thus accounting for the clad residual stress in the calculations. Any prior plasticity that may be present in the specimen was ignored as there is no quantitative method for measuring it.

Figure 3 *Example of the simulation mesh and results, the contour plot shows the thermal flux vector (HFL) magnitude in W/mm^2 .*

The model procedure comprised a heat transfer analysis followed by a stress analysis. The heat transfer analysis calculated the temperatures in the specimen at discrete time intervals during thermal shock. The calculated temperatures were then prescribed to the stress analysis, which calculated the stress from thermal strain. The models are three-dimensional and correspond to a quarter model of the specimens with appropriate boundary conditions applied. Twenty-node quadratic brick elements of type DC3D20 were used to construct the mesh for the heat transfer analysis, and eight-node linear brick elements of type C3D8R were used for the stress analysis. The mesh used for the stress analysis contained a refined region around the crack tip where the side length of each element was 20 μm to ensure mesh insensitivity of the analysis. A row of 20 elements through the thickness of the models was used.

For the heat transfer analysis, the mesh was set to a uniform initial temperature of 360°C, which represents an average of the experimental temperatures measured in the specimens under steady-state conditions before thermal shock. Thermal shock was then simulated by instantaneously adjusting the temperature of free surfaces to 20°C. Instantly cooling the surfaces in this manner represents perfect heat transfer. The transient temperatures were calculated at progressively larger increments of time after applying surface cooling, starting with 0.02 seconds.

For the stress analysis, the model was initially considered to be crack free. The mesh was set to an initial stress-free temperature of 580°C and was then uniformly cooled down to 20°C. This uniform cooling step is a simple way of generating the cladding residual stress from the difference in thermal expansion coefficient between the cladding and parent materials. This method has been shown to be reasonably accurate compared with measurements on stainless steel cladding in previous work by Rybicki et al [7]. The crack was then introduced by removing the symmetry boundary condition along the crack face. Finally, the transient stress during thermal shock was simulated by prescribing the temperatures calculated by the heat transfer model. Stresses were averaged in a cuboid ahead of the crack tip equivalent to the X-ray diffraction measurement volume (i.e. $0.2 \times 0.2 \times 2 \text{ mm}^3$ with the centre located 0.15 mm from the crack tip). A separate stress analysis was carried out to represent each of the three different crack lengths studied in the experiment: 7.4 mm, 10 mm, and crack-free. Material properties were required for the three different regions of parent, HAZ (heat-affected zone), and cladding. Values used for the HAZ are listed in Table 4, and values used for the cladding are in Table 5. The thermal conductivity, specific heat, density, thermal expansion coefficient, and Poisson's ratio were derived from values published for similar alloys in the open literature [21,28–30]. The thermal expansion coefficient is defined in this paper as the mean linear coefficient from 20°C to the indicated temperature, so that free linear thermal expansion is calculated by Equation (5):

$$\varepsilon_{th} = \alpha(T - 20) \quad (5)$$

where ε_{th} is the thermal strain α is the thermal expansion coefficient (in $1/^\circ\text{C}$), and T is the current temperature (in $^\circ\text{C}$). Values for Young's modulus at 20°C were calculated from tensile tests described elsewhere [31], and were reduced with increasing temperature by factors

derived from data published for similar alloys [29,32]. A series of temperature-dependant elastic-plastic stress-strain curves were derived for each material, which were prescribed to the model as incremental plasticity with isotropic hardening. The stress-strain curves used for the parent, HAZ, and clad materials are shown in Figure 4a, b, and c respectively. The solid curves are tensile test results and the markers are the discrete data points used to define the material in the model. The tensile test curves are from room temperature tensile tests [33]. It was assumed that no further strain hardening occurred beyond the points of maximum strain plotted in Figure 4.

