Correlation between the presence of structural defects, impurities and the electrical activity in silicon for photovoltaic applications

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During the fabrication of Si crystalline material for photovoltaic (PV) solar cells, several factors such as thermomechanical stresses, crucible and impurity contamination are at the origin of deformation, structural defects and impurity segregation [1,2] which can ultimately degrade the electrical properties. In this work, we combine complementary structural, chemical and charge transport investigations that are respectively carried out by EBSD (Electron Backscattered Diffraction), SIMS (Secondary Ion Mass Spectrometry), FTIR (Fourier-Transform Infra-Red spectroscopy), PL (Photoluminescence) and SPV (Surface Photovoltage). Correlating these techniques enables to better understand the dependence between structural defects, impurities and charge transport.

Figure 1 presents structural and interstitial oxygen composition maps of the same region of a Si wafer characterised by the presence of sub-grain boundaries (sub-GBs) and grain boundaries (GBs). It can be seen that sub-GB and GB positions on the EBSD map (Figure 1 left) are correlated to the local distribution of interstitial oxygen (Figure 1 right). FTIR and μ FTIR characterisations indicate that light impurities segregate preferentially at the level of the structural defects, forming micro-precipitates, whereas inside the grain, oxygen is predominantly found in interstitial position. The experimental investigations conducted on Si material of several origin and with different levels of impurity contamination show how the presence of defects of different dimensions, from dislocation to grain size, influence the charge recombination in silicon, and consequently, degrade the solar cell quality and efficiency all the more as they interact with impurities.

References:

[1] J. Huang *et al.*, Growth and Defects in Cast-Mono Si for Solar Cells: A Review, physica status solidi (a) (2022) 2200448.

[2] H. Ouaddah *et al.*, Crystal distortions and structural defects at several scales generated during the growth of silicon contaminated with carbon, ActaMaterialia 252 (2023) 118904.



Fig. 1. Grain and sub-grain boundary EBSD map, b) Interstitial oxygen composition map obtained by μ FTIR in the same area.