Atomic-layer approaches towards 'extremely thin' chalcogenide-based photovoltaics: A unique combination of advantages

Pascal Büttner,[1] Vanessa Koch,[1] Dirk Döhler,[1] Florian Scheler,[1] Craig Pointer,[2] Tadahiro Yokosawa,[3] Marcel Rey,[4] Sofia Korenko,[1] Ivan Kundrata,[5] Selina Kern,[1] Maksym Plakhotnyuk,[5] Maïssa Barr,[1] Ignacio Mínguez Bacho,[1] Nicolas Vogel,[4] Ryan Crisp,[1] Erdmann Spiecker,[3] Elizabeth R. Young,[2] **Julien Bachmann**,[1,5,*]

[1] Friedrich-Alexander-Universität Erlangen-Nürnberg, Chemistry of Thin Film Materials, IZNF, 91058 Erlangen, Germany
[2] Lehigh University, Department of Chemistry, Bethlehem, Pennsylvania 18015, United States
[3] Friedrich-Alexander-Universität Erlangen-Nürnberg, Center for Nanoanalysis and Electron Microscopy, Institute of Micro- and Nanostructure Research, IZNF, 91058 Erlangen, Germany
[4] Friedrich-Alexander-Universität Erlangen-Nürnberg, Institute of Particle Technology, 91058 Erlangen, Germany
[5] ATLANT 3D Nanosystems, Kongens Lyngby 2800, Denmark

* julien.bachmann@fau.de

Atomic layer deposition (ALD) and variants of the technique are ideally suited to the generation of 'extremely thin absorber' (ETA) solar cells, in which three distinct semiconductors are combined as electron transport layer (SnO_2, TiO_2, ZnO), light absorption layer (Sb_2S_3, Sb_2Se_3), and hole transport layer (V_2O_5 or spin-coated organics). We have demonstrated six main advantages.

(1) ALD can deliver a material quality significantly improved with respect to solution processing techniques, with crystals of 10 µm lateral size obtained in planar films of 50 nm thickness.

(2) It enables the experimentalist to vary the thickness of layers within the semiconductor stack systematically and optimize the geometric parameters for overall energy conversion efficiency.

(3) It offers the opportunity to engineer interfaces with the use of interfacial layers providing chemical or physical functions (adhesion layers, tunnel barriers) with extreme thickness sensitivity, on the length scale of 0.5 to 1.5 nm.

(4) It provides the capability, unique among the deposition techniques from the gas phase, to deliver conformal coatings of non-planar substrates. Parallel arrays of cylindrical p-i-n heterojunctions in a coaxial geometry allow for decoupling the path lengths for light absorption and charge separation. Ordered monolayers of nanospheres can be exploited to scatter light of near-bandgap energy, enhancing the conversion of light incident in the red spectral range and/or under oblique angle.

(5) Our extension of ALD to the use of precursors dissolved in the liquid phase, instead of classically delivered from the gas phase ('solution ALD' or sALD) expands the range of materials accessible by ALD. It also provides additional experimental tools to adjust the deposit's morphology, and it provides an inexpensive access to ALD.

(6) The recent invention of 'atomic-layer additive manufacturing' (ALAM) circumvents the limitations associated with traditional blanket layering methods. It opens the door to rapid prototyping approaches in the photovoltaics field that mirror the use of 3D printing in manufacturing.

In summary, each major material family exploited in photovoltaics has been associated with a certain set of processing techniques, and our research indicates that atomic-layer processing provides all ingredients required for the success of the group 5 chalcogenides and similar light absorbers.