Interpretation of a capacitance in polycrystalline solar cells: time domain simulations

Konrad Wiśniewski
Faculty of Physics
Warsaw University of Technology
konrad.wisniewski.dokt@pw.edu.pl

***Abstract*—In this work, we presented simulations of capacitance of polycrystalline solar cells using time-dependent calculations based on the finite element method. Our starting point was capacitance transient measurements of thin-film CIGS solar cells, which to this day, after twenty years of investigations, do not have the correct theoretical description. We showed, that there exists a model that can be used to explain experimental data, however, it will be not valid without further modification, which will incorporate grain boundaries in it. We developed our software based on deal.ii C++ library using Local Discontinuous Galerkin Method (LDG) and Mixed Finite Element Method (MixFEM) to check how spatial defects can influence the performance of thin-film devices. The results of simulations show that (i) even grain boundary set in parallel to current flow can significantly change properties of a solar cell and the interpretation of its capacitance and that (ii) presence of barriers set perpendicular to current flow, can be indeed responsible for capacitance transient which we know from experiment.**

***Index Terms*—solar cells, LDG, MixFem, capacitance, transient, grain boundaries**

I. Introduction

In standard interpretation, solar cells should work as perfect pn-junction, but nowadays a lot of modern devices deviate significantly from their archetype. CIGS solar cells can be used as an example. One of the longest disputes in the field of these thin-film devices concerns its capacitance characteristics, especially the behavior of their capacitance during pulse response of the system occurring in Deep Level Transient Spectroscopy (DLTS). This very powerful technique is used extensively for the detection and characterization of deep defects in semiconductor junctions. However, if applied to more complicated structures the interpretation of DLTS signals faces serious difficulties. Standard theory, as well as existing simulation software, does not provide a proper procedure to calculate transients in polycrystalline structures containing spatial defects such as grain boundaries. In the article [1] we show, that if secondary barriers are an origin of experimental capacitance dependencies, then a current flow over those barriers cannot be described by thermionic emission theory - otherwise this current will be too high. The simplest way to improve previous calculations was to use the diffusion transport theory. The comparison between simulation and experiment is shown in Fig. 1.

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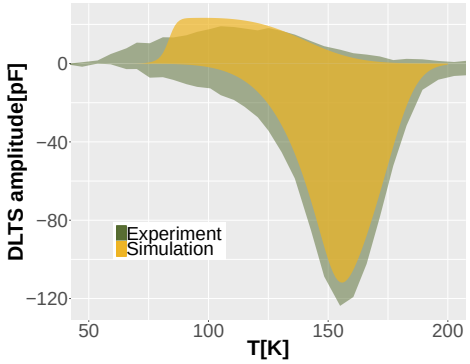

Fig. 1. Comparison between simulation and experimental data from DLTS experiment. The experimental data were multiply by 3; the mobility used in simulations was $\mu_h = 2 \cdot 10^{-7}(cm^2/Vs)$. This plot was created based on analysis of capacitance transient after voltage step: upper part from 0V to -0.5V and the bottom part from -0.5V to 0V.

Unfortunately, in this new framework decent fit to experiment can be achieved only when the holes mobility is very low, in some samples even lower than $10^{-6}cm^2/Vs$. Those results suggest that what we observe as mobility is not a physical parameter of a material, but it reflects a complicated internal structure of a device. As derived in [2] such a low mobility can be a consequence of an additional trap states located on the grain boundary.

II. 2D simulations

The method proposed in [3] was used to calculate IV- and CV-curves, as well as capacitance transient in solar cells. This method solves Poisson equation and continuity equations consecutively, by using the Mixed Finite Element Method and Local Discontinuous Galerkin Method respectively. The deal.ii finite element library was used with a connection with UMFPACK direct solver similarly as in [3]. The time was updated via an implicit-explicit time-stepping algorithm, where recombination parts were treated explicitly. Only a first-order time discretization scheme was considered.

Three geometries were simulated. Each of them combined pn-junction with a different secondary barrier: i) Schottky barrier (e.g. between absorber and back electrode), ii) horizontal grain boundary set parallel to current flow Σ^{II} and iii) vertical grain boundary set perpendicular to current flow Σ^{I}.

