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Calculations of Optimal Source Geometry and Controlled Combinatorial Gradients in Fixed- and Rotating-Substrate PVD Systems

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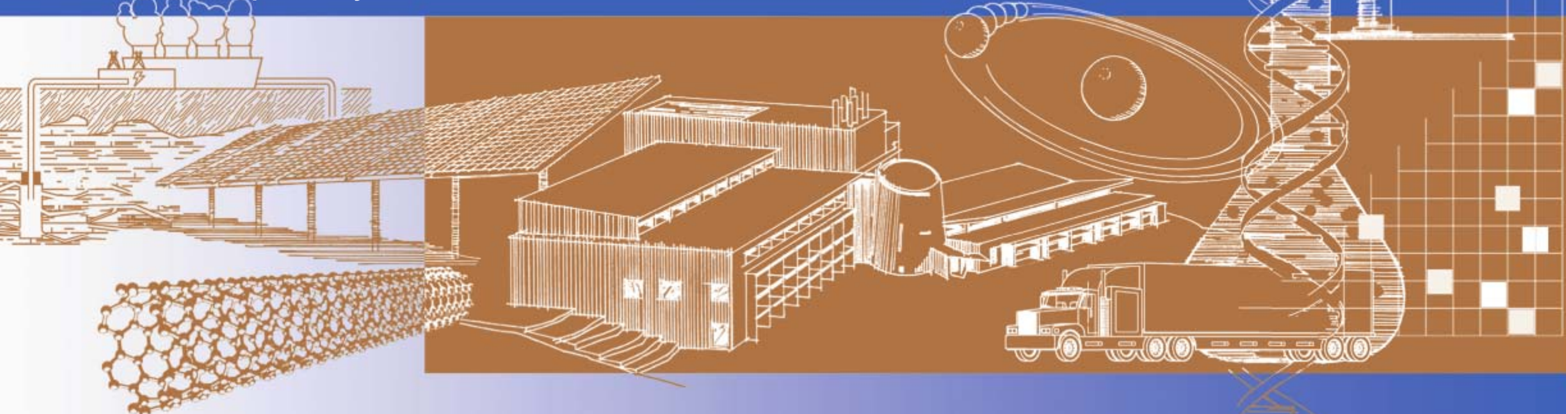

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Calculations of Optimal Source Geometry and Controlled Combinatorial Gradients in Fixed- and Rotating-Substrate PVD Systems

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ABSTRACT

Normalized forms of conventional flux-distribution formulas are applied to physical-vapor deposition from open-boat type sources onto static and rotating substrates. For the rotating-substrate case, the deposition geometry that yields optimal film-thickness uniformity for different source-substrate separations is derived empirically. In addition, flux-distribution formulas are used to develop a novel method for combinatorial physical-vapor deposition. With this method, a single deposition system may be used, without modification, to deposit either highly uniform or graded-composition thin-film materials.

1. Objectives

The goal of the Process Integration (PI) project at the National Renewable Energy Laboratory (NREL) is to integrate deposition, processing, and characterization techniques for research and development of thin-film, crystalline, and polycrystalline photovoltaic (PV) devices.[1] The purpose of this work is to explore the principles of deposition uniformity[2-5] to provide a starting point for the design of PI-compatible physical-vapor-deposition- (PVD-) based deposition and/or processing tools capable of uniform deposition on substrates up to 6” x 6” square. In addition, flux-distribution formulas for static and rotating substrates are employed to demonstrate a novel method for combinatorial thin-film synthesis that is applicable to the research of PV materials and devices.

2. Technical Approach

The deposition geometry used in this work is depicted in Fig. 1. For PVD sources that are characterized by a $\cos\theta$ angular distribution, the substrate-radius-normalized formulas that express the flux distributions on static and rotating substrates, respectively, are

$$J_{static} = K\left(\frac{h_n^2}{R_s^2\left(h_n^2+\rho_n^2+d_n^2-2\rho_n d_n\cos\phi\right)^2}\right), \text{ and} \quad (1)$$

$$J_{rot} = K\left(\frac{h_n^2\left(h_n^2+\rho_n^2+d_n^2\right)}{R_s^2\left[\left(h_n^2+\rho_n^2+d_n^2\right)^2-4\rho_n^2 d_n^2\right]^{3/2}}\right), \quad (2)$$

where K is a constant that depends on the evaporant material and temperature. The subscript ‘n’ denotes geometrical parameters that are normalized with respect to substrate radius R_s, *e.g.*, $h_n = h/R_s$. Substrate radius is defined as the radius in the deposition plane over which film-thickness uniformity is required.

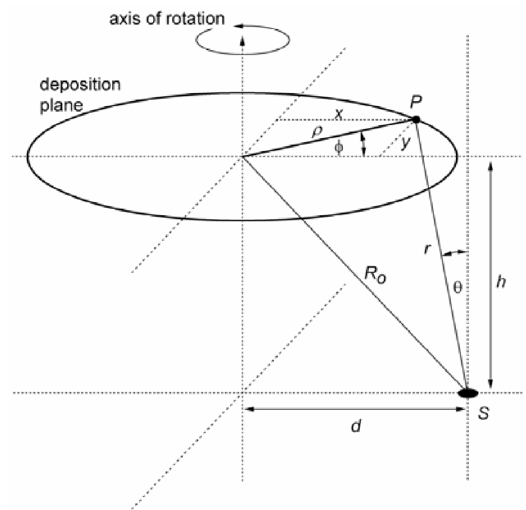

Fig. 1. Deposition geometry parameters.

