

**TOWARDS A BETTER UNDERSTANDING OF GIUM MICROSTRUCTURE
CHARACTERISATION BY GRAIN-SCALE FINITE ELEMENT SIMULATION**

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ABSTRACT

We present numerical simulations of the grazing incidence ultrasound microscopy (GIUM) for microstructure characterisation of a coarse-grained austenitic weld. Comparing the results from different weld models with the experimental data, we draw some observations about the contrast mechanisms of GIUM.

Keywords: elastodynamic wave propagation, grain structure, EBSD, FEM, austenitic weld characterisation

1. INTRODUCTION

Experimental characterisation of the microstructure of coarse-grained materials is most often performed using costly and time consuming methods, such as electron backscatter diffraction. Several years ago an alternative approach, based solely on ultrasound, was presented [1,2]. Grazing incidence ultrasound microscopy (GIUM) was shown to be capable of extracting the grain structure by processing ultrasonic signals recorded with a laser vibrometer aligned along the normal to the propagation plane. The method can reveal details significantly smaller than the wavelength of the ultrasonic wave which is one of its main strengths. The additional information contained in the surface skimming ultrasonic wave was discovered during laser doppler vibrometry studies of the wave propagation and we think a reasonable explanation of the contrast mechanism was given [2]. It is the aim of this contribution to better understand the process of image forming in GIUM and hopefully support the claimed contrast mechanism.

2. MAIN IDEA AND PERFORMED WORK

The main idea of the present contribution is to reproduce the experimental GIUM procedure in a numerical model. Based on the microstructure obtained by EBSD measurements of the austenitic weld sample, we developed several grain-scale finite element models. The mesh was synthesised from the EBSD map and relevant crystallographic information was used to define the topology and the average orientation of the elastic tensor in each grain. Each EBSD measurement covers only a small area of the weld, hence a large number of ‘tiles’ needed to be stitched before full reconstruction. A series of filters applied to raw stitched data in DREAM3D [3] allowed for the detailed grain data to be extracted. Additionally, to retain better flexibility in generating the mesh we used the raster tessellation meshing facility from Neper [4].

To investigate deeper into the physical mechanism behind GIUM we constructed both a 2D and 3D model. The former represented the EBSD data directly; the latter was an extruded version of the same grain structure. Wave propagation simulations were executed using Pogo [5], a GPU-based finite element solver. The weld was insonified with a P-wave propagating across the plane of the weld (x-y), and the response was read along the normal to (z - 3D simulations) or over (x-y - 2D simulations) that plane. The data collected over a grid of points covering the whole cross-section of the weld was then fed into the GIUM data evaluation procedure.

Comparing the results from 2D and extruded 3D simulations allows us to get insight into the physical mechanisms beyond the revealed microstructure signatures, leading into a better understanding of the images obtained from experiments. Further, we simulate several other microstructural configurations assessing the effect of the parameters on the level of detail revealed by GIUM imaging.

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3. RESULTS AND DISCUSSION

As this is an ongoing work, at the moment of abstract submission we only mention the results of the 2D simulation. Fig. 1 shows the EBSD inverse pole figure of the investigated austenitic weld. The propagation of a longitudinal ultrasonic wave with frequency $f = 2$ MHz and a propagation angle of 45° (incident from the upper right corner in the figures) was simulated. Different components of the wave, namely particle displacement and strain, were used as an input into the GIUM procedure. Figure 2 gives the GIUM evaluation for the dilatation calculated from both the horizontal and the vertical components (the only components available in the 2D simulation). This can be compared to the GIUM result from the experiment in Figure 3.

At this point we summarise the observations gathered so far.

Both the GIUM evaluation based on the 2D numerical simulation and the GIUM evaluation of the experimental data show the same global grain structure (see especially the encircled area), but there are differences in the details. The contrast in the GIUM images depends on the wave signatures (displacement components and strain components) available as an input for evaluation. For the 2D simulation, from the tested quantities, dilatation produced GIUM images with apparently the best contrast (not shown). As observed already experimentally [1], the details in GIUM images depend on the propagation direction of the ultrasonic wave, which is now confirmed by the 2D simulation. Furthermore, acknowledging that shear waves are more sensitive to the microstructure, we simulated shear wave excitation and subjected resulting response to GIUM evaluation. However, in this case the GIUM image was distorted. We interpreted this distortion as a consequence of increased grain scattering interfering with the principles behind GIUM image synthesis described in [1, 2]. Moreover, mode converted pressure waves travel faster than the primary shear wave and overlay the image. In case of primary pressure waves there is scattering too, but the mode converted shear waves are slower as the pressure waves and can be well separated. Consequently, the GIUM evaluation algorithm reads the wavefront signatures of only one wave, and backwall-reflected waves do not influence the image.

