Control of atom fluxes for the production of solar cell devices

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Motivation: thin film CIGS solar cell production

Collaboration with IRDEP (Institut de Recherche et Développement sur l'Energie Photovoltaïque, EDF, CNRS, Chimie Paristech).

Optimal control of the production process of thin film CIGS (Copper, Indium, Gallium, Selenium) solar cell devices

Typical composition of a CIGS solar cell

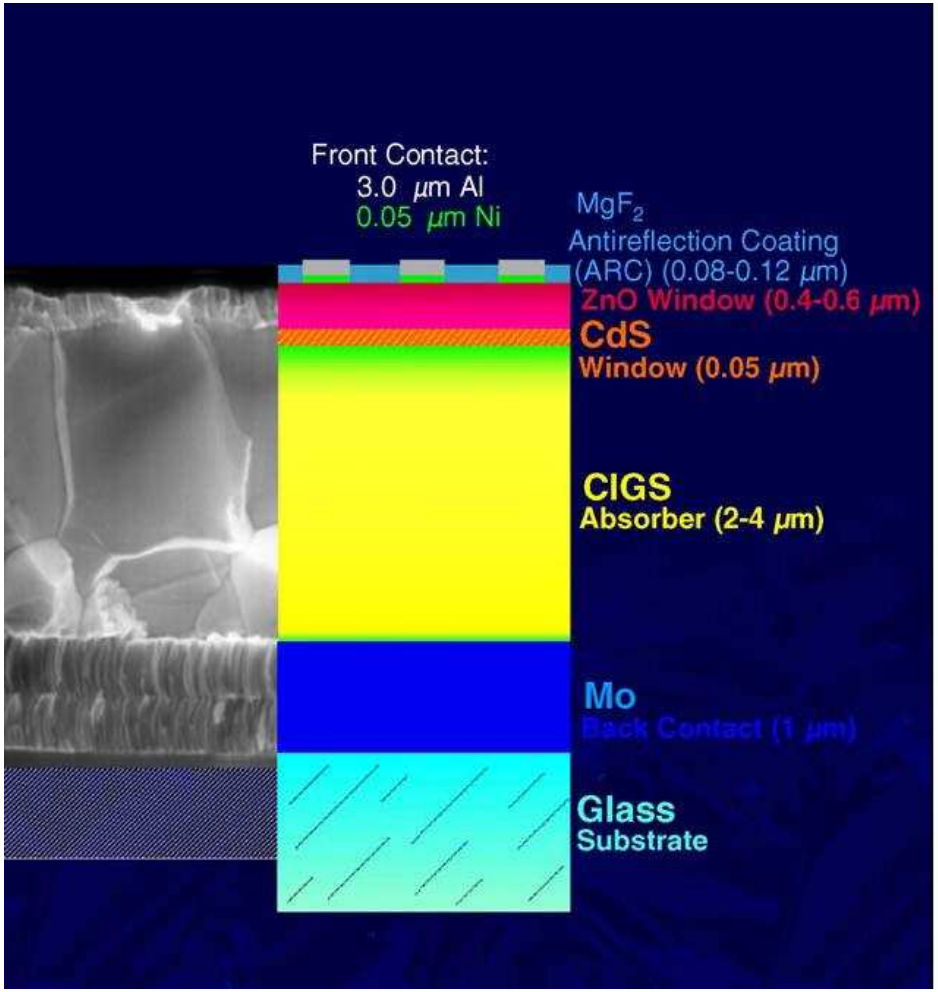
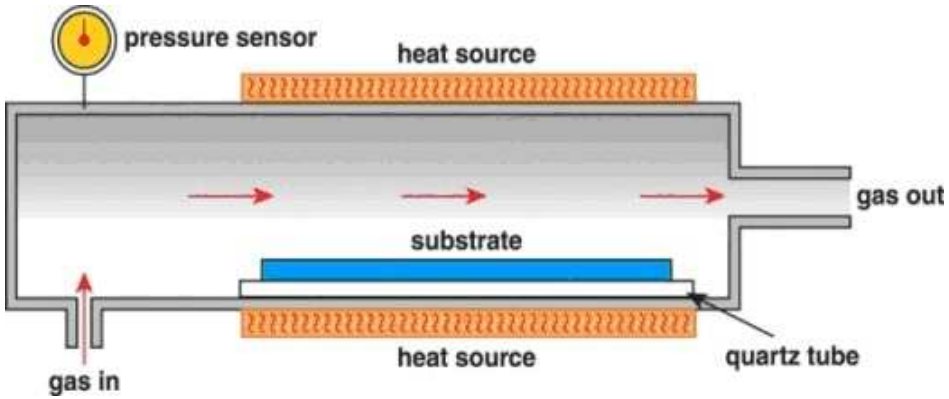
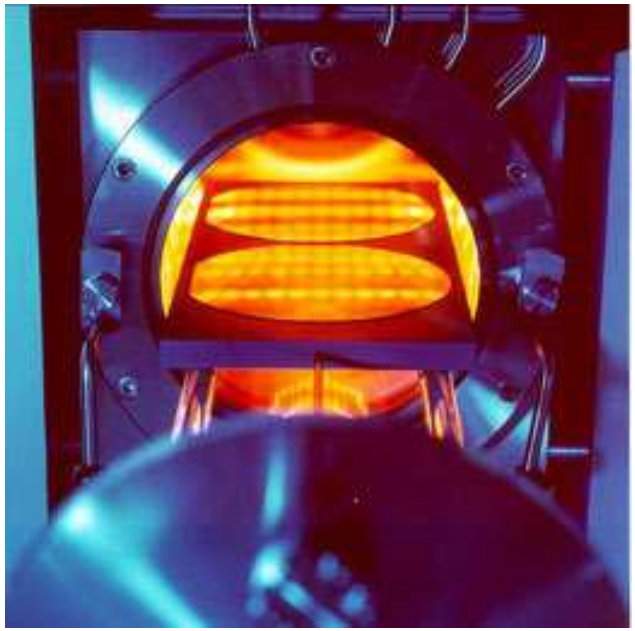


