EPR

EPR to Improve Solar Cells Quality and Performance

Application Note

Innovation with Integrity

Introduction

In the past three decades photovoltaic (PV) modules have experienced an average price reduction of 20% for every doubling of the accumulated sales. The availability of sufficiently pure silicon or polymers (for organic PVs) has been an important limiting factor for rapid growth. Therefore, there is a strong need for low-cost technologies for production of silicon and polymer synthesis for PV applications. However, such low-cost production will most likely compromise the purity of the resultant silicon or polymer. It is crucial to have accurate specifications for concentrations of defects and impurities without risking the production yield and cost targets, and achieving shorter energy pay-back times.

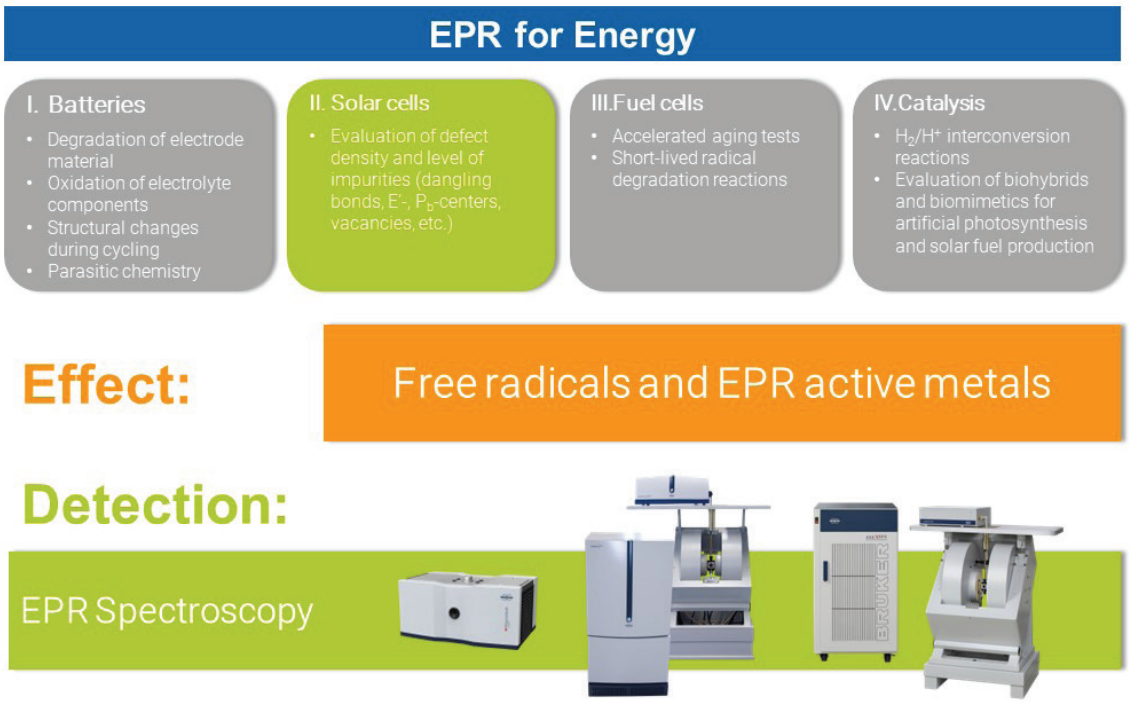
Paramagnetic defects and impurities in PV materials include:

- E' centers in SiO_2
- Atomic H^0 in SiO_2 or c-Si
- Dangling bonds (P_b centers at Si-SiO_2 interfaces)
- Grain boundary defects
- Intra grain defects
- Transition metals
- Free radicals

Challenge: It is not possible to remove all defects and impurities from photovoltaic materials. Evaluating the defect density and level of impurities during the production process is important for solar cell efficiency.