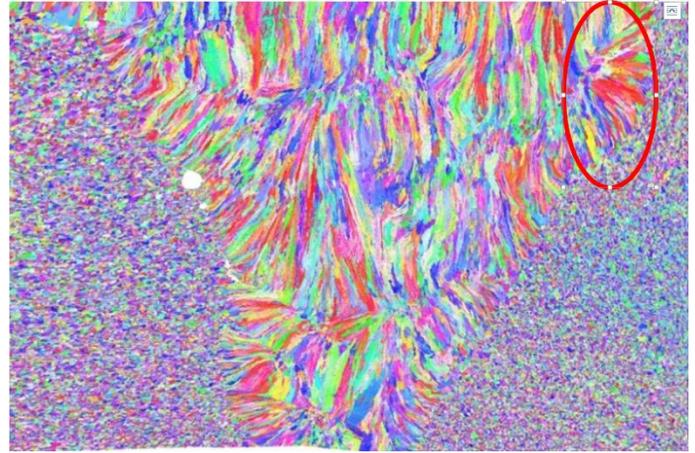


FIGURE 1: EBSD MAP OF THE GRAIN STRUCTURE OVER THE CROSS SECTION OF THE AUSTENITIC WELD

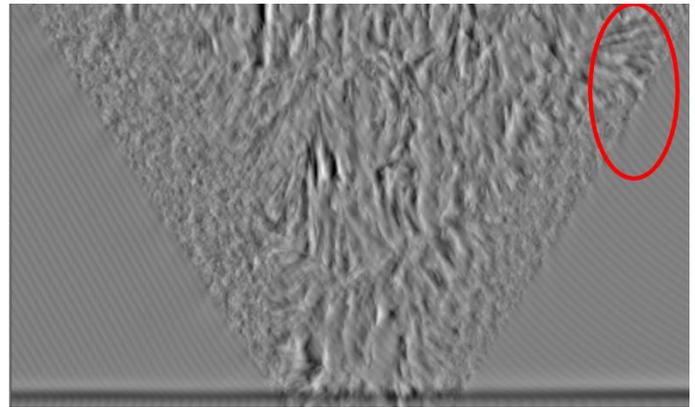


FIGURE 2: GIUM EVALUATION OF THE DATA FROM THE 2D FINITE ELEMENT SIMULATION

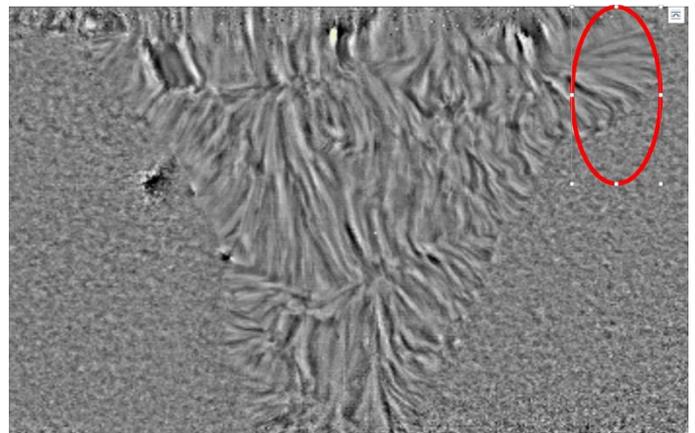


FIGURE 3: GIUM EVALUATION OF EXPERIMENTAL DATA

The 2D finite element simulation of the GIUM procedure gave already promising results. But let us recall the proposed GIUM contrast mechanism. An average strain in the pressure wave extends over several grains. The out-of-plane displacement at the free surface will depend on the orientation of the grain at a given position with respect to the wave propagation direction (the direction of the average strain) and with respect to the free surface. Therefore, the out-of-plane displacement will vary from grain to grain. The GIUM algorithm maps that variation. There is no “out of plane displacement” in the 2D simulation. We used the dilatation instead, but this might be not that grain orientation dependent. That is why we expect a significantly better agreement between 3D simulation and experimental GIUM. This simulation is running now (that is, at the time of the abstract submission deadline) and we will report about that at the conference.

4. CONCLUSION / FURTHER WORK

In this contribution, we reproduced GIUM microstructure mapping setup in numerical simulations and attempted at investigating deeper into the mechanisms behind GIUM image synthesis and the level of detail available. Based on the raw EBSD data collected from scanning an austenitic steel weld, we reconstructed the microstructure and generated finite element meshes. We simulated wave propagation across the weld both using a 2D representation and a full 3D setup. Displacements recorded over a grid of points were processed and fed into the GIUM evaluation procedure. We obtained good qualitative agreement between the experiment and the 2D simulation and provided explanation on the differences. Further, several other configurations were tested to reveal the effect of different excitation direction, wave type and microstructure characteristics on the level of detail available for GIUM. Full 3D simulations are underway and will be reported during the conference. Given that they represent the experimental setup more closely, they are expected to shed more light on the fundamental physics behind this imaging method.

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