Five-fold Branched Si Particles Studied with Orientation Imaging Microscopy

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Introduction

Many five-fold branched Si particles (Si_p) were observed in Al-40wt%Si functionally graded materials (FGMs) produced by a single step laser process on cast Al-alloy substrate (reference is made to our recent publications [1,2]). The fascinating result is that the five-fold branched silicon particles are much bigger in size (25~40µm) than the previously reported nanometer-sized particles in literature. Microstructural features of Si_p were scrutinized with orientation imaging microscopy (OIM with TSL software packages).

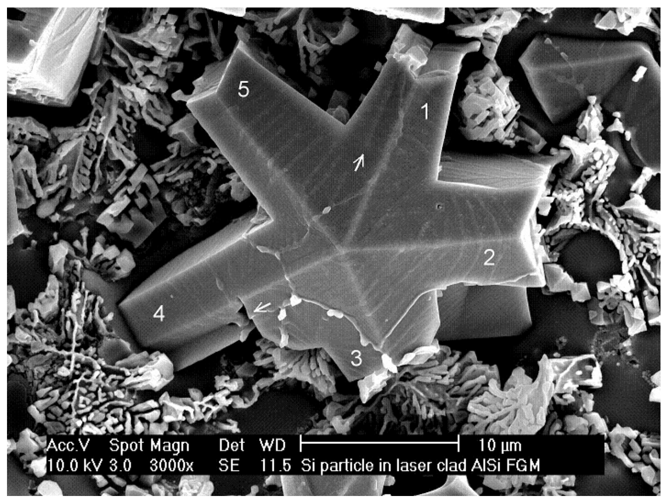

Figure 1 – SEM micrograph of a five-fold branched Si particle in laser clad AlSi40 FGM layer. The twins are numbered clockwise and the arrows mark extra re-entrant grooves.

Figure 1 shows a typical Si_p that was partially etched from the FGM layer to exhibit its three dimensional structure. Five flat faces are on the top of the particle and together five ridges are formed. The re-entrant growth groove at the branch tips is clearly demonstrated by the three-dimensional view, which intersects with the ridge at the center of the branches. It is interesting to note that the five-fold Si particle not only grows along the branched tips, but also thickens in the perpendicular direction, i.e. along the common [110] axis of the branches, pointing to the so-called twin plane re-entrant edge (TPRE) growth mechanism [3, 4].

In order to study the multiply twinned structure of the five-fold Si_p, OIM was applied. The crystallographic nature of these multiply twinned structures is notable because there is a 7.5° mismatch between the twinning structure and the five-fold branched structure. The accommodation of this mismatch is accomplished in two ways: 1) at a single twin boundary and 2) distributed among multiple constituent twin boundaries.

Single Twin Mismatch

An orientation map of a five-fold twinned Si particle is presented in Fig.2 (b). The Si particle consists of five twins that are represented by different colors, which are assigned on the basis of the local details of the lattice orientation as indicated by the inserted unit triangle of the inverse pole figure (IPF). In the pole figure depicted in Fig.2 (c), <110> poles of all the five twins are plotted on the projection plane of the sample coordinates TD and RD, with corresponding colors to that of the twins in Fig.2 (b). Similarly, <111> poles are plotted in Fig.2 (d). It can be concluded from Figs.2 (c) and (d) that the five twins share a common <110> axis and that they join through five <111>-twinning planes, which are located at the center of each branch. Such a configuration results in an angular mismatch of 7.5° because the angle between each pair of twinning planes is 70.5° and the total angle summed up to 352.5°.