Figure: Typical composition of a thin film CIGS solar cell device

Production process: Chemical Vapor Decomposition (CVD)





Production process: Chemical Vapor Decomposition (CVD)

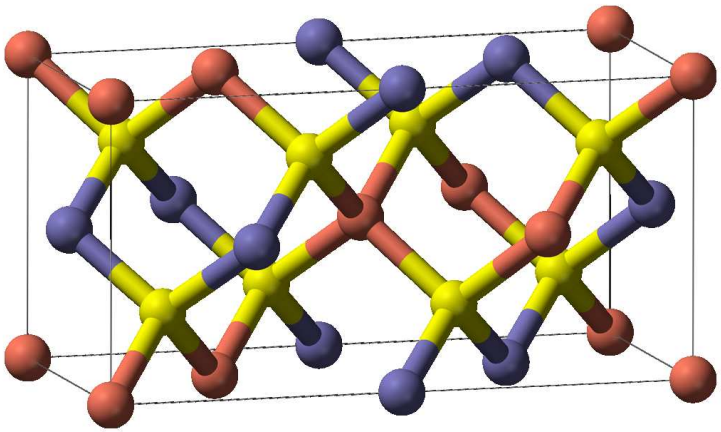


Figure: CIS unit cell

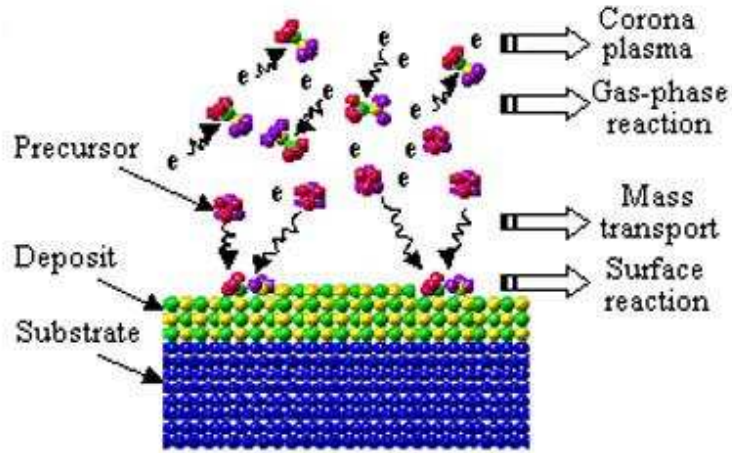
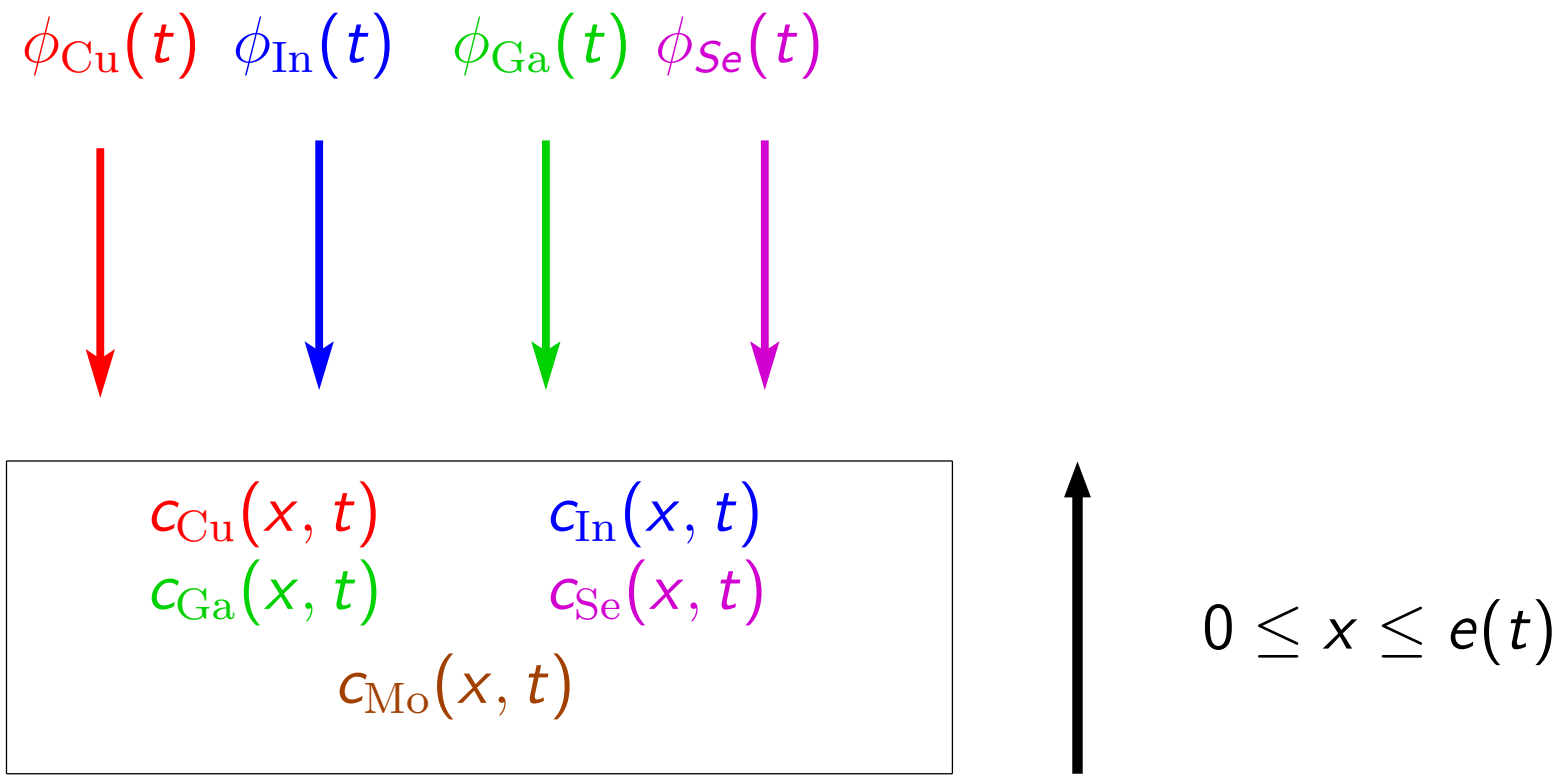