Table 4 *Material properties used for the HAZ and parent materials in the finite element model.*

Temperature (°C)	Thermal conductivity, κ (W m ⁻¹ K ⁻¹)	Specific heat, c_p (J kg ⁻¹ K ⁻¹)	Thermal expansion coefficient, α ($\mu\text{m m}^{-1}$ K ⁻¹)	Young's modulus, E (GPa)
20	41.6	466	11.80	203
100	41.3	495	12.14	201
200	40.5	532	12.29	194
300	39.3	570	12.51	189
400	37.2	623	13.01	181
500	34.7	695	13.59	170
600	31.6	795	14.04	162

Table 5 *Material properties used for the cladding in the finite element model.*

Temperature (°C)	Thermal conductivity, κ (W m ⁻¹ K ⁻¹)	Specific heat, c_p (J kg ⁻¹ K ⁻¹)	Thermal expansion coefficient, α ($\mu\text{m m}^{-1}$ K ⁻¹)	Young's modulus, E (GPa)
20	14.9	444	11.03	172
100	15.9	465	11.33	169
200	17.3	486	11.35	165
300	19.0	502	11.35	160
400	20.5	519	12.45	155
500	22.1	536	14.03	151
600	23.9	578	16.22	145

(a)

(b)

(c)

Figure 4 Elastic-plastic stress-strain curves used in the finite element model for: (a) the parent, (b) the HAZ, and (c) the cladding.

4 Results

4.1 Steady-state measurements before and after thermal shock

X-ray diffraction measurements were made under steady conditions at room temperature and at elevated temperature. The temperature in the specimens was uniform at room temperature (20°C) but non-uniform at elevated temperature as shown in Figure 5a which is the temperatures measured by the thermocouples during elevated temperature steady state conditions. The temperature gradient occurred because the strip heaters did not cover the whole specimen and did not provide perfectly uniform heating.

The steady state measurements carried out before thermal shock on the crack-free specimen at room temperature should be comparable to residual stress measurements made on the original

clad plate in previous work [5]. Figure 5b compares the stresses measured in a crack-free specimen by X-ray diffraction (XRD) in this work with those measured in the original clad plate by deep hole drilling (DHD) in previous work [34]. Briefly, DHD operates on a similar basis as centre hole drilling in which by removing the material, the residual stress is relieved in stages and by measuring the relaxation strain during the process, the residual stress is back-calculated. In DHD, a guide hole is drilled in the material whose spatially resolved diameter is measured by an air probe. The material around the guide hole is then separated from the component by electro-discharge machining a core, thus changing the diameter of the guide hole as the residual stress is relaxed. By remeasuring the diameter of the hole, the residual stress in the material can be calculated [35]. The X-ray diffraction measurement is the average of four measurements made on one of the crack-free Specimen D. The error bars on the XRD measurement indicate the range of values obtained from the different measurements made horizontally and averaged to be comparable with those measured by DHD. The single error bar on the DHD measurement represents the typical uncertainty of approximately 35 MPa obtained in previous work [31].

Figure 6 shows contour maps of room-temperature steady-state stress in Specimen B (7.4 mm crack) before (a) and after (b) thermal shock, and the corresponding maps for Specimen F (10 mm crack) are shown in (c) and (d). The stress shown in the figures are the component normal to the crack (σ_{11}). Before thermal shock, the stress is the cladding residual stress which has been redistributed by inserting a crack. In both specimens, the stress around the crack tip is tensile before thermal shock, whereas after thermal shock a smaller region of compressive stress has formed around the crack tip.

The steady-state stresses were extracted from contour maps along the crack line (at $x_1 = 0$) and are plotted in Figure 7. Results for Specimen B (7.4 mm crack) are shown in Figure 7 (a) and results for Specimen F (10 mm crack) are shown in Figure 7 (b). Stresses are plotted under three different steady-state conditions: before thermal shock at room temperature (RT); before thermal shock at elevated temperature (ET); and after thermal shock at room temperature. In both specimens, high tensile stresses exist near to the crack tip before thermal shock at room temperature. The magnitude of the near-tip stresses is reduced at high temperature. After thermal shock, the near-tip stresses are high-magnitude and compressive.

Figure 5 Comparison of residual stress measurements in the clad plate (by DHD in previous work [5]) with measurements in a crack-free specimen (by XRD in this work). Error bars on the XRD results indicate scatter.

Figure 6 Contour plot of stress normal to the crack (σ_{11}) measured by XRD (a) Specimen B (7.4 mm crack) before thermal shock (b) after thermal shock (c) Specimen F (10 mm crack) before thermal shock and (d) after thermal shock.

