

# Determination of microscopic residual stresses using diffraction methods, EBSD maps, and evolutionary algorithms

## Project Presentation

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## ABSTRACT

Residual stresses, both macroscopic and microscopic, are originated during conventional metallurgical processes. Knowing their magnitude and distribution is of great importance in the structural design of applications where fatigue, stress corrosion or thermal cycling occur (e.g., in the nuclear industry). The importance of these stresses is reflected in the large number of articles published in recent years, mainly focused on studying macroscopic stresses. However, there are no experimental studies that quantify the magnitude of microscopic triaxial stresses. This lack is due in part to the limitations of diffraction techniques (neutrons and synchrotron radiation). Since the measurement volume is much higher than the variation of these microscopic stresses, its calculation is greatly complicated, because the methods used in the case of macroscopic stresses are not valid for microscopic ones. Furthermore, there is no reliable procedure to obtain the relaxed lattice parameter value, a key factor in the calculation of residual stresses. The aim of this project is to develop a methodology for mapping microscopic stresses, particularly in aluminium alloys. The procedure will use experimental diffraction results from large European facilities, mainly by neutron diffraction, which will be analyzed using evolutionary algorithms, computational techniques that handle a large number of variables. The procedure will be based on the analysis of the displacements of the peaks of diffraction and, fundamentally, its widening.

## CCS CONCEPTS

• **Computing methodologies** → **Search methodologies**; • **Applied computing** → **Physical sciences and engineering**; • **Applied computing** → *Aerospace*;

## KEYWORDS

Aluminium alloys, Multi-objective optimization, EBSD maps

### ACM Reference Format:

J. Ignacio Hidalgo, Ricardo Fernández, Oscar Garnica, J, Manuel Colmenar, Juan Lanchares, and Gaspar González-Doncel. 2019. Determination of microscopic residual stresses using diffraction methods, EBSD maps, and evolutionary algorithms: Project Presentation. In *Genetic and Evolutionary Computation Conference Companion (GECCO '19 Companion)*, July 13–17, 2019, Prague, Czech Republic. ACM, New York, NY, USA, 2 pages. <https://doi.org/10.1145/3319619.3326769>

## DESCRIPTION

Periodically, Mass media report incidents at industrial facilities, oil platforms, factories, etc. Accidents such as bursting pipes, deposits collapsing due to corrosion or fatigue problems, and failures in various components which, before the end of the planned life cycle, fail suddenly and sometimes tragically. Those news usually do not focus on the technical details of the accident or its causes. Attention is mainly focused on the economic cost involved and, fundamentally, on the human factor; the people involved, injured or dead. Usually, there is a technical question behind the accident, such a bad design, an inadequate selection of the material. Undoubtedly, the detailed analysis of these faults and the knowledge of their cause has served to advance in new designs and to improve the performance of new components. These analyses are often complex and not always accurate. A reliable diagnosis requires a whole history of data on materials, their conditions of use, their microstructural characteristics, etc., information that is not always available. Therefore, it is common to resort to tolerance margins that alleviate the ignorance of these factors in anticipation of their possible relevance during the service life of the component. This is the area where the residual stresses are found. These stresses are generally present in materials and components. They are originated in the different stages of their manufacturing process. Whenever there is a non-homogeneous dimensional change (deformations and/or expansions), residual stresses are generated. In the case of macroscopic stresses, they can be determined without great complexity, but there are other stresses, the microscopic ones, whose magnitude is still unknown.

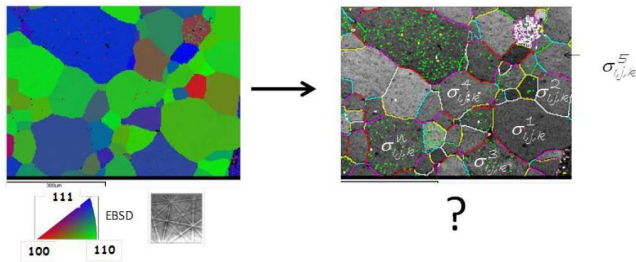
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GECCO '19 Companion, July 13–17, 2019, Prague, Czech Republic

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ACM ISBN 978-1-4503-6748-6/19/07...\$15.00

