Correlation of grain structure, impurities and electrical properties in photovoltaic silicon using in situ and ex situ techniques

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Silicon (Si) remains the most used material for photovoltaic solar cells with a market share over 90%. However, the fabrication methods of Si ingots including the most advanced ones face common challenges in order to improve the resulting PV efficiency of the solar cells. Some of the main issues are related to the crystallization of Si and to the control of defect generation. In particular, it is essential to understand the formation and, as a further step, to control the final grain structure, to decrease the density of structural defects, such as dislocations, and to understand the role of impurities that interact with the crystal structure during growth.

In this work, two types of samples have been studied: model laboratory scale-samples containing different kinds and levels of impurities characterized by *in situ* X-ray imaging during their solidification, and samples issued from large ingots grown by industrial processes. The growth of crystalline silicon is characterized using the *in situ* X-ray imaging a unique device named GaTSBI (**G**rowth at high **T**emperature observed by X-ray **S**ynchrotron **B**eam **I**maging) at ESRF (European Synchrotron Radiation Facility, Grenoble, France). Both techniques recording data during solidification, radiography and Bragg diffraction, allow revealing the morphology and kinetics of the solid/liquid interface as well as the defect formation and crystal lattice distortion during growth. These methods provide precise knowledge about the fundamental mechanisms of growth and of defect formation during growth. Moreover, contactless minority carrier lifetime maps of selected samples containing different levels of impurities and showing different crystalline structure arrangements are determined by the microwave phase-shift (µw-PS) technique. A comparison between the lifetime measurements by µw-PS (Figure 1-b) and the crystal and defect structure and, e.g., the coincidence site lattice map (CSL) calculated from EBSD measurements (Figure 1-a) is carried out. Presence of light impurities, such as O and C, is found to increase the grain density. In addition, there is a clear evolution from a high proportion of ∑3 twin grain boundaries to higher order twin and random grain boundaries when the light impurity concentrations are increased. Furthermore, the results show the influence of metallic impurities such as copper (Cu) on the electrical properties.

X-ray spectroscopy photoemission followed by surface photovoltage experiments were performed on identical areas of the sample at Soleil Synchrotron in order to evaluate the level of Cu impurity and to measure the relative electrical activity of grain boundaries, respectively (Figure 1).

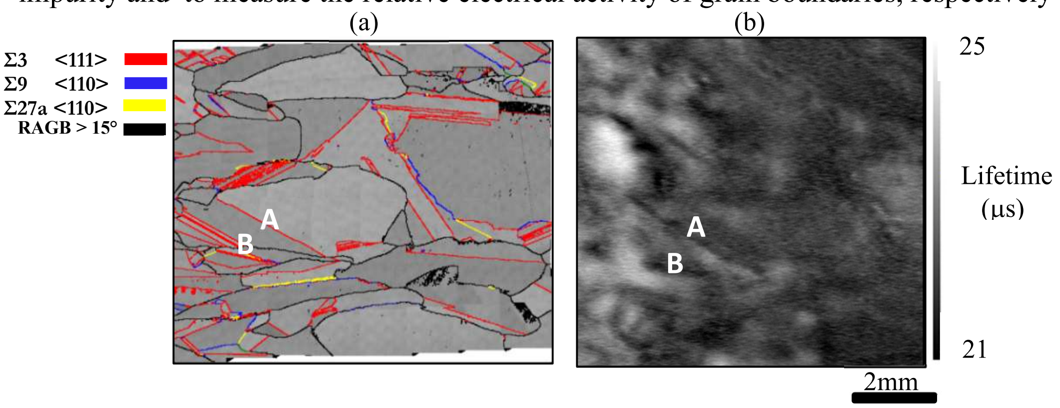

Figure 1*: Silicon sample grown by cold crucible casting process :(a) CSL map showing different grain boundary types; (b) lifetime map obtained by microwave phase shift, without surface passivation. The scale is the same for a) and b). A: active ∑3 twin grain boundary, B: active random angle grain boundary.*