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# The topology of three-dimensional grain boundary network and its influence on stress corrosion crack propagation characteristics in austenitic stainless steel in a simulated BWR environment

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## ABSTRACT

The intergranular cracking and the grain boundary network along the cracks in an austenitic stainless steel 316L after stress corrosion cracking (SCC) test in simulated BWR water were investigated in terms of three-dimensional characterization. It was found that the twin boundaries not only show a strong resistance to cracking, but they could also prevent their neighboring boundaries from cracking, as the cracking probability is lower for boundaries that have higher fraction of neighboring twin boundaries. The propagation of intergranular SCC can be hindered by triple junctions or quadruple junctions in the presence of twin boundaries.

## 1. Introduction

Stress corrosion cracking (SCC) occurs in materials under the synergistic action of stress and a corrosive environment, as in the case of austenitic stainless steel in pressurized water reactor (PWR) or boiling water reactor (BWR) environment. After a long-term service at the reactor operating conditions or even new materials if heat-treating is not done properly, grain boundaries become a susceptible path to SCC initiation and propagation, and intergranular SCC (IGSCC) is a severe problem in the nuclear industry in particular [1,2]. Therefore, improvement of SCC resistance through grain boundary enhancement are getting more and more attentions in recent years [3–10].

In coincident site lattice (CSL) approach, the extent of grain-to-grain fit ( $\Sigma$ -value) between the atoms in the two grains is characterized by the reciprocal of the ratio of the number of ‘coincidence sites’ to the total number of sites. A coincidence site is one that is shared by both grains at the two sides of the grain boundary (GB). For instance, when  $\Sigma$  equals to 3, it means that there will be one atom for every three atoms that is shared by the two lattices. Therefore a boundary with low  $\Sigma$  would be expected to have a lower energy than one that has a high  $\Sigma$  [11]. GBs with different  $\Sigma$ -values have different lattice-structures and therefore different properties. The twin boundary (TB, i.e.  $\Sigma 3$  boundary) has lower boundary energy, and stronger resistance to impurities segregation/precipitation and intergranular degradation compared with random boundaries ( $\Sigma > 29$ ) [3–10,12]. So the concept of GB-

engineering [13–18] was proposed to improve the GB-related properties by increasing the proportion of special boundaries (low- $\Sigma$  CSL boundaries, boundaries with  $\Sigma \leq 29$ ) in materials. Many experiments [3–10,19–22] in high temperature or corrosive solutions have shown that the GB-engineered austenitic stainless steel and Ni-based alloy 690 had remarkably higher resistance to intergranular corrosion/SCC than conventional materials, because the proportion of low- $\Sigma$  CSL boundaries were increased to about 75% after GB-engineering from the original level, which was about 30 ~ 50%. However, all these studies were based on two-dimensional (2D) microstructure characterization of the tested alloys, using optical microscope (OM), scanning electron microscope (SEM) and electron backscatter diffraction (EBSD) mapping. GB character distribution in 3D microstructure and its relationship to IGSCC are rarely studied.

While 2D studies had shown that some special boundaries have stronger resistance to cracking during SCC test, the effect of these special boundaries on IGSCC was still not understood comprehensively in terms of crack propagation, because it is more important to study the topological characteristics of GB network rather than individual interfaces. The topological characteristics are correlated with not only the proportion of special boundaries but also the distribution of special boundaries in spatial GB network, and it really should be studied in 3D. It is generally found that the IGSCC propagates along random boundaries [3–5]. If the distribution of special boundaries is such a way that breaks up the long-range connectivity of IGSCC-susceptible random

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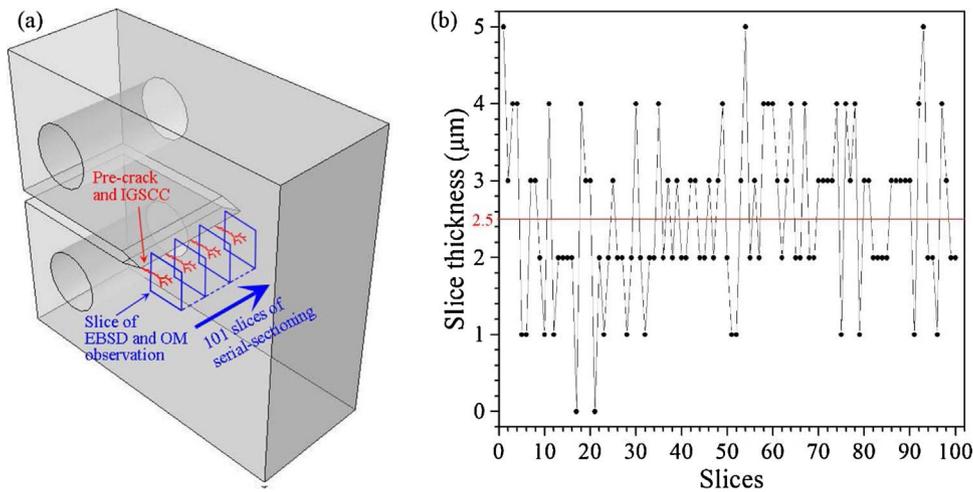


Fig. 1. (a) Schematically showing the slices of 3D characterization in the CT sample. (b) The thicknesses distribution of the total of 101 slices.

