Modeling the role of grain boundaries on electrical activity in $Cu_2ZnSnSe_4$ solar cells

D. Cozza, C.M. Ruiz, D. Duché, M. Pasquinelli, J.J. Simon and L. Escoubas
Aix Marseille Université, CNRS, IM2NP UMR 7334, 13397, Marseille, France
S. Giraldo, A. Pérez-Rodríguez, E. Saucedo
IREC, Catalonia Institute for Energy Research, Jardins de les Dones de Negre 1, 2ª, 08930 Sant Adrià del Besòs, Spain

Kesterite based photovoltaics is a promising thin film technology with the potential of future large scale production: $Cu_2ZnSnSe_4$ absorbers are made of cheap/earth-abundant elements and present optimal band gaps (between 1 and 1.5 eV) for solar cells. Devices with efficiency higher than 11% have been demonstrated by different groups. Nevertheless, performances are still far away from the other technologies of the thin film family, in particular a significant V_{OC} deficit impairs the final efficiency of the devices.

One of the possible origins of these limitations can be the electrical activity on the grain boundaries. While on CIGSe the mechanism of passivation of grain boundaries are understood, there are still much to do on the kesterite case. In particular, some studies in literature suggested that the Grain Boundaries (GBs) inside the polycrystalline absorber can play a dominant role as a source of V_{OC} loss [1].

In this work, we employ 2D modeling and the software Silvaco® to perform electrical simulations of $Cu_2ZnSnSe_4$ solar cells structures including GBs inside the absorber and a $MoSe_2$ layer between the absorber and the Mo back contact. The GBs are modeled both as thin vertical and horizontal stripes presenting different properties and physical mechanisms than the surrounding Intra-Grain kesterite: lower bandgaps, higher recombination, presence of static charges (positive or negative) and n-conductivity; these different conditions are considered both independently and combined. The analysis of the results gives an insight about the possible correlations between the electrical activity of GBs and their impact on the performances of the device.

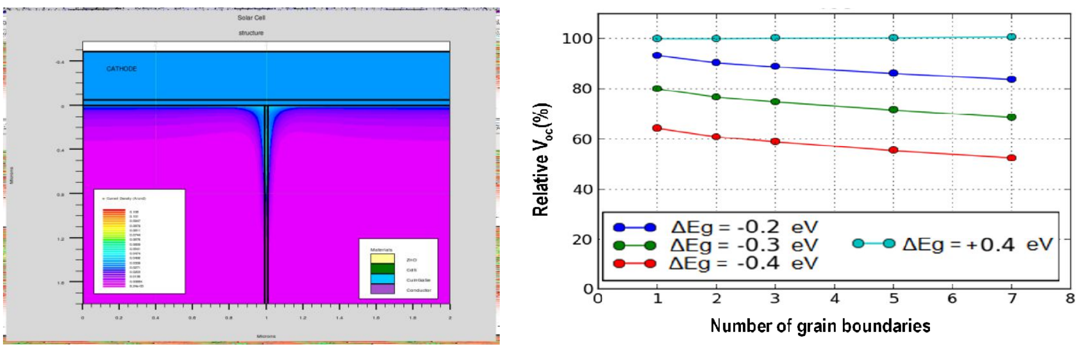

Fig 1: On the left, plot of the current density near a grain boundary. On the right, the relative loss of V_{oc} as a function of number of grain boundaries.

[1] A. Kanevce, I. Repins, S.-H. Wei, "Impact of bulk properties and local secondary phases on the $Cu_2(Zn,Sn)Se_4$ solar cells open-circuit voltage", Solar Energy Materials and Solar Cells, Volume 133, pp119-125, 2015.