Nuclear Instruments and Methods in Physics Research A 841 (2017) 12–16

Contents lists available at ScienceDirect

Nuclear Instruments and Methods in Physics Research A

journal homepage: www.elsevier.com/locate/nima

Sample positioning in neutron diffraction experiments using a multi-material fiducial marker

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ARTICLE INFO

Keywords:
Neutron diffraction
Strain scanning
Sample positioning
Artificial neural network

ABSTRACT

An alternative sample positioning method is reported for use in conjunction with sample positioning and experiment planning software systems deployed on some neutron diffraction strain scanners. In this approach, the spherical fiducial markers and location trackers used with optical metrology hardware are replaced with a specifically designed multi-material fiducial marker that requires one diffraction measurement. In a blind setting, the marker position can be determined within an accuracy of ± 164 μm with respect to the instrument gauge volume. The scheme is based on a pre-determined relationship that links the diffracted peak intensity to the absolute positioning of the fiducial marker with respect to the instrument gauge volume. Two methods for establishing the linking relationship are presented, respectively based on fitting multi-dimensional quadratic functions and a cross-correlation artificial neural network.

1. Introduction

1.1. Strain scanning using neutron diffraction

An inherent advantage of using neutron (and X-ray) diffraction techniques in the investigation of stresses in materials and components is the non-destructive nature of the measurements. Specific volumes are examined by the accurate positioning with respect to the instrumental gauge volume defined by the intersection of the primary and diffracted beam paths. The size and position of the respective beams are set by apertures. Internal strain caused by various inhomogeneous lattice displacement mechanisms is determined from the direct comparison of the measured diffraction peak position in the polycrystalline solid to its stress-free reference.

1.2. Traditional sample positioning

Accurate sample positioning with reference to the instrumental gauge volume is one of the most important parameters in diffraction based strain investigations. It is suggested that positional accuracy should typically be 10% of the largest dimension of the gauge volume in the diffraction plane [1]. Experience has shown that positional accuracy of about ± 0.5 mm can be achieved by aligning a sample with a laser and ± 0.2 mm by using theodolites. This can be further improved by performing neutron beam sample entry scans and fitting the diffracted intensity values as a function of relative position to an appropriate analytical solution [2] to give accuracies in the order of ± 10 μm. The method works well for samples with a simple geometrical shape, but becomes less efficient to apply for samples exhibiting an arbitrary form which may require multiple entry scans. This becomes time-consuming with subsequent loss of the useful beam time for strain investigations.

1.3. Advanced positioning methods

To speed up the sample alignment procedure, a number of alternative positioning methods have been reported of which two are briefly introduced:

Ratel et al. has proposed a 'direct sample positioning and alignment methodology' where a sample of arbitrary shape is mounted on an accurately machined baseplate and sample holder [3]. The baseplate can be rapidly repositioned on the instrument within ± 100 μm accuracy using locating dowels. By digitizing the sample and baseplate using a coordinate measuring machine (CMM), or laser scanner, most of the sample alignment and experiment planning can be performed off-line. A common reference point between the digitized sample plate and the physical instrument is determined by performing x, y and z

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http://dx.doi.org/10.1016/j.nima.2016.10.020
Received 19 September 2016; Received in revised form 4 October 2016; Accepted 10 October 2016
Available online 13 October 2016
0168-9002/

entry scans on an alignment pin mounted on a separate baseplate.

Strain Scanning Simulation Software (SScanSS), developed by the Open University, UK, facilitates arbitrary sample alignment, experiment planning and measurement automation [4]. SScanSS utilizes 3D computer models of the sample and instrument in combination with spherical fiducial markers and a CMM to determine the sample's position on the instrument to within ± 100 μm relative to a laboratory coordinate system.

2. Multi-material fiducial marker positioning

2.1. Considerations

Since not many neutron facilities have access to CMM's, an alternative method has been explored to determine the sample position within the SScanSS system approach. The hypothesis has been to replace the traditionally used spherical fiducial marker with a composite marker that can be directly measured with the neutron diffraction beam to determine its position. This eliminates the need of a CMM for positioning.

In order to resolve the marker position in three dimensions the following essential requirements have to be considered:

- The marker has to comprise three different materials, where each material defines a different orthogonal dimension with their intercept defining zero as a unique position;
- The materials need to render diffraction angles that are in close proximity to each other, but adequately separated, to enable their analyses from one instrument setting.

The neutron pathlength through the marker, the different scattering lengths and attenuations of the constituent materials, as well as the gauge volume filling fraction will be different for each position in the marker since the gauge volume is partially submerged in all three materials throughout. This will lead to a distinct ratio of peak intensities with respect to the marker position. The peak intensities can therefore be used to determine the marker position relative to the gauge volume.

This approach requires a *characterization dataset* of the instrument fiducial marker combination, against which, the position of subsequent blind setups can be determined from a single diffraction detector data frame measurement.