Figure: Chemical Vapor Deposition process

Simplified 1d model (1)

Let us denote by $\mathcal{A} := \{\mathrm{Cu}, \mathrm{In}, \mathrm{Ga}, \mathrm{Se}, \mathrm{Mo}\}$ the set of the different atomic species involved in the process.

The production process lasts during a time $T > 0$. The aim is to control the fluxes of the different atomic species $(\phi_A(t))_{A\in\mathcal{A}, 0\le t\le T}$ in order to obtain a desired thickness of the cell $e^{\mathrm{opt}}(T)$ and desired profile of concentrations $(c_A^{opt}(x))_{A\in\mathcal{A},\, 0\le x\le e^{\mathrm{opt}}(T)}$ at time $t = T$.



Simplified 1d model (2)

At time $t \in (0, T)$, $e(t)$ denotes the thickness of the cell, and for all $0 \leq x \leq e(t)$, $c_A(x, t)$ denotes the local concentration of entity A at time t and depth x.

Time $t = 0$: $e(0) = e_0 > 0$, $c_A(x, 0) = c_A^0(x), \quad \forall 0 \leq x \leq e_0, \quad \forall A \in \mathcal{A}$.

We also assume that for all $0 \leq x \leq e_0$, $c_A^0(x) \geq 0$ and $\sum_{A \in \mathcal{A}} c_A^0(x) = 1$.

Evolution of the thickness of the solid: $e'(t) = \sum_{A \in \mathcal{A}} \phi_A(t), \quad \forall t \in (0, T)$

Cross-diffusion of the different species in the solid:

$$\partial_t c_A = \mathrm{div}_x \left[\sum_{B \in \mathcal{A},\ B \neq A} k_{AB} (c_B \partial_x c_A - c_A \partial_x c_B) \right], \ \forall (t, x) \in (0, T) \times (0, e(t))$$

Boundary conditions:

$$F_A(x, t) := \sum_{B \in \mathcal{A},\ B \neq A} k_{AB} (c_B(x, t) \partial_x c_A(x, t) - c_A(x, t) \partial_x c_B(x, t)).$$

$$F_A(0, t) = 0, \quad F_A(e(t), t) + e'(t) c_A(e(t), t) = \phi_A(t), \quad \forall t \in (0, T).$$

Properties of the model

The diffusion equations are derived from a lattice-based hopping model, leading to a cross-diffusion system for $n = |\mathcal{A}|$ species, incorporating volume-filling effects.

It follows from this model that

$$\forall (t,x) \in (0,T) \times (0,e(t)), \quad c_A(t,x) \geq 0 \text{ and } \sum_{A \in \mathcal{A}} c_A(t,x) = 1. \tag{1}$$

Besides, we have the following mass conservation property (due to the choice of boundary conditions):

$$\partial_t \left(\int_0^{e(t)} c_A(x,t)\, dx \right) = \phi_A(t). \tag{2}$$

Remark: In the case when all the diffusion coefficients k_{AB} are identical and equal to k, the system can be equivalently rewritten as

$$\partial_t c_A(x,t) = k \Delta_x c_A(x,t), \quad \forall (t,x) \in (0,T) \times (0,e(t)).$$

Questions

Theoretical questions:

- Well-posedness of the model? (existence, uniqueness...)
  In the case when $\phi_A(t) = 0$, this model was derived and studied for particular values of the diffusion constants k_{AB} in [Burger, Di Francesco, Pietschmann, Schlake (2010)].