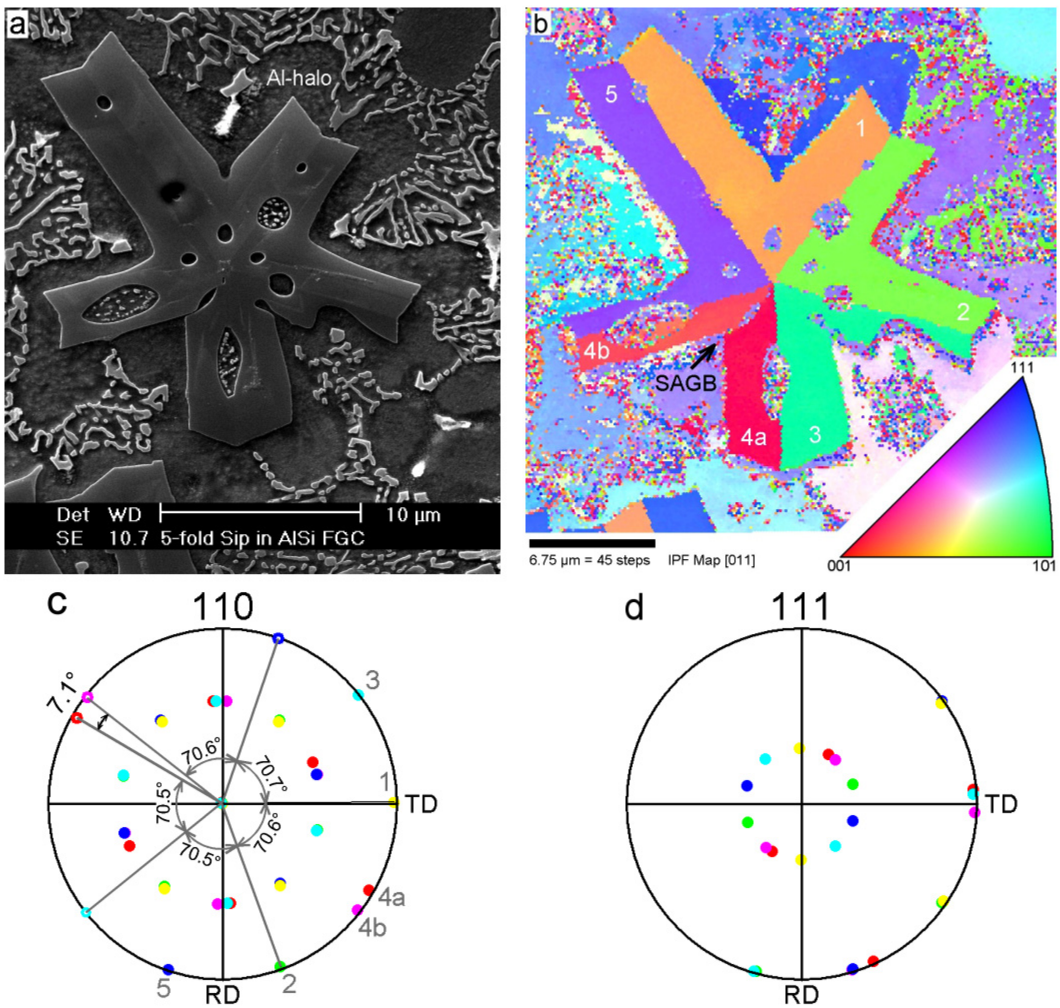

Figure 2 – Orientation imaging microscopy of a five-fold branched Si particle: (a) SEM micrograph; (b) [011] inverse pole figure (IPF) map showing the configuration of its five twins numbered clockwise. An arrow points to a single SAGB in the twin No.4. The inserted unit triangle of IPF indicates the color shading assigned to local orientation of the lattice and is valid for the following IPF map. (c) <110> pole figure showing the 7.1° tilt angle of the SAGB and the coincided <110> poles among all the twins aligned to the normal direction (ND) of the sample by rotating the scan data. The gray numbers indicate the corresponding twins. (d) <111> pole figure showing pairs of coincident <111> poles between two neighboring twins.

To answer the question how the 7.5° mismatch is accommodated in a five-fold twinned particle, we concentrated on the misorientation distribution over all the twins of a particle. The first possibility is identified with the particle displayed in Fig.2 where a single twin contributes nearly to the entire 7.5° mismatch. As one may note on Fig.2 (b), twin No.4 shows two parts with a slight difference in color, i.e. one in red and the other in red-orange. These two parts are distinguished from each other by a small angle grain boundary (SAGB) of about 7.1° misorientation (indicated with an arrow). This small angle misorientation can be more easily recognized from Fig.2 (c) where the two corresponding groups of <110> poles rotate 7.1° about their common <110> axis.

Distributed Twin Mismatch

Other examples of accommodation where the 7.5° mismatch is divided into two or more twins of a particle are more frequently observed. Fig.3 shows a particle exhibiting four SAGBs in four different twins and a further twinning in the twin No.5. The detailed misorientation distribution over each twin is visualized in Fig.3 (c) by mapping the misorientation of all scanning points on