EPR solution:

- Detecting and quantifying structural defects and traces of impurities that affect the electrical properties of PV
- Monitoring processes that result in degradation of semiconductor properties



Influence of deep defects on device performance of thin film poly-Si solar cells

Thin films with high electronic quality are a prerequisite for the development of next generation silicon-based thin film solar cells. Numerous polycrystalline Si (poly-Si) thin film approaches on glass have been explored in a quest to produce crystalline thin film solar cells that can compete with state-of-the-art Si wafer-based solar cells. However, it is known that the open circuit voltage (V_{OC}) for poly-Si solar cells is significantly lower compared to wafer-based Si solar cells. EPR studies on solid phase crystallized Si solar cells revealed that deep level paramagnetic defects are major recombination centers in poly-Si and hence the most important limitation of the electronic quality of poly-Si. Conclusions based on EPR:

- Grain boundary and intra-grain defects are often present in poly-Si solar cells
- With the Bruker SpinCount module defect concentrations (defect density N_s) can be determined
- Post-deposition treatments (SPC, RTA, HP) improve electronic qualities - an increase in V_{oc} correlates to a decrease of the defect density
- EPR confirms that poly-Si solar cells performance limitation correlates to the density of paramagnetic defects

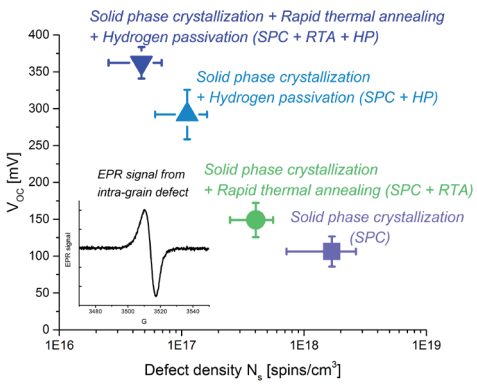


Figure 1: Performance of thin-film poly-Si solar cells as a function of defect density. Reproduced from reference [1] in accordance with Creative Commons Attribution 4.0 License.

Identifying intra-grain and grain boundary defects in polycrystalline Si thin films

Having shown that paramagnetic defects are limiting the device performance of poly-Si solar cells, it is important to discuss the microscopic origin of the observed defects in order to identify them. The intra-grain and grain boundary defects in polycrystalline Si films can be characterized by employing quantitative EPR measurements on liquid phase crystallized layers with an average grain size of 200 µm and tailored solid phase crystallized Si layers with similar intra-grain morphology but systematically varied grain sizes between 0.25 µm and 1 µm. The defect characteristics are found to be composed of signals with two distinctive g-values: g = 2.0055 and 2.0032, which are attributed to grain boundary defects and intra-grain defects, respectively.

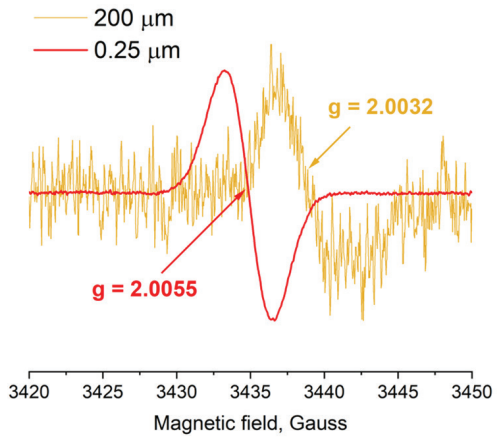


Figure 2: EPR spectra of polycrystalline Si film with 0.25 µm and 200 µm large grains. EPR data revealed the existence of intra-grain defects located at g = 2.0032 (dark yellow) and grain boundary defects at g = 2.0055 (red trace). Reproduced from reference [2] in accordance with Creative Commons Attribution 4.0 License.

