EVALUATION OF RESIDUAL STRAINS AND STRESSES USING TWO-DIMENSIONAL X-RAY DIFRACTION

SAKSL Karel[1,2], SZULC Zygmunt[3], GLOC Michał[4], MILKOVIČ Ondrej[1], ĎURIŠIN Juraj[5], CIUPIŃSKI Łukasz[4], ARNBJÖRNSSON Adalsteinn[6], OSTROUSHKO Dmytro[7], MAZANCOVÁ Eva[7], BERTRAM Florian[8]

[1]Slovak Academy of Sciences, Institute of Materials Research, Slovakia, EU
ksaksl@saske.sk, ondrej.milkovic@tuke.sk
[2]Faculty of Sciences, Pavol Jozef Šafárik University in Košice, Košice, Slovakia, EU
[3]Explomet - Opole (High-Energy Techniques Works), Opole, Poland, EU, zygmunt.szulc@explomet.pl
[4]Warsaw University of Technology, University Research Centre "Functional Materials", Warsaw, Poland, EU, michalgloc@poczta.fm, lciupinski@gmail.com
[5]Technical University of Košice, Faculty of Electrical Engineering and Informatics, Košice, Slovakia, EU, juraj.durisin@tuke.sk
[6]Innovation Center Iceland, Materials, Biotechnology and Energy, Reykjavík, Iceland, ada@nmi.is
[7]VSB - Technical University of Ostrava, Faculty of Metallurgy and Materials Engineering, Ostrava, Czech Republic, EU, dimitrij.o@seznam.cz, eva.mazancova@vsb.cz
[8]DESY Photon Science, Hamburg, Germany, EU, florian.bertram@desy.de

Abstract

Residual stresses exist in material independently of the presence of any external loads. Their presence may not be readily apparent and so they may be overlooked or ignored during a process of engineering design. This however can cause great design risk because they can have profound impact on material strength, dimensional stability and fatigue life. Almost all manufacturing processes create residual stresses that can further develop during service life of the manufactured component. Several comparative, qualitative and quantitative methods for stress analysis are nowadays applied in engineering praxis. Among them X-ray diffraction is one of the most used and developed over the past 90 years. In this article we describe novel concept of two-dimensional X-ray diffraction (XRD^2) and we demonstrate its applicability on determination of residual strains and stresses in a bimetallic austenite/ferrite steel system. Our analysis is based on X-ray micro-diffraction experimental utilizing hard monochromatic X-rays focused down to micrometer size. In this way bimetal in bulk form was analyzed and microstructural differences between the joined materials and their interface were determined.

Keywords: X-ray diffraction, XRD^2, explosive welding, bimetal

1. INTRODUCTION

Residual stresses exist in materials and structures, independently of the presence of any external loads. Stresses are self-equilibrating, where local areas of tensile and compressive stresses sum to create zero force and moment resultants within the whole volume of the material or structure. The mechanisms for creating residual stresses in materials include:

- non-uniform plastic deformation during manufacturing processes that change the shape of a material including forging, rolling, bending, drawing, extrusion, etc.
- surface modification during machining, grinding, plating, peening, and carburizing, as well as in service for example by corrosion or oxidation.
- material phase and/or density changes, often in the presence of large thermal gradients.

Several comparative, qualitative and quantitative methods for stress analysis are nowadays applied in engineering praxis. Among them well-established are: hole drilling, ring coring, slitting, contour, X-ray and neutron diffraction, magnetic, ultrasonic and optical methods. In this paper we describe a relatively novel approach of the two-dimensional X-ray diffraction method (XRD²) developed by B.B. He [1] and demonstrate its applicability on an XRD data collected at a synchrotron source.

2. THEORY OF STRESS ANALYSIS WITH XRD²

The basic concept underlying the non-destructive measurement of residual strain and stresses from XRD measurement is based on the fundamental relation formulated by W. L. Bragg in 1913 connecting the spacing, $d_{\{hkl\}}$, between certain crystal lattice planes families $\{hkl\}$ to the diffraction angle, $2\theta_{\{hkl\}}$, at which the radiation is scattered coherently and elastically for a given wavelength of the radiation, λ

