Light-induced degradation and defects in amorphous and microcrystalline silicon - a new approach to an old problem with novel EPR techniques

K. Lips[1], J. Behrends[1], B. Rech[1], M. Brandt[2], M. Stutzmann[2], O. Astakhov[3], F. Finger[3], R. Bittl[4], K. Holldack[5], Ch. Freysoldt[6], J. Neugebauer[6], A. Schnegg[1]

[1]Hahn-Meitner-Institut Berlin, Abt. Silizium-Photovoltaik, Kekuléstr. 5, 12489 Berlin, Germany
[2]Technische Universität München, Walter-Schottky-Institut, Am Coulombwall 3, 85748 Garching, Germany
[3]Forschungszentrum Jülich, Institut für Energieforschung - 5, Photovoltaik, D-52425 Jülich, Germany
[4]Freie Universität Berlin, Fachbereich Physik, Arnimallee 14, 14195 Berlin, Germany
[5]Berliner Elektronenspeicherring - Gesellschaft für Synchrotronstrahlung mbH (BESSY), Albert-Einstein-Str. 15, 12489 Berlin, Germany
[6]Max Planck Institut für Eisenforschung, Max-Planck-Straße 1, 40237 Düsseldorf, Germany

In materials applicable for photovoltaic energy conversion, in particular thin-film silicon, impurities, defect states and light-induced structural changes can drastically influence the solar conversion efficiency. Knowledge about the genesis and structure of defect states is a necessary prerequisite for optimisation strategies leading to thin-film solar cells with higher efficiency. Defect states in solids are often paramagnetic; this renders Electron Paramagnetic Resonance (EPR) the method of choice to get nanoscopic insight into their structural and functional properties. In spite of the success of EPR spectroscopy in elucidating defect structures and impurities in the field of energy research, recent EPR studies were limited by insufficient spectral and time resolution as well as detection sensitivity. This situation dramatically changed with the advent of novel multi-frequency EPR spectrometers and detection schemes, which allowed EPR specotroscopists in recent years to determine highly desired information about spin coupling parameters inaccessible until then.

In order to exploit and further develop the outstanding potential of advanced EPR techniques for solar energy research, an interdisciplinary German network is established that follows a strategy which comprises

- the application of top of the line high-field EPR techniques, multi frequency (electron nuclear double resonance, electron double resonance, high field/ high frequency) and indirect (pulsed electrically and optically detected resonance; pEDMR and pODMR, respectively) detection schemes to amorphous (a-Si:H) and microcrystalline silicon (µc-Si:H) to get a detailed picture of their defect states and impurities in absorber materials and solar cells,
- mapping the electron spin density distribution of amorphous and crystalline defect structures by density functional theory based calculations of the respective magnetic interaction parameters.
- the development of novel instruments and detection schemes leading to unmatched spectral, temporal and spatial resolution as well as sensitivity in the detection of defect states,
- the proof of concept of a THz-EPR spectroscopy using coherent IR-radiation with frequencies from 30 GHz to 3 THz as is supplied by a unique BESSY operation mode.

In this presentation we will give a brief review of the basic contributions of EPR to the current understanding of defects and defect creation in a-Si:H and µc-Si:H and discuss in detail the limitations of the currently discussed defect models. An introduction to the various EPR-based methods is given and first experimental results on THz EPR using synchrotron radiation and pEDMR will be given. It will be discussed how these novel methods with their unprecedented spectral and spatial resolution and detection sensitivity will be able to boost the knowledge about the nanoscopic picture of defects in thin-film silicon.