In situ synchrotron X-ray imaging of the crystal growth of Si containing high and low levels of light impurities

Hadjer Ouaddah, Mame Cor Sané, Maike Becker, Isabelle Périchaud, Guillaume Reinhart, Gabrielle Regula, Nathalie Mangelinck-Noël

Aix Marseille Univ, Université de Toulon, CNRS, IM2NP, Marseille, France

Aiming to the production of low cost and high efficiency crystalline silicon based solar cells for photovoltaic (PV) applications, current research focuses on several key targets among which the optimization of silicon growth processes, to improve the crystalline quality of the final ingot. Three alternative technologies have recently been proposed to master the initial grain nucleation and defect generation at the bottom of the crucible during the first stage of solidification: the dendritic casting method, the mono-like solidification (ML-Si) and the high performance multi-crystalline silicon (HP mc-Si).

All those growth techniques share challenges to improve the final PV properties. It concerns the control of the final crystalline grain structure, the decrease of the density of structural defects, namely dislocations, and the control of the impurities that interact with the crystalline features during crystal growth. However, the *post-mortem* study of the solidified ingots is limited by the difficulty of accessing and understanding the mechanisms occurring during the crystallization, their symbiosis or competition and their kinetics.

Within this context, our contribution consists in characterizing the fundamental growth mechanisms of crystalline silicon using *in situ* X-ray imaging in a unique device named GaTSBI (**G**rowth at high **T**emperature observed by X-ray **S**ynchrotron **B**eam **I**maging). Two imaging characterisation techniques are combined during silicon growth using X-ray synchrotron radiation at ESRF (European Synchrotron Radiation Facility, Grenoble, France): X-ray radiography and X-ray Bragg diffraction. The X-ray radiography method brings information on the morphology and kinetics of the solid/liquid (S/L) interface. The X-ray Bragg diffraction gives additional information about the evolution of the grain shape and structure, the defect formation and the local level of crystal lattice distortion during growth.

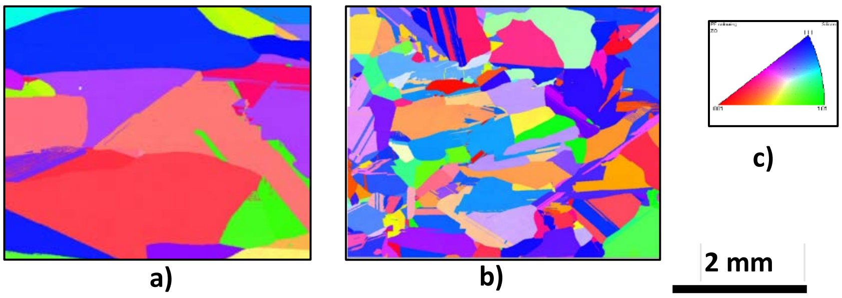

Figure 1. *Inverse pole figure (IPF) along the growth direction obtained by EBSD: a) Sample D ([C] = 0.21 ppmw, [C_s] = 0.4 ppmw, [O] = 0.058 ppmw, [O_i] = 3.5 ppmw, [Cu] = 0.28 ppmw), c) Sample B ([C] = 3.1 ppmw, [C_s] = 2.1 ppmw, [O] = 0.098 ppmw, [O_i] = 3.1 ppmw), c) Grain orientation legend.*

Using both imaging modes, essential features of twinning and grain competition in crystalline silicon are characterized. Complementary *ex situ* techniques are used to investigate the crystallographic orientation of the grains in particular, EBSD: electron backscattered diffraction. Besides, the contribution of the light impurities is studied by measuring their concentration and distribution using FTIR: Fourier Transform Infra-Red spectroscopy in relation to the crystalline structure. The main focus of the present contribution is the grain structure formation in relation to the presence of two light impurities frequently found in silicon material: carbon and oxygen. It is shown that the presence of light impurities increases the grain density (Fig.1). Moreover, a clear evolution from a high proportion of Σ3 twin grain boundaries to higher order twin boundaries and random grain boundaries is observed when increasing the light impurity concentration. Grain boundary type role in dislocation emission and development is also discussed knowing that dislocations are major defects regarding electrical properties.