Figure 7 Stress normal to the crack (σ_{11}) measured under steady state conditions in (a) Specimen B (7.4 mm crack) and (b) Specimen F (10 mm crack). Stresses are plotted along the crack line (at $x_1 = 0$). RT = room temperature (20°C), ET = elevated temperature.

4.2 Transient measurements during thermal shock

Figure 8 shows the temperatures measured in Specimen G (10 mm crack) during thermal shock. Results from only one specimen have been shown for clarity, although these results are representative of the temperatures experienced by all the specimens. Temperatures were measured by thermocouples T1, T3, and T5, which were 0, 7, and 17 mm from the bottom of the specimen. The cooling rate measured at the bottom of the specimen at the start of thermal shock (at zero seconds) was $-235^\circ\text{C s}^{-1}$.

The stresses measured by X-ray diffraction during thermal shock are plotted for three specimens, one for each crack length, in Figure 9 over (a) 10 minutes and (b) 30 seconds. In the specimens containing cracks, the stresses were measured 150 μm ahead of the crack tip. In the crack-free specimen, the stress was measured 10.15 mm from the bottom of the specimen (i.e. at the same point as the specimens with 10 mm long cracks). In the cracked specimens, the stress rises rapidly after the start of thermal shock and reaches a maximum tensile value within one second and then rapidly becomes compressive. The peak tensile stress was 966 MPa in the specimens with 10 mm cracks and 902 MPa in the specimens with 7.4 mm cracks. The stress in the cracked specimens change sign from tensile before thermal shock (before zero seconds) to compressive towards the end of the transient where conditions are tending towards steady state. This sign change was also observed in the steady state measurements shown in Figure 7. The crack-free specimen experienced a much smaller change in stress during thermal shock than the specimens with cracks.

Figure 8 *Temperatures during thermal shock plotted over (a) 10 minutes and (b) 30 seconds. Measurements from the experiment are compared with calculations by the finite element model.*

Figure 9 *Stress normal to the crack measured 150 μm ahead of the crack tip during thermal shock in one of each type of specimen plotted over (a) 10 minutes and (b) 30 seconds.*

The temperatures measured during thermal shock in a single representative specimen are also shown in Figure 8 and are compared with results from the finite element model. Results are plotted over 10 minutes (a) and 30 seconds (b). Before the start of thermal shock, the temperature is non-uniform in the experiment because of non-uniform heating as discussed before, whereas the finite element model is at a uniform temperature of 360°C. Cooling is generally faster in the finite element model for two reasons: first, the cooling boundary condition in the model represented perfect heat transfer and was therefore more severe than in the experiment; second, the model did not account for the thermal energy stored in the heaters which retarded the cooling rate in the specimen. The latter effect explains the large difference between the experimental and numerical results over 10 minutes. The effect is stronger in thermocouple T4 (see Figure 1c) because it was closer to the heaters than thermocouple T1. However, agreement between the model and experiment is reasonable over shorter time periods as shown in Figure 8 (b).

The stresses calculated using finite element analysis are shown in Figure 9 for three models, one for each crack length studied: (a) 7.4 mm, (b) 10 mm, and (c) zero (crack-free). The results for each crack length are compared with the experimental measurements. The results are only plotted over 30 seconds because agreement between the heat transfer model and the measured

temperatures degraded beyond this point (see Figure 8). Before the start of thermal shock (i.e. from -5 to 0 seconds) there is an initial error between the model and experiment of around 200 MPa for the specimens with 7.4 mm cracks (Figure 10 (a)) and around 100 MPa for the crack-free specimen (Figure 10 (c)). The time during thermal shock at which peak stresses were calculated shows good agreement with the experimental measurements for all crack lengths. Agreement diverged beyond the point of peak stress, with experimental measurements in the cracked specimens becoming compressive much faster than in the model. The error between the model and experiment was much smaller in the crack-free specimen.

(a)

(b)

(c)

Figure 10 Stress 150 μm ahead of the crack tip during thermal shock calculated using finite element analysis (FEA) and compared with the experimental results for specimens containing: (a) a 7.4 mm crack, (b) a 10 mm crack, and (c) no crack (stress at the same point as the specimen with a 10 mm crack). The stress component, σ_{11} , is normal to the crack.