Numerical questions:

- How to design a stable algorithm such that (1) and (2) are satisfied at the discrete level?

With zero fluxes ($\phi_A(t) = 0$, $e(t) = e_0$): gradient flow structure

Without fluxes, this system has a gradient flow structure [Jordan, Kinderlehrer, Otto, 1998], [Zinsl, Matthes, 2014], [Mielke, Liero, 2013], [Jungel, 2014], [Daneri, Savaré, 2010] , in the sense that it can be rewritten as

$$\partial_t C = \mathrm{div}_x \left[M(C) \partial_x \nabla \mathcal{E}(C) \right], \quad C(t,x) = (c_A(t,x))_{A \in \mathcal{A}}$$

where

- $C : \left\{ \begin{array}{ccc} (0,T) \times (0,e_0) & \to & S \\ (t,x) & \mapsto & (c_A(t,x))_{A \in \mathcal{A}} \end{array} \right.$, with $S := \{ C = (c_A)_{A \in \mathcal{A}} \in \mathbb{R}_+^{|\mathcal{A}|} \mid \sum_{A \in \mathcal{A}} c_A = 1 \}$, is the set of profile concentrations;
- $\mathcal{E} : \left\{ \begin{array}{ccc} S & \to & \mathbb{R} \\ C & \mapsto & \mathcal{E}(C) := \sum_{A \in \mathcal{A}} c_A (\ln c_A - 1) \end{array} \right.$ is the driving entropy functional of the system;
- $M : \left\{ \begin{array}{ccc} S & \to & \mathbb{R}^{|\mathcal{A}| \times |\mathcal{A}|} \\ C & \mapsto & (M_{AB}(C))_{A,B \in \mathcal{A}} \end{array} \right.$ is the mobility tensor defined by

$$\forall A \neq B \in \mathcal{A}, \quad M_{AA}(C) := \sum_{A' \in \mathcal{A},\ A \neq A'} k_{AA'} c_A c_{A'} \text{ and } M_{AB}(C) := -k_{AB} c_A c_B.$$

Optimal transport formulation: distance generated by a mobility matrix

[Benamou, Brenier, 2000], [Zinsl, Matthes, 2014]

Optimal transport metric associated to a moblity matrix for nonlinear cross-diffusion systems: For $C_0, C_1 : (0, e_0) \to S$,

$$W_M(C_0, C_1)^2 = \inf \left\{ \int_0^1 \int_0^{e_0} W^T M(C)^{-1} W \, dx \, dt, (C, W) \in \mathcal{C}^1(0, T; C_0, C_1) \right\},$$

where

$$\mathcal{C}^1(0, T; C_0, C_1) := \left\{ C, W : (0, T) \times (0, e_0) \to \mathbb{R} \mid \begin{array}{c} C(0) = C_0, \ C(1) = C_1, \\ \partial_t C + \partial_x W = 0 \end{array} \right\}.$$

For some diffusion equations (linear mobility matrix), this distance can be reinterpreted in terms of the standard Wasserstein distance.

Numerical scheme: de Giorgi's minimizing movement method

Without fluxes: Minimizing movement method [Jordan, Kinderlehrer, Otto, 1998], [Daneri, Savaré, 2010] for the numerical resolution of the system:
Let $\tau > 0$ be a time step.

$$C_{n+1} \in \inf_{\substack{C=(c_A)_{A\in\mathcal{A}}:(0,e_0)\to S,\\ \forall A\in\mathcal{A},\ \int_0^{e_0} c_A(x)\,dx = \int_0^{e_0} c_A^0(x)\,dx}} \mathcal{E}(C) + \frac{1}{2\tau} W_M(C_n, C)^2.$$

Possible advantages:

- implicit scheme, hopefully stable;
- mass and volume constraints satisfied exactly at each iteration;
- using a regularized entropic distance? [Benamou, Carlier, Cuturi, Nenna, Peyré, 2014]
- With fluxes, use of a splitting scheme (minimizing movement method for the diffusion step, explicit scheme to treat the fluxes).

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