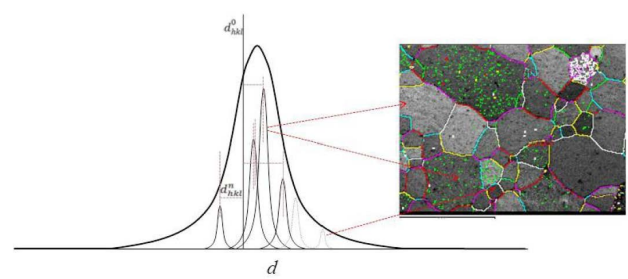
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**Figure 1: Map of individual orientations of a microstructure and the equivalent map of residual stresses to be determined. The first one is obtained by means of EBSD. The second will require diffraction peak data and evolutionary algorithms, as proposed in the project.**

However, their influence on the problems described may also be relevant. This project is focused on determining these microscopic stresses. Specifically, an attempt will be made to develop a procedure for mapping these microscopic stresses for structural materials. The different residual stresses in materials [1] are distinguished in the dimensional scale in which they are manifested. Although this scale differs in orders of magnitude, its amplitude, however, is not necessarily very different. In a first approach, these stresses are divided into macroscopic and microscopic. In order to understand the origin of microscopic stresses, it is necessary to delve deeper into the microstructure of the materials. These microscopic stresses are classified into intergranular (type II) and intragranular (type III). The microscopic stresses of type II (or mRS), which are of interest in this research, vary between neighbouring grains, as a consequence of the different degree of plastic (and elastic) deformation that a grain has suffered with respect to its neighbours during a given metallurgical process (e.g., rolling). The diffraction techniques used to calculate macroscopic stresses also reveal, albeit in different ways, the presence of microscopic stresses. Since the gauge volume is much larger than the grain size and these have different stresses, the effect on diffraction peaks is more complex as they experience displacement and widening. This circumstance entails an enormous difficulty in calculating the stresses of individual grains to the extent that it has not yet been possible to map the triaxial state of type II stresses. The EBSD technique, based on retrodispersed electrons, is the most convenient one for the study of micro-texture or the determination of the individual orientations of a significant number of crystalline grains. Some attempts have been made using EBSD maps, from the changes or distortions that occur in the Kikuchi lines as a result of a stress state, but is limited to 2D. The EBSD technique, however, will be essential in this study to determine the crystallographic orientation of the grain map whose stresses are being estimated. From the images of the micro structure we will obtain the following information:

- The number, size and aspect ratio of the grains. We will work with homogeneous structures, with the purpose of assuming only one size for all the grains.
- The macroscopic texture to establish the preferential orientations of the grains.
- The map of individual orientations of the grains of these microstructures. With this, it will be possible to associate



**Figure 2: Simplified description of the effect of the different stress of individual grains on the displacement and widening of the diffraction peak. Each peak is generated by a group of grains that have a given  $hkl$ , normal to the observation surface, but each grain has different stress.  $hkl$  identifies a plane, which is used as a reference to measure the strains in different regions of the sample.**

diffraction peaks of a specific  $hkl$  to specific grain collectives. The microtexture maps obtained by EBSD must be congruent with the macrotexture measurements.

With this information, which contains a large number of variables, it should be possible to determine the triaxial state of the individual grains, Figure 1, given appropriate assumptions. The objective is to obtain the stress tensor of each of the grains, which supposes 3000 variables for a microstructure with 1000 grains. This enormous size prevents the use of deterministic algorithmic techniques, since their execution time would be unaffordable. In this type of problems with such large search spaces, algorithmic techniques based on metaheuristics enable acceptable solutions to be found in affordable execution times. The search is carried out by assuming a relaxed value,  $d^0$ , of the lattice spacing of a given  $hkl$  plane, which is used as a reference to measure the strains in different regions of the sample. In addition, it must comply with those states of stress of the set of grains that meets certain conditions of mechanical equilibrium at the microscopic level. These algorithms have successfully solved the problem faced by this group of the stress state in a welded plate [1] [2].

**ACKNOWLEDGMENTS:** The work is supported by the synergic R&D projects in new and emerging scientific areas at the frontier of science and of an interdisciplinary nature, co-financed by the Operational Programs of the European Social Fund and the European Development Regional Fund, 2014-2020, of the government of Madrid, Project Y2018/NMT-4668 (Micro-Stress- MAP-CM)

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