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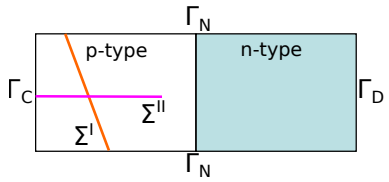

Fig. 2. The sketch of a physical domain of polycrystalline solar cells. Left and right border represents electrodes - Γ_D: Ohmic metal contact, Γ_C: Ohmic contact with the presence of grain boundary (Σ^I or Σ^{II}), or Schottky junction without them. The top and the bottom border were simulated by Neumann boundary conditions which did not allow current flow outside of a device.

The sketch of a structure is shown in Fig. 2. Grain boundaries were represented as an additional thin layer ($0.1\mu m$), with donor-like traps characterize by a single energy level situated in the middle of the bandgap. A horizontal grain boundary does not touch the border of pn-junction to prevent leakage current.

Two main parameters were describing a state of a system: uncompensated charge in p-type material Q, and total current I. The calculations were terminated when a current reach the accuracy: $\epsilon = 1\mu A$. An exponential character of capacitance decay was assumed to determine this moment. The derived condition for the change of the value of the current is then: $\Delta I < \epsilon\tau^{-1}\Delta t$, where: τ is a characteristic time of a decay and Δt is a current time step. The value of τ was approximated and set before the start of the simulation.

The capacitance was calculated by looking at the derivative of parameter Q with respect to potential: $C = \frac{\Delta Q}{\Delta V}$ (where ΔV used in simulations was 1mV) in some specific time Δt_C. Inversion of Δt_C can be ascribed to the frequency of alternating current at which the capacitance would be measured in an experiment.

III. Results

There were two main goals concerning two-dimensional calculations. First, to check if in the framework of the finite element method there will be possible to recreate the results from Sec.I (e.g. to check if capacitance will increase with time after voltage step from -0.5V, to 0V). Second, to check how horizontal grain boundaries will change capacitance measurements. Fig. 3 shows that indeed Schottky barrier will cause a capacitance transient, but what is more, the fact that the capacitance is measured only within specific time Δt_C, will distort measurements even further. Fig. 4 shows the doping profile derived from CV-cures, which can deviate significantly from the reference profile (without traps on grain boundary).

Those two examples show, that without a proper understanding of the physics of spatial defects and the way they influence capacitance there is impossible to propose a reasonable physical model of a polycrystalline solar cell. The better tool distinguishing between point and spatial defect is needed to achieve higher energy conversion efficiencies.

IV. Limitations

The main drawback of the method used in this article is that it works only for small time steps. The real transients last

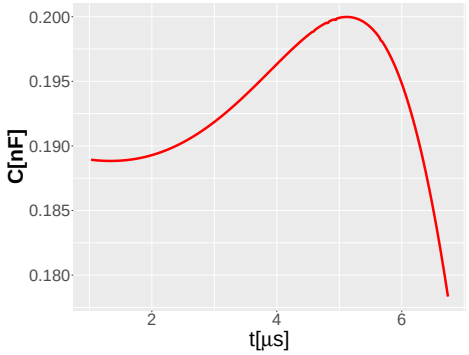

Fig. 3. Capacitance transient after voltage step from -0.5V to 0V in 300K in a structure containing Schottky junction. The first part of the transient, when capacitance increase, is caused by the change in potential on the Schottky junction which will increase with time. The second part results from the way the capacitance is calculated - it is not connected to any physical phenomenon.

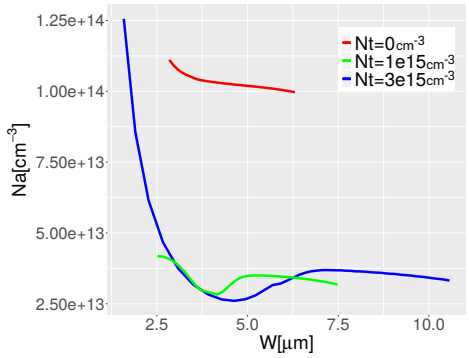

Fig. 4. Doping profiles for three different trap densities on grain boundary.

for milliseconds or even longer, while the most common time step used in calculations was 0.1ns. Without an algorithm that will enable adaptive time-stepping, there is impossible to trace all transient.

Negative charge density appears in the region with the biggest spatial derivative of charge density. It does not influence global parameters significantly, however, it is unphysical.

In the case of simulations of a structure with a vertical grain boundary, the amplitude of the voltage step was limited to the tenths of volts. There was possible to check that vertical grain boundary work similar to the Schottky junction, but a direct comparison with the experiment was not possible.

References

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