$$2d_{\{hkl\}}\sin\theta_{\{hkl\}} = \lambda \tag{1}$$

Polycrystalline materials consist of a large amount of crystallites of various sizes, shapes, and orientations. When a solid material is elastically deformed by a force, each crystallite changes its shape or size. Assuming that the stresses in each crystallite represent the stresses in the solid, the stresses can be measured by measuring the lattice *d*-spacing change in the crystallites. The stress in a sample can be compressive or tensile, so that the *d*-spacing in the corresponding direction will be smaller or larger than the stress-free sample, respectively. This *d*-spacing change can be measured by the diffraction peak position change based on the Bragg law. In this case, the *d*-spacing in the crystallites serves as a gauge to the deformation. The methods of stress measurement by X-ray diffraction can be classified as conventional, that is one-dimensional and two-dimensional (XRD²). Stress measurement with two-dimensional X-ray diffraction (XRD²) is based on the fundamental relationship between the stress tensor and the diffraction cone distortion. **Figure 1** shows the difference between diffraction patterns collected from unstrained and strained crystallites.

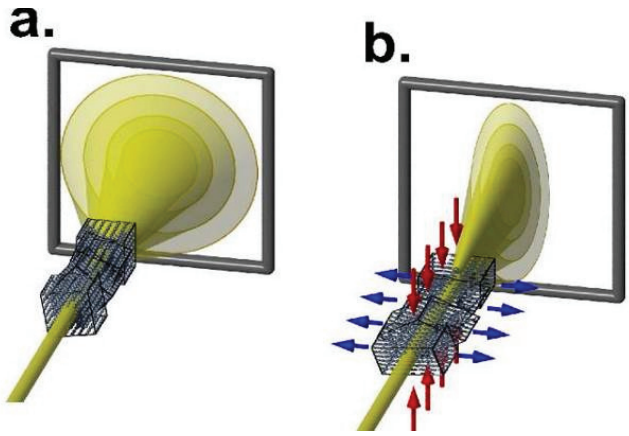

Figure 1 Schematic drawing of 2-dimensional X-ray diffraction **a.** from unstrained and randomly oriented crystallites **b.** from strained - compressed and elongated crystallites. Differences between the two diffraction patterns are largely exaggerated in the picture.

The diffraction cones from a stress-free polycrystalline sample are regular cones in which diffraction angle 2θ is a constant, see **Figure 2**. The stress in the sample distorts the diffraction cones shape so they are no longer regular cones. For a stressed sample, 2θ becomes a function of the azimuthal angle γ and the sample orientation (ω,φ,ψ), that is, $2\theta = 2\theta(\gamma,\omega,\varphi,\psi)$. This function is uniquely determined by the stress tensor. The strain measured by the 2θ shift at the azimuthal angle γ is $\varepsilon^{\{hkl\}}_{(\gamma,\omega,\varphi,\psi)}$ based on the true strain definition:

$$\varepsilon^{\{hkl\}}_{(\gamma,\omega,\varphi,\psi)} = \ln\frac{d}{d_0} = \ln\left(\frac{\sin\theta_0}{\sin\theta}\right) \tag{2}$$

where d_0 and θ_0 are the stress-free values of interplanar distance and diffraction angle, while d and θ are the measured values from a point on the diffraction ring corresponding to $(\gamma,\omega,\varphi,\psi)$.

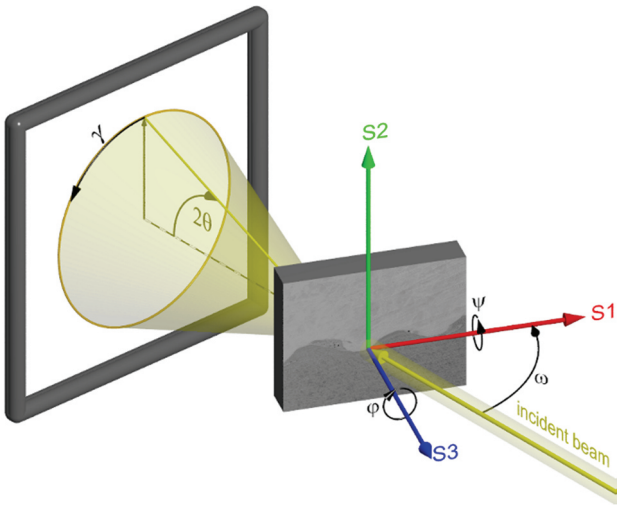

Figure 2 Orientation of laboratory diffraction and sample coordinate system S1, S2, S3

