

Research Project #12

Conformal wet-coating of perovskite on random pyramid texture by controlling the perovskite crystallization process (IET-2 & IMD-3)

Perovskite–silicon tandem solar cells are attracting intense interest because they surpass the efficiency limits of conventional silicon photovoltaics. By combining a wide-bandgap perovskite top cell with a silicon bottom cell, tandems harvest a greater portion of the solar spectrum and have already achieved record efficiencies that surpass those of single-junction silicon. Their compatibility with low-cost, low-temperature processing makes them a practical route to higher-performing, scalable solar modules. Continued work is essential to improve stability and large-area integration so these laboratory breakthroughs can translate into durable, commercially viable clean-energy technologies.

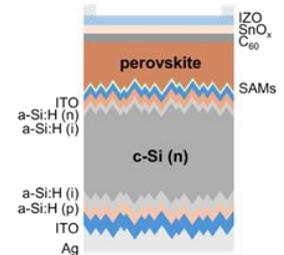


Figure 1: Schematic view of a silicon - perovskite tandem solar cell.

At present, several technologies exist for depositing perovskite layers onto randomly textured silicon pyramids. The most used approach is a hybrid process, in which the inorganic component of the perovskite is first deposited by evaporation, followed by a wet-chemical deposition of the organic component, allowing the two to react and form the perovskite crystal. An alternative method is one-step co-evaporation of all precursors, or sequential evaporation of the inorganic and then the organic species. These vacuum-based routes are used instead of the simpler one-step or two-step solution processes because wet-processed perovskite films typically fail to achieve conformal coverage on micrometer-scale random pyramids. For pyramid textures with heights of about 2–3 μm , the perovskite layer often fails to fully cover the pyramid tips. Increasing the perovskite thickness could, in principle, solve this, but it would result in excessively thick layers at the pyramid valleys, which is detrimental to device performance.

If conformal coating could be achieved using low-cost wet processing, this would be far more attractive than vacuum-based technologies. However, conformality requires that crystallization begins homogeneously across the entire textured surface, independent of whether the location is at the valley or the tip of a pyramid. Achieving these demands requires precise control over heterogeneous nucleation and very rapid, uniform seed formation. Ultimately, this challenge leads back to a deeper understanding of how perovskite crystallization is influenced by substrate morphology, surface energy, and quenching conditions.

The PhD project aims to uncover the crystallization mechanisms of perovskites as a function of texture geometry, surface properties, and processing methods, and to develop a roadmap for engineering truly conformal, wet-processed coatings. This will be demonstrated on high-efficiency perovskite silicon tandem solar cells. This work will combine computational and experimental approaches, and the candidate is expected to spend approximately 50% of their time in Nuremberg at IET-2 and 50% of their time in Jülich at IMD3.

IET-2 will provide the computational infrastructure necessary, including a mesoscale phase field simulation framework that allows for the simulation of crystallization processes in drying solutions deposited on textured surfaces, as well as access to a state-of-the-art high-performance computing infrastructure. The simulations allow for investigation of a wide spectrum of material- and process parameters on the impact of substrate texture, wetting properties, drying, and crystallization kinetics on the perovskite film morphology.

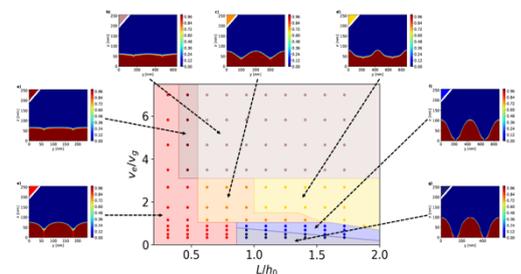


Figure 2: Example of phase field simulations: Morphology of crystals grown in a drying film, depending on the ratio between evaporation rate and growth rate v_e/v_g and on nucleus density L/h_0 .

IMD3 will provide the full experimental infrastructure necessary, including the capability to fabricate different texture morphologies, use various TCO and SAM materials, and apply tailored surface treatments that modify surface energy prior to perovskite deposition. IMD3 can also fabricate complete perovskite–silicon tandem devices, with the current reference efficiency reaching 33.4%. With successful conformal coating, the targeted efficiency exceeds 34–35%.

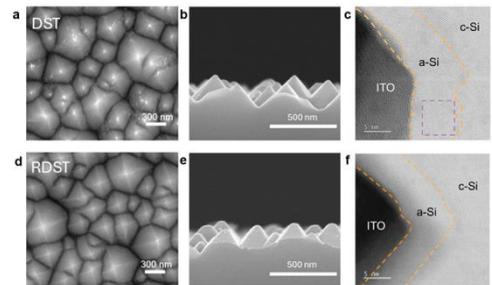


Figure 3: Pyramid morphology modification

The combination of the expertise at IET2 and IMD3 enables a combined experimental–theoretical strategy to accelerate the fundamental understanding of the underlying physical mechanisms and to guide process optimization.

Key tasks in this project:

1. **Set up a phase field model for heterogeneous crystallization of perovskite on textured surfaces:** Based on the existing implementation, include controllable surface energies at the substrate that are valid for arbitrary geometries, as well as a large number of relevant materials. Perform large-scale simulations for a wide spectrum of parameters to investigate the interplay of texture and process parameters on the crystallization of perovskite.
2. **Experimental validation of the simulation results based on the model:** Produce test samples to investigate the impact of texture, surface (TCO/SAM), and quenching on crystallization and compare the results with simulation results for validation.
3. **Define a roadmap for conformal wet-coating of perovskite on random pyramid texture:** Based on insight from (1) and (2), define a strategy for how to obtain a conformal coating using wet chemistry. Potential solutions could be a two-step wet process and/or adaptation of the quenching process.
4. **Develop a working approach for conformal wet-coating of perovskite on a random pyramid texture:** After the roadmap is defined, it should be systematically tested experimentally and supported by simulations. Optimize the process by improved experiments guided by detailed simulations.
5. **Develop a perovskite silicon tandem solar cell using the conformal wet-chemical process:** A high-efficiency perovskite silicon tandem solar cell will be demonstrated using the developed process. Optimization to achieve efficiency beyond 34% should be targeted.

Location of the HITEC Fellow	Forschungszentrum Jülich, Institute of Energy Technologies - Helmholtz-Institute Erlangen-Nürnberg for Renewable Energy (IET-2 / HI ERN), Director: Prof. Dr. Karl Mayrhofer https://www.hi-ern.de/en
Partners of the HITEC Project	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
Specific requirements	M. Sc. in Physics, Chemistry, Materials Science, or a related discipline
For project specific questions please contact	Prof. Dr. Jens Harting, IET-2, j.harting@fz-juelich.de Dr. Kaining Ding, IMD-3, k.ding@fz-juelich.de