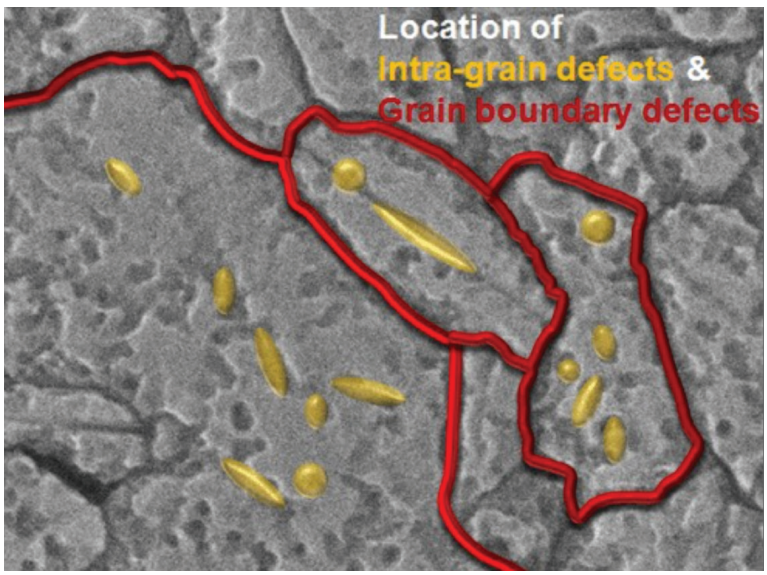


Figure 3: Scanning electron microscopy (SEM) image of poly-Si film. The two types of defects identified by EPR are shown in dark yellow and red colors. Reproduced from reference [2] in accordance with Creative Commons Attribution 4.0 License.

Perovskites: a new avenue of research and development for low-cost and high-efficiency solar cells

In recent years, the perovskite structure has shown great prospects in photovoltaic cells and energy storage applications. The perovskite-based photovoltaic cells have a low cost and long lifetime. These types of solar cells possess desirable features such as tunable bandgaps, excellent light absorption capacity, high charge carrier mobility, and have remarkably improved their power conversion efficiencies (PCEs). However, perovskites suffer from extrinsic defects at their interfaces and grain boundaries, ultimately affecting the perovskite film crystallinity and making their structure in solar cells susceptible to decomposition. The types of paramagnetic defects and their concentration in the crystal lattice is successfully studied by EPR.

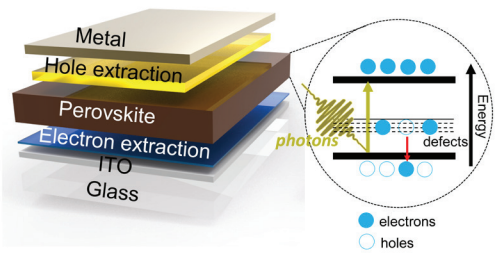


Figure 4: Schematic of a perovskite solar cell. Reprinted from the website of Okinawa Institute of Science and Technology (OIST) graduate university in accordance with Creative Commons Attribution 4.0 License.

Focused-ion-beam induced paramagnetic defects in perovskite films

Ion beam irradiation is known to induce structural changes such as phase transitions and amorphization. Under focused ion beam irradiation conditions, EPR detects isolated and localized paramagnetic spins in perovskite films containing manganites. These defects show Curie behavior at low temperatures (5 to 50 K), which is indicative of localized electrons at the defect sites.

Detecting and identifying the types of defects and their distribution by EPR is important to enable researchers and manufacturers to find appropriate solutions to eliminate them. The use of perovskites in energy storage applications has shown very promising results not only in solar cells but also as electrodes in fuel cells and air batteries as well as electrolytes in solid-state lithium-ion batteries. As a result, the aspect of defect engineering may tune these novel materials for a better understanding of their light-harvesting properties.

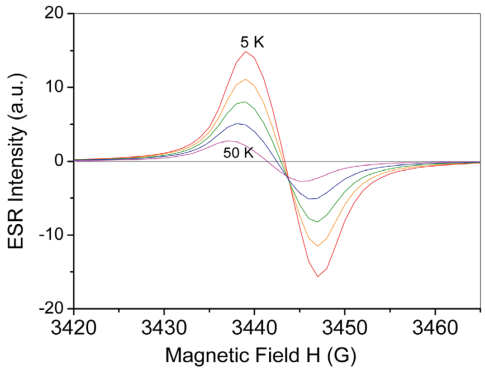


Figure 5: Temperature dependence of the EPR spectra of focused beam irradiation induced defect center in perovskite films. Reproduced from reference [5] in accordance with Creative Commons Attribution 4.0 License.

References:

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