Innovative approach for efficient encapsulation of perovskite-based solar cells: combination of analytical models and experimental investigations.

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In the context of decarbonization of energy production, new types of photovoltaic solar cells are elaborated to achieve higher power conversion efficiencies at lower manufacturing costs. Perovskites based solar cells are on of the most promising technologies currently, in particular tandem silicon-perovskite cells that have reached 33.9 % efficiency [1]. However, those new architectures come with new challenges: for example perovskite materials are highly sensitive to humidity permeation, which severely limits their long-term stability. One possible solution to protect them from that extrinsic degradation is the use of efficient encapsulation layers [2].

Thin Film Encapsulation (TFE) is a powerful method to meet the encapsulation needs of perovskite-based cells: to achieve WVTRs (physical quantity, Water Vapor Transmission Rate, used to quantify barrier properties [3]) of between 10^{-4} and $10^{-6}\ g.m^{-2}.d^{-1}$ [5], to offer laminated films with high flexibility (Young's modulus $\leq 20\ MPa$ at 25 °C [5]), and to ensure good light transmission between 400 and 1100 nm (> 80% [5]); all this with soft deposition conditions (deposition temperature ≤ 100 °C). Among the various thin film deposition methods available, Atomic Layer Deposition (ALD) is an attractive technique since it enables the deposition of uniform and dense [4] thin films of controlled thickness (below the nm), with very low pinhole defect densities and at low temperature (≤ 100 °C thus avoiding damage to the perovskite materials [6]).

Inorganic or organic-inorganic hybrid nanolaminate structures synthesized by ALD are very promising, with WVTRs reaching values close to $10^{-6}\ g.m^{-2}.d^{-1}$ [6]. Concerning the nature of the nanolaminates, there are many candidate materials, most of which are metal oxides (e.g. Al_2O_3 [7], TiO_2 [8]). They are often combined in nanolaminate structures with their "metalcones" counterparts, which are organic-inorganic hybrid materials typically synthesized by ALD-MLD (ALD-Molecular Layer Deposition) using metal precursors and various organic coreactants that yield metal alkoxide films [9]. As a result, numerous combinations of materials and nanolaminate structures (different monolayer thicknesses) are conceivable, and require a high amount of time to synthesize and characterize. A need has therefore been identified to speed up the selection of encapsulating layers. This study therefore proposes to combine experimental measurements and numerical simulation to improve the screening of encapsulating layers.

We thus first suggest screening metal oxides and hybrid materials using helium permeation measurements; assessing Helium Transmission Rates (HeTR) of ALD samples deposited on ITO-recovered PET substrates (less time-consuming than water permeation measurements – *Figure 1 and 2*) and morphological characterizations (density, roughness, mechanical properties) as good layers for encapsulation. We also propose two ways of refining the 1D classical analytical model [3] for predicting the WVTR within multilayers (*Figure 3*), as well as a dependence relationship between the effective diffusion coefficient of the diffusing species within a material and the concentration at the upstream interface of the same material (*Figure 4*), validated by experimental measurements and enabling more accurate prediction of the barrier properties of multilayers than the 1D models used nowadays.

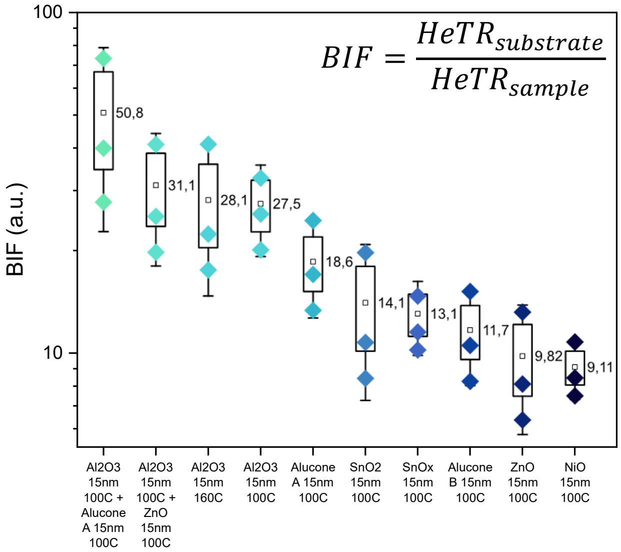

Figure 1. Helium permeation improvement factor of different ALD layers (substrate: 50nm ITO recovered PET).

Figure 2. Photo of the helium permeameter used at CEA Liten (QHV-4 Vinci Technologies).

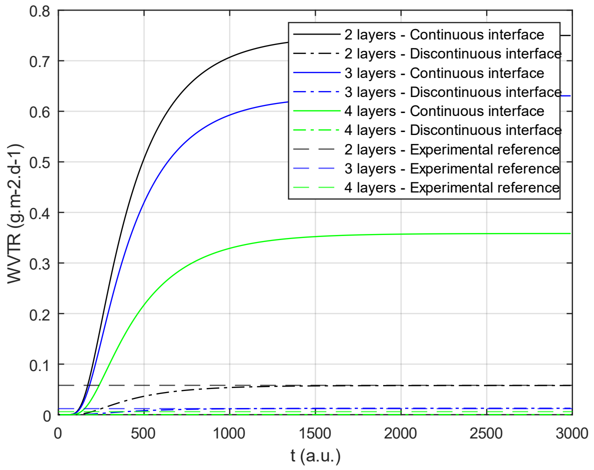

Figure 3. Simulated WVTR curves (without and with analytical model refinement) compared with experimental values from the work of Kiese et al. [10].

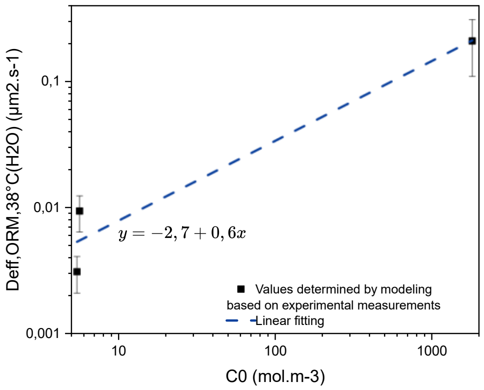

Figure 4. Evolution of the water diffusion coefficient within the ORM as a function of concentration at the upstream interface, based on model refinement and enabling the prediction of effective diffusion coefficient values within multilayers.

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