2.2. Marker composition and geometry

The multi-material fiducial marker (MMFM) selected for this feasibility study comprised three materials specifically chosen to have Bragg peaks close to 2θ=90° at a neutron wavelength of 1.646 Å as used on the Materials Probe for Internal Strain Investigations (MPISI) instrument at the SAFARI-1 research reactor in South Africa [5]. The MMFM shown in Fig. 1 consists of a 20×8×4 mm^3 sized beryllium slab attached to a 10×8×3 mm^3 sized mild steel (ferrite; α-Fe) slab, and an 8×8×8 mm^3 sized 316L-stainless steel (austenite; γ-Fe) cube. Table 1 indicates the expected Bragg peak positions from this composite sample.

2.3. Experimental procedure

The MMFM was precisely constructed and set up on MPISI as shown in Fig. 2. In this configuration the beryllium and mild steel are measured in transmission geometry and the stainless steel in reflection geometry. As the neutron pathlength remains constant through the material measured in transmission geometry, the intensity of the diffracted beam will only be a function of the filling fraction of the gauge volume. The diffracted peak intensity will systematically increase as the gauge volume moves deeper into the material and remain constant when the entire gauge volume is fully submerged in the material. In the reflection scattering geometry the neutron pathlength increases as the gauge volume moves deeper into the material. The diffracted intensity is now dependent on both the material neutron attenuation factor and the filling fraction. Subsequently, as the intercept gauge volume increases the diffracted intensity will correspondingly increase up to the position where it is fully submerged. The

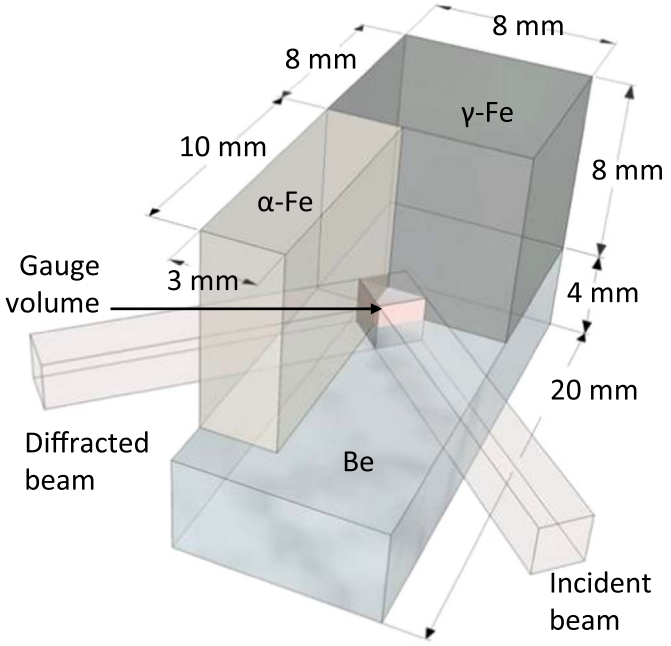

Fig. 1. Illustration showing the marker geometry and dimensions.

Table 1
MMFM diffraction peak positions when using 1.646 Å neutrons.

Material	Crystal plane	Diffraction angle (2θ)
Mild steel	211	88.6°
Beryllium	110	92.1°
316L Stainless steel	311	99.6°

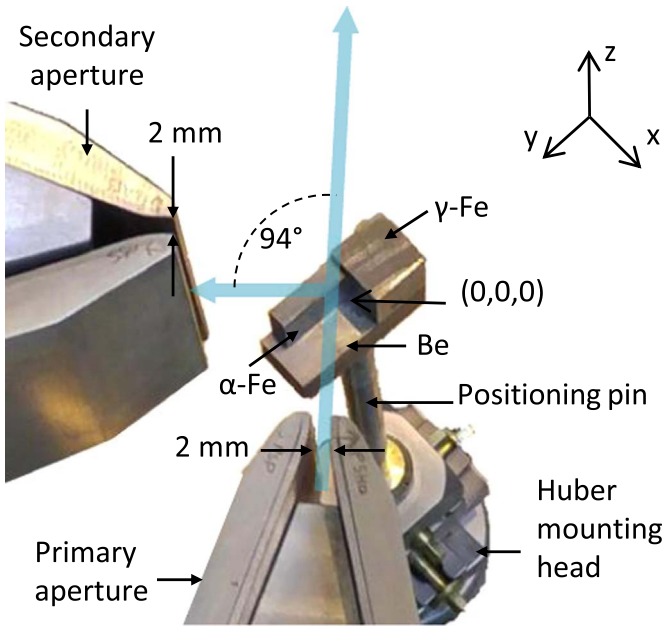

Fig. 2. Diagram showing the setup and positioning of the MMFM on MPISI.