The direction of $\varepsilon^{\{hkl\}}_{(\gamma,\omega,\varphi,\psi)}$ in the sample coordinates S1 S2 S3 can be given by the unit vector $\boldsymbol{h}_{hkl}$:

$$\boldsymbol{h}_{hkl} = \begin{bmatrix} h_1 \\ h_2 \\ h_3 \end{bmatrix} \tag{3}$$

and the $\boldsymbol{h}_{hkl}$ vector components can be express for Eulerian geometry by the following:

$$\begin{aligned} h_1 &= \sin\theta(\sin\varphi\sin\psi\sin\omega+\cos\varphi\cos\omega)+\cos\theta\cos\gamma\sin\varphi\cos\psi \\ &\quad -\cos\theta\sin\gamma(\sin\varphi\sin\psi\cos\omega-\cos\varphi\sin\omega) \\ h_2 &= -\sin\theta(\cos\varphi\sin\psi\sin\omega-\sin\varphi\cos\omega)-\cos\theta\cos\gamma\sin\varphi\cos\psi \\ &\quad +\cos\theta\sin\gamma(\cos\varphi\sin\psi\cos\omega+\sin\varphi\sin\omega) \\ h_3 &= \sin\theta\cos\psi\sin\omega-\cos\theta\sin\gamma\cos\psi\cos\omega-\cos\theta\cos\gamma\sin\psi \end{aligned} \tag{4}$$

The measured true strain can be expressed as a scalar product of the strain tensor components with the unit vector $\boldsymbol{h}_{hkl}$

$$\varepsilon^{\{hkl\}}_{(\gamma,\omega,\varphi,\psi)} = \ln\frac{d}{d_0} = \ln\left(\frac{\sin\theta_0}{\sin\theta}\right) = h_1^2\varepsilon_{11} + 2h_1h_2\varepsilon_{12} + h_2^2\varepsilon_{22} + 2h_1h_3\varepsilon_{13} + 2h_2h_3\varepsilon_{23} + h_3^2\varepsilon_{33} \tag{5}$$

By substituting for the γ the value from 1º to 360º, the above equation establishes the relationship between the diffraction cone distortion and the strain tensor. Therefore, this equation is the fundamental equation for strain measurement by two-dimensional X-ray diffraction. The equation can be used to calculate the strain tensor components from the measured strain (2θ shift) values at corresponding directions. The fundamental equation for stress measurement by XRD² is a linear equation of the strain tensor components. The strain

tensor can be obtained by solving the linear equations if at least six independent strains at significantly different orientations (at different azimuthal angles γ) are measured.

Stress tensor components can be calculated from the strains by the following equations:

$$\sigma_{ii} = \frac{E}{1+\nu}\varepsilon_{ii} + \frac{\nu E}{(1+\nu)(1-2\nu)}HS$$
$$\sigma_{ij} = \frac{E}{1+\nu}\varepsilon_{ij} \qquad (6)$$
$$HS = (\varepsilon_{11} + \varepsilon_{22} + \varepsilon_{33})$$

where E is the Young's modulus, ν is the Poisson's ratio and term HS is the sum of the normal strain tensor components.

3. EXPERIMENT

3.1. Explosively welded material and sample preparation

A sheet of pressure vessel steel P355NH of the following chemical composition (wt. %): Fe-97.75, C-0.18, Mn-1.19, Si-0.35, Ni-0.22, Cu-0.2, Al-0.041, Cr-0.02, Nb-0.02, P-0.015, Mo-0.004, V-0.003, Ti-0.003, S-0.002, B-0.0002 was clad (explosively welded) by austenitic stainless steel 254SMO Fe-53.87, C-0.014, Cr-19.99, Ni-17.96, Mo-6.05, Cu-0.69, Co-0.41, Si-0.39, Mn-0.38, N-0.213, P-0.021, Nb-0.012, S-0.001. The thickness of the ferritic base material was 10 mm and of the clad 3 mm. Dimensions of the welded sheets were 800 × 520 mm. Both the materials were explosively welded by the EXPLOMET-Opole company, Poland under mild conditions. From a material cube of 5 mm an edge length was cut out so that the interface was roughly in the middle parts of four faces. The two parallel faces of the cube subjected to the micro-diffraction experiment were finely ground, polished and etched in order to remove the residual stresses introduced by the cutting process.

