COMPUTER-AIDED DESIGN OF THE CHEMICAL VAPOR DEPOSITION OF SILICON FOR APPLICATION IN SOLAR CELLS

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ABSTRACT

The chemical vapor deposition (CVD) of Silicon (Si) is a key process for the manufacturing of solar cells and photovoltaic (PV) panels owing to the inertness and abundance (~ 22% in the earth crust) of Si, its long-term stability and the maturity of the technology as compared to Cd solar cells, dye sensitized and organic cells and perovskites, respectively. Although at a first glance the electricity production from Si PVs looks financially attractive and environmentally-friendly, in reality their fabrication requires huge energy amounts, produced by conventional energy sources, which in turn, releases green- house harmful gases and other pollutants in the atmosphere and yields high-level electric energy prices. This work focuses on the CVD of p-i-n Si on metallic filaments for the direct development of Si cells applied in photovoltaic applications with the aim to reduce the energy required for the production of PV panels. However, CVD is a complex process owing to the interplay between transport phenomena and chemistry mechanisms occurring within the reactor. Thus, a computational framework is employed to assist the design of the process and its optimization. The modeling procedure consists of a computational fluid dynamics (CFD) model that takes into account the transport phenomena within the CVD reactor, namely fluid flow, species transport and heat transfer. The mechanistic analysis of the transport phenomena, facilitated with the use of CFD modelling, allows the optimization of the reactor and process design with regard to deposition thickness and uniformity. This model will serve as a basis for the development of a detailed and experimentally validated model, which will include chemical reactions for the deposition of p-i-n Si. Furthermore, the experimentally-validated CFD model will be applied for the production of an extended dataset based on the different CVD parameters (gas flow rates, deposition) which will trigger the data-driven analysis of the process. This hybrid computational framework not only provides invaluable information for the CVD of Si on filaments but more importantly, it will result in the efficient design and optimization of the process under investigation, enabling the fabrication of low-cost and environmentally-friendly solar cells for PV applications.

KEYWORDS: CVD of Si, p-i-n Si, deposition on filaments, solar cells, CFD modelling

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