5 Discussion

5.1 Steady state

The near-tip stresses shown in Figure 7 change from high-magnitude tensile before thermal shock to high-magnitude compressive after thermal shock. The compressive stresses are caused by reverse plasticity may occur during unloading. The unloading occurs beyond the point of peak stress during thermal shock, for example shown in Figure 9(b). This behaviour is consistent with predictions by warm pre-stress models that the stress immediately adjacent to the crack tip becomes compressive as soon as any unloading occurs [36].

5.2 Transient

During thermal shock, the X-ray diffraction measurement was carried out at the same position in the specimens containing 10 mm cracks (Specimen F and Specimen G) and the crack-free specimen (Specimen D). However, the results in the two types of specimens are very different (Figure 9(b)). At the onset of thermal shock, the stress in the crack-free specimen became low-magnitude compressive whereas the stress in the cracked specimens became high-magnitude tensile. This is because the stresses in the cracked specimen are the near-tip stresses, typically described by fracture parameters such as the stress intensity factor, which depend on the stresses acting over the entire length of the crack, whereas the stress in the crack-free specimen is just a point measurement which is not affected by the presence of a crack. The peak near-tip stresses measured in the cracked specimens are tensile because the stresses acting over the majority of the crack faces at that point in time, comprising residual stress and thermal stress, are tensile. However, in the absence of a crack the stress at the measurement point is compressive.

Agreement between the temperatures calculated by the finite element model and those measured in the experiment was reasonable during the first 30 seconds of thermal shock in crack-free samples (Figure 8). However, in terms of stress, agreement with the specimens containing cracks was poor over the same period (Figure 10(a) and(b)). This could have been caused by experimental error or by the incompatibility between the model and the experiment. Agreement between the model and experiment was better without a crack (Figure 10(c)). For example, in the specimens containing 7.4 mm cracks and the crack-free specimen, there is an initial discrepancy in the stress calculated by the model just before thermal shock. The difference can be seen between -5 and 0 seconds in Figure 10(a) and Figure 10(c). This is an inaccuracy in the finite element model caused mainly by imperfect simulation of the residual stress. The error in the crack-free model represents the error at the measurement point (around 100 MPa), whereas the error in the model with a 7.4 mm crack is larger because it is magnified by the measurement point being close to the crack tip. It should be noted that the experimental stress measurements from diffraction experiments were elastic only therefore Figure 9 shows the elastic component of the simulated stress in FE to ensure compatibility between the technique is maintained.

Figure 11 Stress normal to the crack (σ_{11}) measured during thermal shock and normalised by the temperature dependent yield stress measurement point

Plane stress assumptions are used to calculate stress from the X-ray diffraction measurements which may not be a true representation of the stress condition in a 2 mm thick samples. The peak stresses measured during thermal shock are high compared to the yield stress of the material. Figure 11 shows the magnitude of one component of the stress tensor in the cracked specimens during thermal shock normalised by the temperature dependent material yield stress and as it can be seen that the near-tip stresses calculated by the finite element model are higher than the yield stress of the material. This suggests the stress state is triaxial, which would allow individual components to exceed the uniaxial yield stress without causing the material to yield. However, only the in-plane components of strain (ϵ_{11} , ϵ_{22} , ϵ_{12}) could be measured by X-ray diffraction, therefore either a plane strain or plane stress assumption had to be made for calculation of the stress tensor. Plane stress was assumed ($\sigma_{33} = \sigma_{13} = \sigma_{23} = 0$) because the specimens were thin (2 mm) and no out of plane distortion was observed after the thermal shock visually. The stresses were therefore calculated using a two-dimensional formulation of Hooke's law (Equation (4)) which does not account for the non-zero σ_{33} , σ_{13} , and σ_{23} components. This is a reasonable assumption for measurements which were made far from the crack tip (or in the crack-free specimens) and at the free surfaces at $x_3 = 0$ mm and $x_3 = 2$ mm. However, it has been previously demonstrated that close to the crack tip σ_{33} is always non-zero within the specimen thickness [37]. The three-dimensional formulation of Hooke's law is given in Equation (6):

$$\sigma_{11} = \frac{E}{1+\nu} \epsilon_{11} + \frac{\nu E}{(1+\nu)(1-2\nu)} (\epsilon_{11} + \epsilon_{22} + \epsilon_{33}) \quad (6)$$