3.2. Instrument used for the microdiffraction experiment

To determine phase composition and residual strains and stresses of the interface and surrounding regions, a hard X-ray micro-diffraction experiment was performed at the beamline P07 at PETRA. During the experiment, monochromatic synchrotron radiation of photon energy 78 keV (λ = 0.015895 nm) was used. The beam of photons was focused by compound refractive lenses down to a spot size of 2.2 μm × 34 μm. The sample was positioned perpendicularly to the direct incident beam by adjusting the tilt of a supporting cradle with precision ± 0.25 degree adjusted by the steepest transition (measured by absorption) between the materials. For the measurement the tilt and rotation angles φ and ψ were fixed to 0º and since the sample was positioned perpendicularly to the incident beam, ω = 90º. The materials interface was scanned shot-by-shot along a straight path (yellow dashed line marked in **Figure 4a** and **5a** of length 0.4 mm with step width of 1 μm. During each step, the sample was illuminated by highly intense hard X-rays for 7.5 seconds. The resulting 2D XRD patterns were recorded using a Perkin Elmer 1621 detector. The recorded XRD patterns were then processed by applying the Fit2D software [2].

4. RESULTS

4.1. Bimetal phase composition

Figure 3 shows the XRD patterns obtained from different parts of the bimetal: 254SMO clad measured 213 μm far from the center of the joint (blue curve on the top), P355NH base metal measured 187 μm from the joint, but in the opposite direction (black curve at the bottom) and center of the joint itself (represented by red

curve in between). The 254SMO consists of sole fcc-Fe (austenite) phase while the P355NH of bcc-Fe (ferrite) and low amount (below 4 vol. %) of orthorhombic Fe_3C (cementite - not visualized in the pattern) phases. Material in the joint center consists of the mixture of all the phases. Any other phase was not detected.

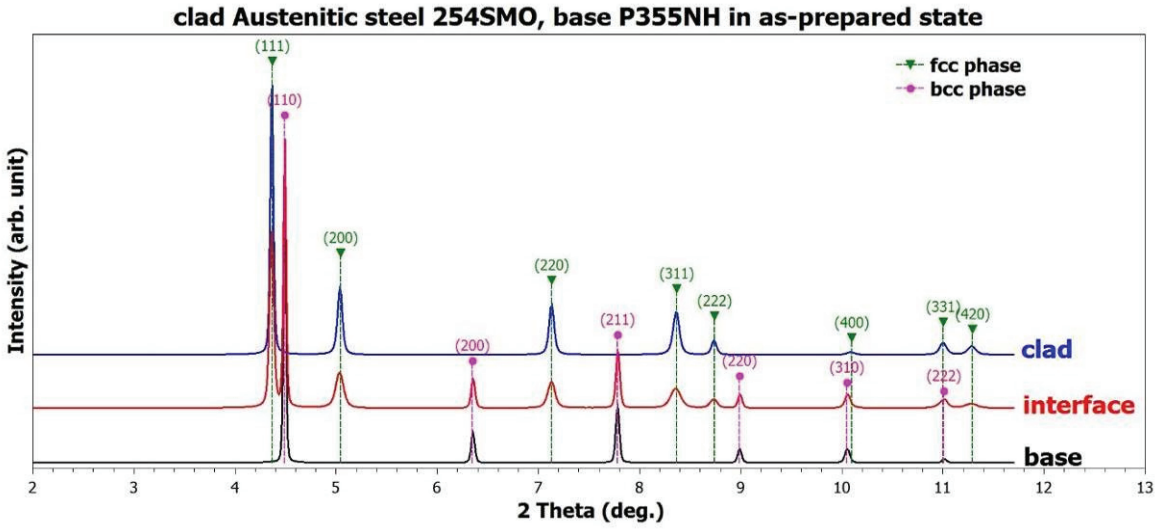

Figure 3 XRD patterns taken from different part of the bimetal

4.2. Residual strains in the material

Amount of elastic strains in the material (**Figure 4a-c**) was calculated applying the above described XRD[2] theory. For the analysis the Debye-Scherrer rings {222} of austenite and {220} ferrite were chosen because rings of the second order slip planes are well separated from the others and have similar interplanar distances of 0.10431 nm, 0.10141 nm and similar planar atomic densities of $1.769.10^{15}$, $1.719.10^{15}$ atoms / cm^2, respectively. The rings were radially integrated $I(2\theta,\gamma)$ in γ steps 1º over the whole azimuthal range 1 - 360º. The θ and d values were calculated from $I(2\theta,\gamma)$ peaks whose position was set to 2θ coordinate of the peak's centre of mass. The whole procedure was applied on 400 individual XRD patterns taken from a sample in the line scan.

