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Physical Vapor Deposition of Tin- and Lead-Based Halide Perovskites Via *in situ* X-ray Diffraction: From Phase Evolution to Formation Kinetics to Thin Film Solar Cells

Pu-Chou Lin[1], J. Damm[1], T. Schulz[1], K. Heinze[1], P. Pistor[2], R. Scheer[1, *]

[1]Institute of Physics, Photovoltaics Group, Martin-Luther-University, Halle, Germany

[2]Departamento de Sistemas F ísicas, Universidad Pablo de Olavide, Sevilla, Spain

Email address:

pu-chou.lin@physik.uni-halle.de (Pu-Chou Lin), roland.scheer@physik.uni-halle.de (R. Scheer)

[*]Corresponding author

Abstract

This study explores advancements in organic-inorganic lead-free perovskite materials, focusing on the film formation process during deposition by thermal evaporation for lead- and tin-based perovskites. It involves growth analysis, solar cell component preparation, and the analysis of optoelectronic properties. Key aspects include *in situ* X-ray diffraction for observing phase changes during growth, analysis of perovskite degradation, and development of multi-stage all-vacuum growth processes for multi-component perovskite thin films. State-of-the-art Pb-based perovskites and potential Sn-based compounds will be examined. We conduct sequential deposition/reaction processes under controlled temperature and flux variations in order to estimate reaction constants, diffusion constants, sticking coefficients, and activation energies. *In situ* X-ray diffraction in real-time will be the primary experimental method, providing insights into phase formation during thin film growth. A sandwich-like material structure design (*e.g.*, PbI_2-CsI-SnI_2) will be used to analyze the perovskite's growth mechanism and diffusion model as well. Further exploration involves understanding how IA-group cations like Cs achieve thermodynamic and kinetic balance in PbI_2 and SnI_2, facilitating the formation of stable and high-quality perovskite layers. There are three possible film growth mechanisms: (a) Precursor vapor reaction: Solid-state precursor films react from the vapor phase to form the perovskite film. (b) Diffusion couple reaction: Two or more solid-state precursor films react via chemical diffusion. (c) Exchange reaction: Another component fully or partly exchanges one component (anion or cation) during annealing processes (*e.g.*, $MAPbI_3$ to $MAPbBr_3$ exchange reaction). This study aims for solvent-free, controllable film deposition, utilizing sequential evaporation for better reproducibility. Different film growth mechanisms will be investigated, including precursor vapor reaction, diffusion couple reaction, and exchange reaction. Both Pb-based perovskites and Sn-based compounds are investigated, with a focus on reaction kinetics and diffusion. The ultimate goal is to advance toward the production of large-area, high-efficiency solar cells through physical processes, including the completion of various layers within a vacuum chamber, paving the way for stable and high-performance commercial applications in solar energy technology.

Keywords

Halide Perovskites, Physical Vapor Deposition, *In Situ* X-Ray Diffraction, Co-evaporation, Diffusion Model, Precursor Vapor Reaction, Exchange Reaction, Perovskite Solar Cells