An estimate was made of the error caused by the plane stress assumption used to calculate stresses from the measured elastic strains. This was achieved by simulating an X-ray diffraction

measurement using elastic strains calculated by the finite element model during thermal shock. Two simulated measurements of stress were made: the first method used the general, isotropic version of Equation (4), which is the plane stress method used in the experiment; the second method used Equation (6), which represents a perfect measurement that makes no prior assumption about the stress state. It was found that the peak magnitude of σ_{11} during thermal shock was up to 17% larger using the perfect measurement compared with the plane stress assumption. Therefore, the peak tensile stress measured in the cracked specimens, for example shown in Figure 10, could be smaller than the true value.

Another possible source of uncertainty in the experimental measurements of stress could exist because of a difference between the temperatures measured by the thermocouples and the true temperature at the measurement point. The calculation of stress from the X-ray diffraction measurements requires reliable knowledge of the temperature at the measurement point so that the correct value of stress-free lattice spacing, d_0^{hkl} , is used in Equation (3). In this experiment, the temperature of the measurement point was inferred from measurements by thermocouples located 12 mm away. This is a reasonable assumption in the crack-free specimen, because the temperature is only expected to vary significantly in the x_2 direction which is normal to the water surface. This may not be a fair assumption in the specimens with cracks because water marks observed in the specimens after thermal shock suggested that water was drawn up the crack, providing additional cooling on the crack faces and around the tip. For example, a trace of the water mark left on Specimen B (7.4 mm crack) after thermal showed that as water evaporated from the surface during thermal shock the depth of submergence was not the uniform 2 mm intended but immersed the full crack in water. The thermocouples were located above the water mark, whereas the X-ray diffraction measurement point was below. Therefore, the true temperature at the measurement point could have been lower than the value measured by the thermocouples, causing the assumed value of stress-free lattice spacing to be unrealistically high. This in turn would make the measured strains and stresses too low. A sensitivity analysis was carried out on Specimen B (7.4 mm crack). It was found that if the measured temperatures were 50°C below the true value at the measurement point, then the peak stress during thermal shock would be 200 MPa too low. This source of error could therefore explain a large amount of the difference between the stresses from the experiment and the model in the specimens containing cracks.

The observation of the water marks also suggested that there could have been extra cooling around the crack than was accounted for in the model. To check this, additional finite element models were made which included extra cooling local to the crack by prescribing the cooling boundary condition to regions on the crack faces and around the crack. It was found that agreement in terms of stress between the model and the experiment was somewhat, but not completely, improved when the model accounted for extra cooling local to the crack [33].

5.3 Fracture

Stress intensity factors were estimated from the measurements of stress made during thermal shock in specimens containing cracks. The stress intensity factors, associated with elastic

strains measurements, were calculated using the solution for the stress fields near to the tip of a crack in a linearly elastic material [38]:

$$\sigma_{11} = \frac{K}{\sqrt{2\pi r}} \cos\left(\frac{\theta}{2}\right) \left[1 + \sin\left(\frac{\theta}{2}\right) \sin\left(\frac{3\theta}{2}\right)\right] \quad (7)$$

where: σ_{11} is the stress normal to the crack, K is the stress intensity factor, and θ and r are polar coordinates with the origin at the crack tip. We accounted for the effect of the measurement averaging the stresses over a projected square area [33]. Equation (7) is strictly valid for sharp cracks, whereas the cracks in the specimens were machined using wire electrical discharge machining and so had a finite tip radius. However, it is reasonable to use Equation (7) in this case because the tip radius is small (54 – 64 μm , measured using a shadow graph). In addition, the equation is only valid in the case of linear elastic conditions which is not necessarily maintained in the case of this experiment as the plastic strains could not be measured by the diffraction method. Nonetheless, the results provide a useful indicator of the proximity of the material to fracture failure. The results were compared with those calculated using a blunt crack form of Equation (7) [39], and it was found that the stress intensity factor only reduced by 2% when the finite tip radius was accounted for.

