The diode factor in solar cells with metastable behaviour

Susanne Siebentritt, Thomas Paul Weiss, Taowen Wang, Valentina Serrano-Escalante
Laboratory for Photovoltaics, Department of Physics and Materials Science, University of Luxembourg

It is well known, that the diode factor (or diode ideality factor) has a strong influence on the fill factor and thus the efficiency of a solar cell. Several models exist to explain diode factors of the complete solar cell, where it is important if the dominant recombination occurs in the neutral zone or in the space charge region and if the absorber is doped [1,2]. This diode factor of the complete device depends on the properties of the absorber, as well as on the contacts. Photoluminescence (PL) offers the possibility to determine the diode factor of the absorber alone by studying the excitation dependence of the PL intensity [3-5]. Naturally, this is the diode factor of the neutral zone. Thus, in a doped semiconductor one would expect a diode factor of 1. If the main recombination channel is through highly asymmetric defects, the minority carrier lifetime can become excitation (or injection) dependent and the diode factor increases [6]. This diode factor increase is due to a non-linear behaviour of the minority carrier concentration with excitation.

Many semiconductors have defects that show metastable behaviour, i.e. under excitation they change their charge state and it takes thermal excitation over a potential barrier, and thus usually long times, for the defects to go back into its equilibrium state even after the perturbation has been removed. In particular, in $Cu(In,Ga)Se_2$ metastable behaviour has been observed as persistent photoconductivity [7,8]. A defect – most likely the Cu-Se double vacancy [9] – changes upon electron capture from a donor state to an acceptor state. The return to the donor state requires rather high activation energy, leading to light soaking and persistent photoconductivity. Such metastable behaviour leads to an increase in the majority carrier concentration (in low injection conditions) and thus to a diode factor larger than 1 [10]. In this case, the increase of the diode factor is due to changes in the majority carrier concentration. This change can be directly observed by CV measurements with light soaking.

The exact extend of the diode factor increase depends on the doping level and on the presence of other major recombination channels. Diode factor measurements are thus suitable to identify the presence of competing recombination channels. The limitations of the fill factor for the final device efficiency can be assessed for the PL measurements of the absorber layer alone.

[1] R. Scheer and H. W. Schock, *Chalcogenide Photovoltaics: Physics, Technologies, and Thin Film Devices* (Wiley-VCH, 2011).
[2] S. M. Sze and K. K. Ng, *Physics of Semiconductor Devices* (John Wiley and Sons, New York, 2007).
[3] T. Trupke, R. A. Bardos, M. D. Abbott, and J. E. Cotter, Applied Physics Letters **87**, 093503 (2005).
[4] F. Babbe, L. Choubrac, and S. Siebentritt, Solar RRL **2018**, 1800248 (2018).
[5] S. Siebentritt, T. P. Weiss, M. Sood, M. H. Wolter, A. Lomuscio, and O. Ramirez, Journal of Physics: Materials **4**, 042010 (2021).
[6] J. Schmidt, A. Cuevas, S. Rein, and S. W. Glunz, Prog. Photovolt. Res. Appl. **9**, 249 (2001).
[7] M. Igalson, M. Cwil, and M. Edoff, Thin Solid Films **515**, 6142 (2007).
[8] U. Rau, K. Weinert, Q. Nguyen, M. Marmor, G. Hanna, A. Jasenek, and H. W. Schock, Mat. Res. Soc. Symp. Proc. **668**, H9.1 (2001).
[9] S. Lany and A. Zunger, J. Appl. Phys. **100**, 113725 (2006).
[10] T. P. Weiss, F. Ehre, V. Serrano-Escalante, T. Wang, and S. Siebentritt, Solar RRL **2021**, 2100063 (2021).