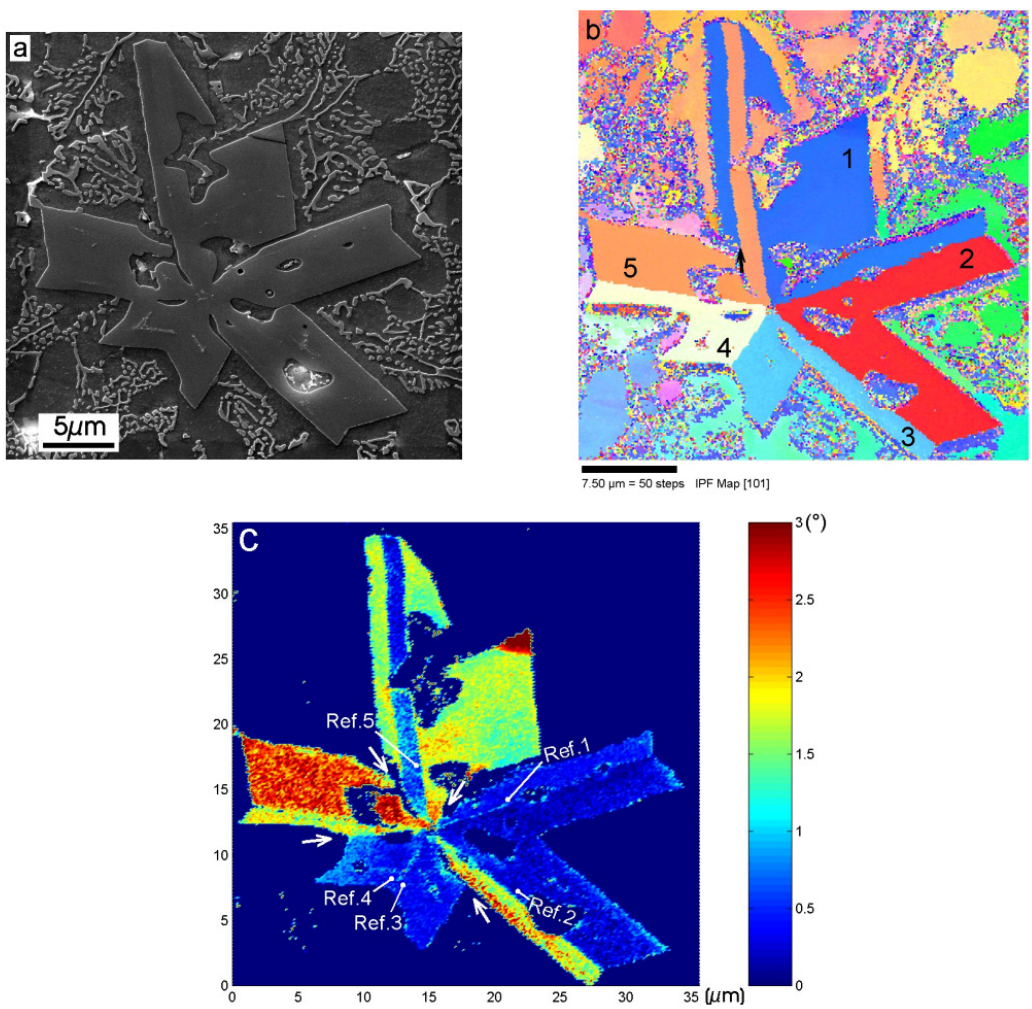

Figure 3 – Combined microstructure and crystallography analysis of a five-fold Si particle: (a) SEM micrograph of the particle. (b) [101] IPF map showing the five twins numbered clockwise and a further twinning in the twin No.5 indicated by an arrow. (c) Misorientation distribution of each twin drawn with respect to a definite reference point marked by a white circle. Arrows indicate the SAGBs in four different twins. The color-shading bar on right scales the misorientation angles.

a twin with respect to a definite reference point nearest to the twin boundary. Except for twin No.2, all the twins show the misorientation distribution in two parts such that, the part containing the reference point exhibits an average misorientation in the range 0.48° to 0.74° and the other part possesses an average misorientation between 1.78° and 3.05°. The misorientation difference between these two parts indicates that there is a small angle grain boundary (SAGB), which can be directly seen from the color difference inside the twins. The SAGBs originate from the center of the particle where the common 110 axis is located and terminate at the fork of the branched twins. The average tilt angles of the SAGB in twin No.1, 3, 4 and 5 are 1.30°, 1.92°, 1.70° and 2.31°, respectively. These four SAGBs contribute to a total deformation of about 7.2° and the rest of the mismatch is assumed to be elastic deformation.

Conclusions

The OIM results show that the 7.5° mismatch that arises when arranging five tetrahedrons around a common <110> axis is accommodated by small-angle grain boundaries (SAGBs). The mismatch is most frequently accommodated by multiple SAGBs as opposed to a single SAGB. The situation in which all five twins of a particle contained an SAGB was never observed. The SAGBs may disturb the progress of growth steps, causing the particles to branch. The most remarkable facts of this study are that the five-fold branched silicon particles are much bigger in size (25~40μm) than the previously reported sizes in literature of nanometer sizes. The examples of a single SAGB reported previously [5] are just a special case of the SAGB mechanism.

Bibliography

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