The stress intensity factors during thermal shock calculated from the stresses measured in the cracked specimens (K_m) are plotted in Figure 12. Equation (7) assumes that the material is linearly elastic, and so the calculation of stress intensity factors is only strictly valid if the region of material encompassed by the measurement point has not yielded (i.e. yielding is limited to a region very close to the crack tip). Therefore, a threshold value was calculated, which is the value of K_m required for half of the area of the measurement point to contain stresses above the uniaxial yield stress. If plane stress conditions are assumed ($\sigma_{33} = 0$), then the threshold is the point at which half of the material in the measurement point has yielded, and so values of K_m which exceed the threshold are clearly invalid. However, the threshold may be conservative because near tip triaxiality allows individual components of stress to exceed the uniaxial yield stress, as discussed in the previous section. The threshold therefore represents a basic criterion which, if exceeded, indicates that using Equation (7) to calculate the stress intensity factor may be inaccurate. The threshold values are indicated in Figure 12. The threshold is different for the different crack lengths because the measurement points are in regions with different yield strengths. The results are summarised in Table 6. The maximum stress intensity factor occurred under transient loading during thermal shock, rather than under steady conditions before or after thermal shock. These results only account for residual and thermal stresses, and do not include a contribution from internal pressure.

Table 6 *Stress intensity factors calculated from measured stresses before (at 20°C), during, and after (at 20°C) thermal shock. ‘Before’ and ‘after’ values were calculated from residual stress measurements made in previous work [5] on the same material. ‘During’ values were calculated from transient measurements carried out during thermal shock in this work.*

Crack length (mm)	Stress intensity factor before thermal shock, K_{RS} (MPa m ^{1/2})	Peak stress intensity factor during thermal shock, K_m (MPa m ^{1/2})	Stress intensity factor after thermal shock, K_{RS} (MPa m ^{1/2})
7.4	14.6	24.3 – 24.6	8.0
10	6.0	20.6 – 26.8	6.3

The maximum stress intensity factor experienced during thermal shock by the specimens with 7.4 mm cracks was 24.6 MPa m^{1/2}. In previous analysis by Udagawa et al [11] a peak stress intensity factor of 95 MPa m^{1/2} was calculated for a 10 mm surface crack in an RPV during a non-pressurised thermal shock caused by a loss of coolant accident. The stress intensity factor calculated from the measurements made in this work is much lower. This is partly because of some of the sources of experimental uncertainty discussed in the previous section, and partly because the geometry of the specimen was different to that of a full-size RPV. The total thickness of the clad plate from which the specimens were extracted was 42 mm, whereas RPVs typically have a wall thickness of 180 - 200 mm. This has two effects. The first effect is that the cladding residual stress will be higher in the thicker RPV because the relative thickness of the cladding is smaller [5,7]. The second effect is that the RPV can sustain tensile thermal stresses to a greater depth from the inner (cooled) vessel wall. For example, in the analysis of an RPV by Udagawa et al [11], when the stress intensity factor during thermal shock was highest the stress normal to the crack (σ_{11}) was tensile all the way from the inner wall to a depth of 65 mm. Clearly it is impossible for the specimen used in this work to sustain a similar stress profile because it was extracted from a plate which is only 42 mm thick. Furthermore, the residual and thermal stresses must be self-balancing therefore the specimen used in this work can only sustain tensile stress down to a much smaller depth. Finally, the specimens used in this experiment were thin (2 mm) and so the thermal stresses were approximately uniaxial, acting normal to the crack (σ_{11}). In an RPV, the thermal stresses are approximately biaxial ($\sigma_{11} = \sigma_{33}$ in which case it can be demonstrated using Hooke’s law that their magnitude in a linear elastic material is increased by a factor of $(1 - \nu)^{-1}$ compared with uniaxial thermal stresses [3].