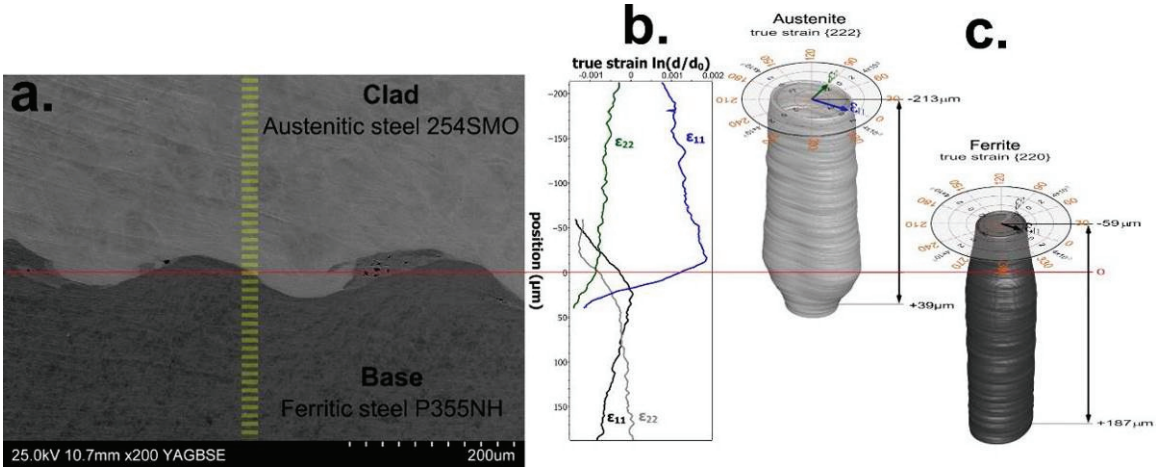

Figure 4 a. Metallographic cross-section of the bimetal, **b.** true strains distributions in the material, **c.** 3D polar plots of the true strains in the material

Figure 4c shows 3D polar plots of the true strains measured from the austenite and the ferrite phases. As one can see, they overlap in the joint region, where the materials are clinched to each other. **Figure 4b** shows plot

of the normal strain tensor components ε_{11} and ε_{22} obtained from the material along the scanned line. From the figure it is obvious that austenite is much more strained than ferrite showing maximal difference (elastic strain anisotropy) 0.28 % in place ~15 μm far from the centre of joint. The austenite "squeezed" in ferrite - the place on the top of the wave is hydrostatically compressed by 0.13 % in comparison to the stress-free sample.

4.3 Stresses in the material

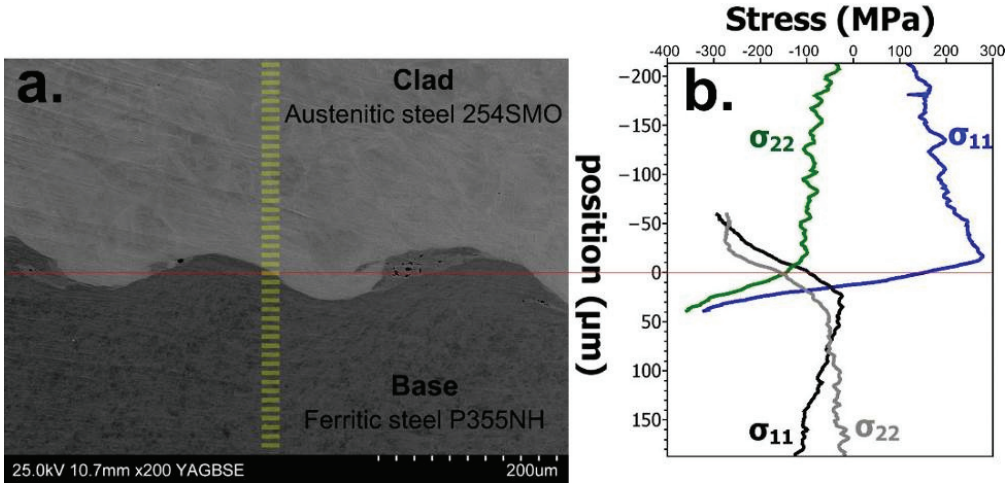

Figure 5 a. Metallographic cross-section of the bimetal, **b.** residual stresses in the material

Knowing strains, Young's modulus E and Poisson's ratio ν, of the materials one can calculate the residual stresses, see **Figure 5**. As one can easily notice, the material is simultaneously under tension and compression. Values of the normal stress components can reach as much as 360 MPa what is at the elastic limit of the austenite steel. More importantly, the difference in a narrow region between compression and tension can sum up to 640 MPa what is comparable to the strength limit of the 254SMO austenite steel (690 - 850 MPa).

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