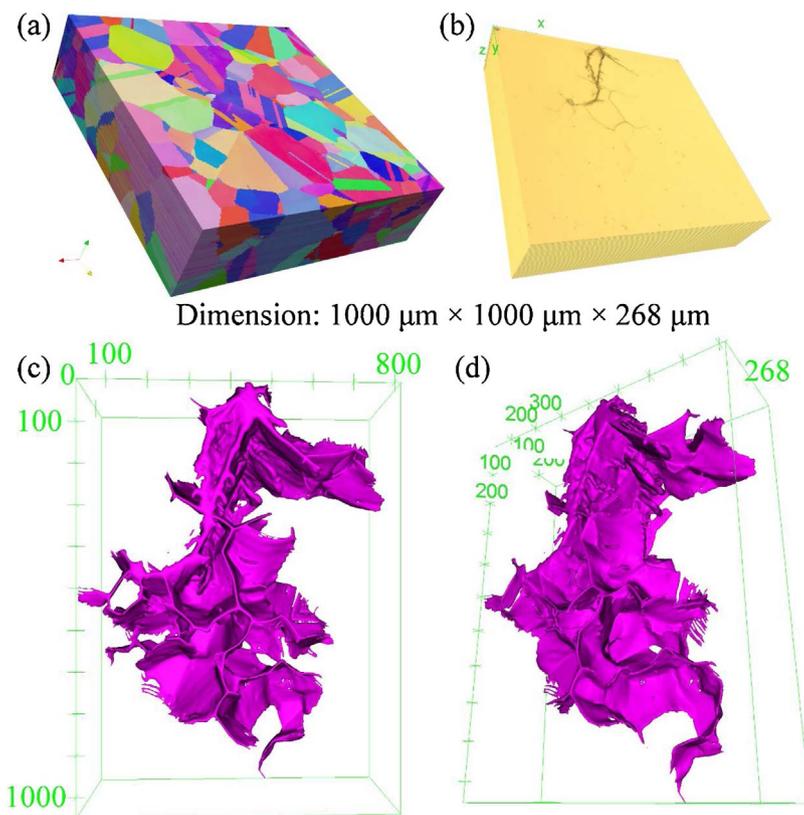


Fig. 2. Visualizations of the reconstructed 3D microstructures: (a) the reconstructed 3D-EBSD microstructure; (b) the reconstructed 3D-OM microstructure; (c, d) 3D visualizations of the IGSC crack from different perspective, which were drawn using the 3D-OM data in ImageJ 3D Viewer. (See supplementary file '3D-crack').

boundaries, it is generally expected to hinder IGSC propagation based on the percolation theory [9,22,23]. For example, triple junctions with two twin boundaries could stop the IGSC propagation [19,20]. However, how other types of topology structures of GB network affect crack propagation is unclear. For example, how the IGSC propagates through a quadruple junction. Quadruple junction [24–26] is a spatial structure so that it cannot be observed in 2D maps. Quadruple junction is an assembly of six boundaries between four mutually neighboring grains, and 3 is the maximum number of twin boundaries in quadruple junction [26]. The arrangement of twin boundaries in quadruple junctions should have significant influence on IGSC propagation. In addition, the observed connectivity of random boundaries depends on whether the observation dimension is 2D or 3D [23,27]. Simulation studies have shown that the connectivity of random boundaries could be broken when proportion of special boundaries is more than 35% in a 2D microstructure [28], but the threshold value is more than 80% for a

3D microstructure [23]. Therefore, further studies on GB network characteristics and their influence on IGSC propagation by using 3D microstructure characterization are needed.

In the present paper, the microstructure and crack of a 316L stainless steel after SCC test in a simulated BWR environment were investigated in three-dimensional by using 3D-EBSD and 3D-OM. Attention was particularly paid to the propagation of cracks through quadruple junctions in the presence of twin boundaries.

## 2. Material and experiments

### 2.1. Material

The material used in this work is a low-carbon austenitic stainless steel 316L with a chemical composition of 17.16 wt.% Cr, 11.90 wt.% Ni, 1.32 wt.% Mn, 2.08 wt.% Mo, 0.028 wt.% C, 0.37 wt.% Si,

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