Grain Boundary Engineering and $\Sigma 3^n$ Multiple Twinning

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1. Abstract

Grain boundary engineering (GBE) suggests that microstructures with a high fraction of "special" grain boundaries have better mechanical properties, like improved corrosion resistance, creep resistance etc. The special $\Sigma 3$ grain boundaries, generally resulting from twinning mechanisms by deformation or recrystallisation, are considered to be the "strongest" ones, and many engineers are trying to elaborate microstructures with a high density of $\Sigma 3$ grain boundaries and large Twinning-Related Domains (TRDs) [1]. TRDs are constituted by grains linked by twins or by twins of twins and so on, i.e. linked by $\Sigma 3^n$ grain boundaries [7]. In that aim, multiple twinned materials are characterised by Electron Back-Scattered Diffraction (EBSD) in a Scanning Electron Microscope (SEM) (see for examples [1],[2]). Although the $\Sigma 3^n$ grain boundaries are easy to identify for $n \leq 4$, there is no method to automatically identify them for higher twinning orders. Indeed, the distribution of the orientations of multiple twinned crystals is very dense and nearly isotropic for $n \geq 5$ [3], and consequently, it is very difficult to distinguish a random misorientation from a special $\Sigma 3^n$ one.

The present study reports the main results of a geometric/algebraic study on the $\Sigma 3^n$ grain boundaries; it explains the method to identify them and to reconstruct the TRDs from EBSD data [4]. Multiple twinning is represented geometrically by a 3D fractal (Fig.1)and algebraically by a groupoid (more details about groupoids are given in [5]). In this groupoid, the variants are the objects, the misorientations between the variants are the arrows between the objects, and the $\Sigma 3^n$ operators are the different types of arrows (expressed by sets of equivalent arrows). Different substructures of this groupoid can be equivalently introduced to encode the operations with strings, such as free groups [6][7] or semigroups [4]. In all the cases, the operators are expressed by sets of equivalent strings and their composition can be determined without any matrix calculation by string concatenations. The composition is multivalued. The composition table of the operators is very useful to identify the $\Sigma 3^n$ grain boundaries and the TRDs in the EBSD maps (Fig. 2). This approach is very similar to the one used to reconstruct the parent grain from EBSD data obtained on the daughter grains (for example the reconstruction of austenitic grains from the martensitic ones) [8]. We illustrate this theoretical approach with some experimental studies on the crystallographic environments of defects in copper interconnections lines.

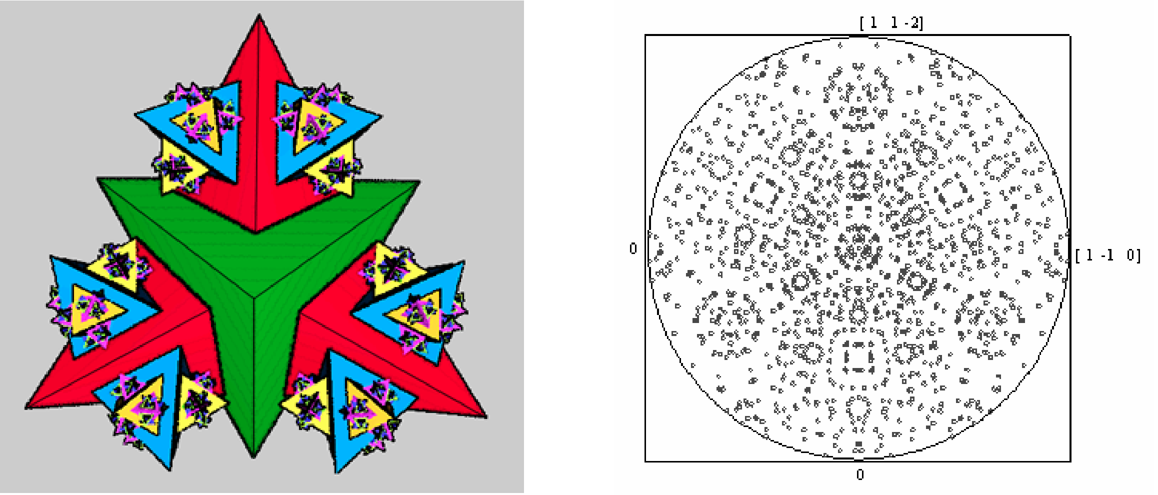

Figure 1 *- 3D fractal representation of $\Sigma 3^n$ multiple twinning and corresponding pole figure*

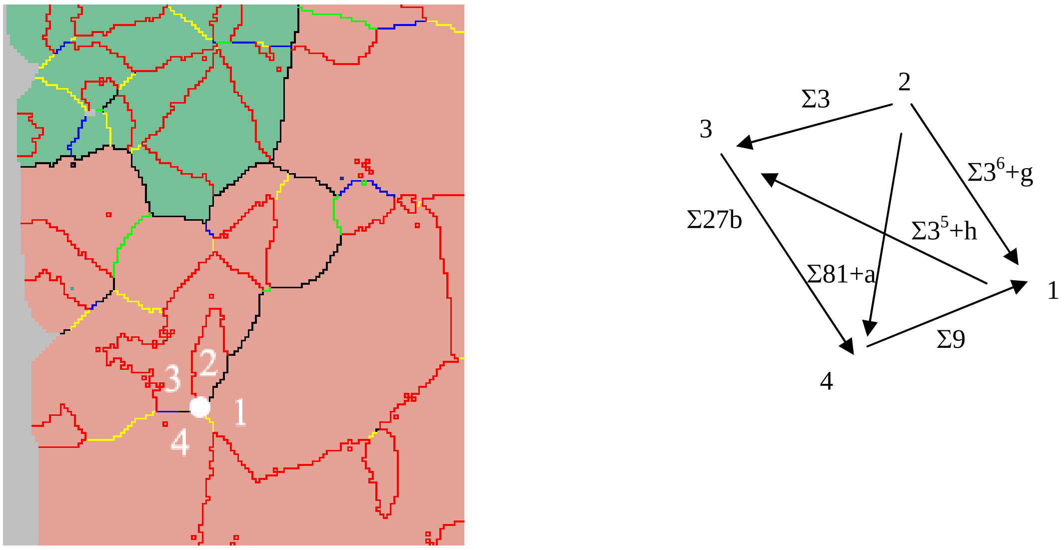

Figure 2 *- EBSD map around a void (the white disk) situated in the junction of four grains. In the figure, the $\Sigma 3$ boundaries are in red, the $\Sigma 9$ in yellow, the $\Sigma 27$ in blue and the $\Sigma 81$ in green. The higher order $\Sigma 3^n$ with $n \geq 5$ or the "random" boundaries are in black. The grains around the void are linked by the following rotationsidentifed to some $\Sigma 3^n$ operators by using the groupoid composition table.*

2. Références

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