5.4 Simulation

It is important to note that, as detailed above, the model could have been fine-tuned so that the finite element results match that of the experimental data. For example, the area which experiences thermal shock was changed from the original nominal area to the area indicated by the water mark; the crack tip radius was measured by an optical microscope and was represented in the simulation instead of choosing the nominal 0.15mm diameter of the wire EDD. There could have been other fine tuning applied on the simulation. For example: the reduction in heat flux due to bubble formation at the hot surfaces could have been considered; or attempts could have been made to identify the correct stress state of the sample instead of a

simplified plane stress condition. However, such practice is not applicable to industrial applications as for example a loss of coolant accidents in a reactor pressure vessel is not monitored at 30 Hz by X-ray diffraction to allow close simulation of the process. The FE presented in this work is representative of engineering practice and it can be argued that the discrepancy between the results of a closely monitored and staged experiment and a well-executed finite element model with sound assumptions (e.g. plane stress, 2 mm water level, uniform temperature, ...) is typical of a simulation carried out by an experienced operator. It is therefore suggested that due to high number of uncertainties associated with a multi-physics phenomenon such as a thermal shock, the results of FE simulation, though an acceptable indicative, cannot replace the critical experiments. This is critically important as our FE study showed that the elastic strains measured by X-ray diffraction less than a second after the thermal shock in a thin sample is close to lower shelf toughness of the material. It therefore could be envisaged that in a thick sectioned reactor pressure vessel, the elastic-plastic stress intensity factor experienced by the material is a considerable fraction of its toughness impacting the integrity of the vessel.

Figure 12 Stress intensity factors calculated from the near-tip stress measured in specimens containing: (a) a 7.4 mm crack, and (b) a 10 mm crack.

The simulation presented here used all the information available from an industrial standard test to produce as comprehensive a model as possible. This included simulating the cladding residual stress and detailed simulation of a thermal shock process. There were other factors influencing the thermal shock process that are very difficult to measure, especially in an industrial setting. The FE, if tuned using the unmeasured values, could result in a close agreement between the experiment and simulation. However, since the aim of the study was not to develop a simulation that matched the experiment using all means necessary but to assess whether a reasonable simulation informed only by easily measurable parameters can be used to assess the safety of the plant in the absence of a full scale test. The model used here is shown not to be capable of replicating experimental values thus confirming the complex industrial processes of thermal shock cannot be analysed by simulation only.

6 Conclusions

This work measured stresses in RPV material under transient conditions during thermal shock. This was achieved by extracting thin specimens from a clad plate and subjecting them to thermal shock whilst simultaneously measuring stress using time-resolved synchrotron X-ray diffraction. Stresses were measured during thermal shock at a single point in the parent material in crack-free specimens, and at the crack tip in specimens with through-cladding surface cracks. Stresses were also measured under steady-state conditions before and after thermal shock. Stresses were only measured in the parent material (SA508 4N) because the grain size in the cladding (Alloy 82) was too large for reliable X-ray diffraction measurements. It was found that:

- Steady state measurement in the specimens containing cracks found high tensile stresses near the crack tip before thermal shock, which changed to high-magnitude compressive stresses after thermal shock.
- Transient measurements of stress during thermal shock made at the crack tip in specimens with cracks showed that peak tensile stresses of up to 966 MPa occurred within a second of the start of cooling. The stresses then rapidly became compressive and remained so for the duration of cooling.
- It was demonstrated entirely from experimental measurements of residual and thermal stresses that the peak stress intensity factor occurred under transient loading during thermal shock, rather than under steady conditions, before or after cooling.
- Stress intensity factors were estimated from the stresses measured during thermal shock. The peak stress intensity factor experienced by the specimens with 7.4 mm surface cracks (through-cladding) was $24.6 \text{ MPa m}^{1/2}$. This is smaller than typical values calculated during analyses of reactor pressure vessels undergoing thermal shock, although this can be explained by geometry effects.
- A finite element model was made as a benchmark thermal shock analysis method. Temperatures calculated by the model showed reasonable agreement with the experiment over the first 30 seconds of thermal shock.
- The stresses found from the FE simulations were in poor agreement with experimental results in specimens containing cracks. Some sources of error were identified in the experiment and model which explain some of the differences between the experimental and numerical results. Agreement between the model and experiment was better without a crack.
- The time dependent stress intensity factor calculated by the finite element was strongly dependent on a number of parameters (e.g. thermal flux between the quenching liquid and the surface in the presence of bubbles) with high level of uncertainty. It was therefore possible to fine tune the model so that experiment and FE stresses match but that would not be representative of the real industrial situation in which the thermal shock is not controlled nor measured. It is therefore unlikely that a practical real-case

simulation could be carried out that is true representative of the condition of the component.

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