Research Project #23

Impact of ion bombardment on photovoltaic materials (IMD-3 & IFN-1)

Solar cells and modules constitute a fundamental component in the transition towards a sustainable and carbon-neutral energy system, while simultaneously remaining cost-effective. Achieving the 'net-zero emission by 2050' target necessitates an average annual growth of 25% in photovoltaic (PV) energy generation until 2030, culminating in a total installed PV capacity of 5 TW by that year. [1] To facilitate this substantial growth and installed capacity, continuous advancements in the power conversion efficiency of solar cells and modules are imperative. Such improvements are essential not only for further reducing electricity costs, thereby expanding potential applications, but also for mitigating land use conflicts with agricultural or residential areas. Consequently, ongoing research and development of both current and next-generation solar cell materials are crucial.

At present, crystalline silicon solar cells predominate in the market. [2] Among these, architectures utilizing hydrogenated amorphous or nanocrystalline silicon as contact layers, known as silicon heterojunction (SHJ), exhibit the greatest potential for power conversion efficiency. [3] Perovskites have emerged as the most promising next-generation materials, either as independent devices or in conjunction with silicon in a perovskite-silicon tandem (PST) configuration. Both SHJ and PST structures require transparent conducting oxides (TCOs) to facilitate efficient charge carrier extraction and establish low-resistive contact with the metallization. Typically, these TCO materials are deposited via sputtering, a process in which particles ejected from a solid target material bombard the sample, forming a thin film. Regrettably, this process can degrade the SHJ structure or perovskite materials, resulting in reduced device voltages and power conversion efficiencies. While the degradation in SHJ solar cells can be mitigated, perovskites suffer irreversible damage, necessitating an additional protective layer. The precise degradation mechanism remains unclear; however, recent findings suggest that ion bombardment is the primary cause of degradation in both cases. [4-6]

This doctoral thesis seeks to investigate the fundamental mechanisms responsible for sputter process-induced degradation in both SHJ and PST solar cells. Through the strategic design of experiments and the application of diverse simulation tools, this study will further explore the effects of particle bombardment on these photovoltaic materials. By integrating various sputtering techniques, such as radio frequency and direct current, with an understanding of the differing dynamics of generated plasmas, a more comprehensive understanding of the material impacts will be achieved. The findings will be underlined with appropriate simulation results to enhance the understanding of different processes. These external influences on the samples will be correlated with the microstructural properties of the materials under investigation and the observed degradation in device performance. From this analysis, the physical degradation processes will be identified. Ultimately, once the degradation mechanisms are determined, sputter processes will be optimized to mitigate this degradation.

The integration of expertise from the Institute for Energy Materials and Devices – Photovoltaics (IMD-3) and the Institute of Fusion Energy and Nuclear Waste Management – Plasma Physics (IFN-1) facilitates promising opportunities for multifaceted collaboration. IMD-3 contributes extensive knowledge regarding the preparation of materials for photovoltaic applications, their characterization, and prior experience in sputter process-induced degradation. Concurrently, IFN-1 offers in-depth expertise in plasma physics, plasma-matter interaction, and simulation capabilities, alongside advanced experimental and microstructural characterization techniques and facilities, mainly the linear plasma generator PSI-2 [7], where samples can be tested under plasma bombardment with a variety of ions and energies. This collaboration, characterized by complementary knowledge, simulation, and experimental capabilities, is well-positioned to address the complexities of this topic and elucidate various critical aspects of the degradation process.

Key tasks in this project:

- **Detangle different impacts during the sputtering process on perovskite materials:** While for SHJ structures ion bombardment is already identified as main degrading mechanisms, investigations for perovskites are in an earlier phase. Through a proven design of experiments, different impacts during the sputter process should be deconvoluted.
- **Quantify the influence of properties of impinging ion on SHJ structures and perovskites:** Correlate the impact of different ion properties like size/mass, energy or fluency on the degradation effect of the samples under test.
- **Correlate microstructural features of the sample under test with degradation:** Test the extent of degradation on different microstructural features of the samples under test, for example void fraction, hydrogen content or oxygen content in the layers for SHJ structures.
- **Assessing different plasma conditions and their resulting impact on the sample through simulations:** Use advanced simulation models to get insights into plasma dynamics and how particles from the plasma reach the sample. In the following, the impact of the impinging particles on the sample can be simulated and evaluated.
- **Develop a model for the degradation process:** Based on the combined findings from previous tasks, a theory about underlying root causes for the degradation should be developed for the materials under test.
- **Development of degradation-free processes:** Based on the previously generated findings and developed theories, design sputter processes so that they can be applied on SHJ and PST solar cells with minimal degradation.

Location of the HITEC Fellow	Forschungszentrum Jülich, Institute of Energy Materials and Devices - Photovoltaics (IMD-3), Director: Prof. Dr. Christoph Brabec https://www.fz-juelich.de/en/imd/imd-3
Partners of the HITEC Project	Forschungszentrum Jülich, Institute of Fusion Energy and Nuclear Waste Management – Plasma Physics (IFN-1), Director: Prof. Dr. Christian Linsmeier https://www.fz-juelich.de/en/ifn/ifn-1
Specific **requirements**	M. Sc. in Electrical Engineering, Materials Science, Physics or comparable Experience in materials science or plasma physics is advantageous
For **project specific** questions please **contact**	Alexander Eberst, IMD-3, a.eberst@fz-juelich.de Dr. Mauricio Gago, IFN-1, m.gago@fz-juelich.de

[1] Haegel, Nancy M., et al. "Photovoltaics at multi-terawatt scale: Waiting is not an option." *Science* 380.6640 (2023): 39-42.

[2] Fischer, Martin, et al. International Technology Roadmap for Photovoltaic, *vdma* (2023).

[3] Allen, Thomas G., et al. "Passivating contacts for crystalline silicon solar cells." *Nature Energy* 4.11 (2019): 914-928.

[4] Yang, Qing, et al. "Origin of sputter damage during transparent conductive oxide deposition for semitransparent perovskite solar cells." *Journal of Materials Chemistry A* 12.24 (2024): 14816-14827.

[5] Qiu, Depeng, et al. "Transparent conductive oxide sputtering damage on contact passivation in silicon heterojunction solar cells with hydrogenated nanocrystalline silicon." *Solar RRL* 6.10 (2022): 2200651.

[6] Eberst, Alexander, et al. "Deeper Insight into the Mechanisms Behind Sputter Damage in Silicon Solar Cells Based on the Example of Nanocrystalline Silicon Carbide." *Advanced Physics Research* 3.9 (2024): 2400036.

[7] Kreter, A., et al. "Linear Plasma Device PSI-2 for Plasma-Material Interaction Studies" *Fusion Science and Technology*, 68.1 (2015), 8–14.