

# The Influence of Crystallographic Orientation on Grain Nucleation, Part 1: Development and characterisation of a model alloy

H. Landheer<sup>1</sup>, S.E. Offerman<sup>1</sup>, W.G. Sloof<sup>1</sup>, N.M. van der Pers<sup>1</sup>, R. Petrov<sup>2</sup>, and L.A.I. Kestens<sup>1,2</sup>

<sup>1</sup>Department of Materials Science & Engineering, Delft University of Technology, Rotterdamseweg 137, 2628 AL Delft, The Netherlands  
<sup>2</sup>Department of Metallurgy and Materials Science, University of Ghent, Technologiepark Zwijnaarde 903, 9052 Zwijnaarde, Belgium

## General Abstract

The steel industry has problems manufacturing products with a constant quality, because of a lack of knowledge of the processes after casting and hot rolling. When these processes are fully understood, industry can control the steel production process completely and use the expertise to develop materials with advanced mechanical properties, like higher strength and better formability.

## Technical Abstract

The mechanical properties of a metal depend on the microstructure, which is the result of a phase transformation, initiated by nucleation. Nucleation takes place at high grain boundary energy sites, which are generated by the misorientation between neighbouring austenite ( $\gamma$ ) grains. For the examination by Electron BackScattering Diffraction (EBSD) of this influence, a high purity iron alloy with 20 w% Cr and 12 w% Ni is examined.

## Introduction

The nucleation rate strongly influences the kinetics of phase transformations and recrystallisation processes that determine the final microstructure and thereby the mechanical properties of the material. Clemm & Fisher<sup>1</sup> found that in terms of grain boundary energy, quadruple junctions are the most favourable sites for nucleation. However, not all quadruple junctions are used and nucleation also happens at interfaces. According to the pillbox model of Lange et al.<sup>2</sup> the grain boundary energy is the total of the interface energy between the  $\gamma$  grains and the interphase energy between the ferrite ( $\alpha$ ) and  $\gamma$  grains. The coherent faces have an orientation relationship of  $\{111\}_{\gamma} // \{110\}_{\alpha}$ , whereas the semi-coherent faces have an arbitrary misorientation.

## Objective

The energy of the austenite/ferrite ( $\gamma/\alpha$ ) interface can be estimated by measuring the crystallographic orientation and the shape of the boundary. To exclude all other influences, like precipitates, the examined material must have high purity. The experiments will be done at RT, and both  $\alpha$  and  $\gamma$  have to be present. Therefore, a carbon free dual phase high purity iron alloy with 20 w% Cr and 12 w% Ni has been developed for these experiments, which will be examined with EBSD to find the factors that influence ferrite nucleation during phase transformation. The results will be used for a model to predict nucleation during phase transformation.

## Preliminary results

The transformation behaviour of model alloy Fe20Cr12Ni has been characterised. The as-received, heavily deformed material was first homogenised to be fully austenitic after quenching and heat-treated at 600°C (873 K) for 15, 66 and 20 hours to obtain a microstructure with 5-10% ferrite. However, no ferrite was observed in the XRD-spectra. Possibly only recrystallisation of the  $\gamma$  phase has occurred.

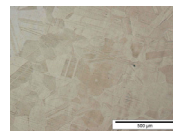


Fig. 1: Microstructure of homogenised Fe20Cr12Ni, fully austenitic; twins.

Fig 2: (a) SEM picture of the microstructure of homogenised Fe20Cr12Ni; (b) Orientation Map (OM) of the microstructure in (a); (c) Legend for the OM in (b).

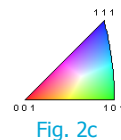
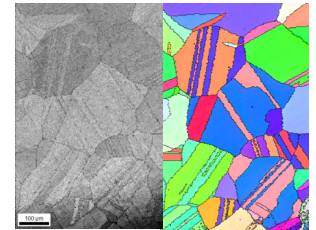


Fig. 2c

Fig. 3: XRD-spectrum of heat-treated samples Fe20Cr12Ni. Possibly, recrystallisation has occurred during heat treatment, of which the higher intensity of the crystal planes is proof.

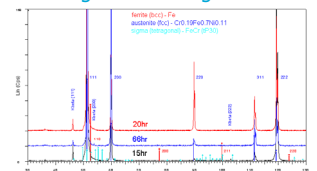
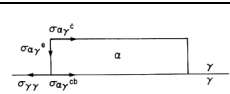
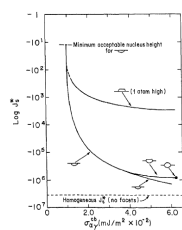


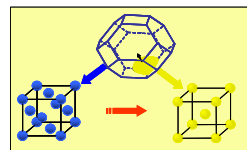
Fig. 3



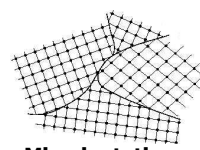
The **nucleus in the pillbox model<sup>1</sup>** grows with a coherent face (OR) and two semi-coherent faces (misoriented).



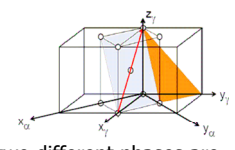
The **nucleation activation energy ( $\Delta G^*$ )** is defined as  $\Psi/\Delta g_v$ .  $\Psi$  comprises the nucleus/parent phase interface energy and the geometry of the nucleus. The models of Clemm & Fisher<sup>1</sup> and Lange et al.<sup>2</sup> predicted  $3.3 \times 10^{-3} \text{ J}^3/\text{m}^6$  and  $2.1 \times 10^{-6} \text{ J}^3/\text{m}^6$ , respectively. Recently, the experimental results of Offerman et al.<sup>3</sup> give  $\Psi = 5 \times 10^8 \text{ J}^3/\text{m}^6$ .



A **phase transformation** is the transition of one crystal structure into another. **Picture:** face centred cubic (fcc) ( $\gamma$ ) to body centred cubic (bcc) ( $\alpha$ ), with bcc nucleating at an fcc grain corner.



**Misorientation:** The difference in orientation of the crystal lattices between the grains.



When two different phases are oriented, such that certain crystal planes and directions are parallel to each other they have an **orientation relationship (OR)**. **Picture<sup>4</sup>:**  $(011)_{\alpha} // (111)_{\gamma}$ ,  $\langle -1-11 \rangle_{\alpha} // \langle -101 \rangle_{\gamma}$ , also known as the Kurdjumov-Sachs OR.

<sup>1</sup>Acta Met. 3, 70, 1955; <sup>2</sup>Met. Trans. 19A, 1988, 247; <sup>3</sup>Science 298, 1003, 2002; <sup>4</sup>Araz Barani, MPIE, Düsseldorf, Germany