Flux variation across the substrate is defined as

$$flux\ variation = \frac{J_{max}-J_{min}}{J_{max}}, \quad (3)$$

where J_{max} and J_{min} are the maximum and minimum values of the flux for $0 < \rho < R_s$.

3. Results and Accomplishments

In this work, the deposition geometry that leads to optimal flux uniformity is determined empirically by systematically varying the source offset d_n for different values of the substrate height h_n, and then calculating the flux variation for each (h_n,d_n) combination according to Eq. (3). In addition, the basic flux-distribution formulas [Eqs. (1) and (2)] are extended to calculate the combinatorial gradients that are produced by specific deposition geometries when the substrate is static for part or all of the deposition.

3.1 Optimal Rotating-Substrate PVD Geometry

Analysis of Eqs. (1)–(3) demonstrates that optimal film-thickness uniformity is achieved when the source offset d_n is related to substrate height h_n according to

$$d_n \cong 0.180 + 0.681 \times h_n. \quad (4)$$

Equation (4) is approximately valid for 2 > h_n > 5, but might not hold in general outside of this range.

3.2 Novel Technique for Combinatorial PVD

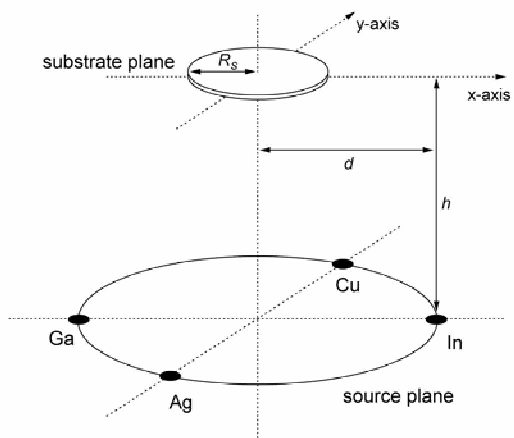

Fig. 2. Schematic of deposition-system geometry for uniform and combinatorial deposition of CAIGS. Complementary sources are placed in opposition on a circle in the source plane defined by Eq. (4).

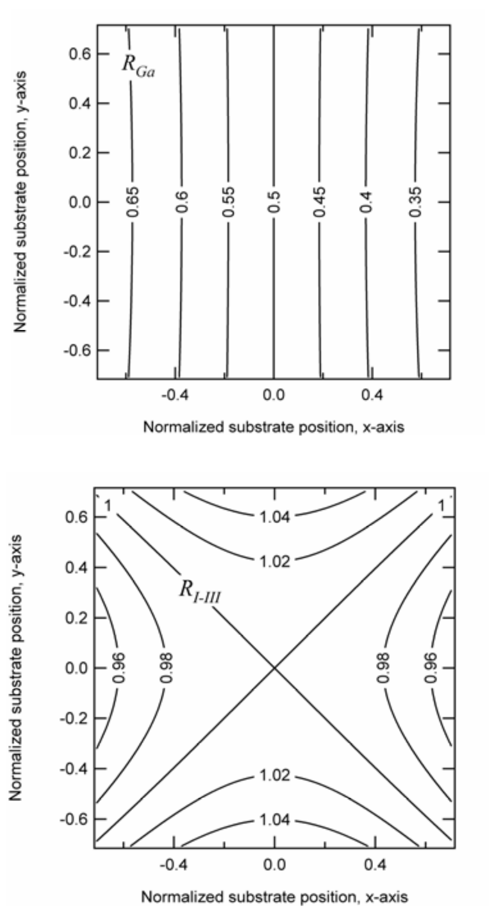

Fig. 3. Contour plots showing calculated Ga content [upper panel, R_{Ga} = *Ga/(In+Ga)*] and Cu content [lower panel, $R_{I\text{-}III}$ = *Cu/(In+Ga)*] for combinatorial deposition of Cu(In,Ga)Se_2.

By performing part or all of a deposition onto a static substrate, it is possible to create combinatorial thin-film libraries with well-controlled compositional gradients. Figure 2 illustrates how sources might be arranged in a deposition system to study the (Cu,Ag)(In,Ga)Se_2 materials system. Complementary metal sources are placed in opposition, and the Se source is not shown.

The deposition geometry in Fig. 2 is capable of producing highly uniform films (when the substrate is rotated during deposition) as well as graded-composition films (when the substrate is static during part or all of the deposition). An example of a combinatorial library sample that may be produced by this arrangement of sources is shown in Fig. 3. In this case, a CIGS thin film is deposited with no Ag. The substrate is rotated during the Cu deposition, and held static during the In+Ga deposition. The calculated Ga content [R_{Ga} = *Ga/(In+Ga)*] varies from about 0.32 to 0.68, while the Cu content is nearly constant at all points on the substrate.

4. Conclusions

To facilitate design of PI-compatible tools, a condition for optimal-uniformity deposition during rotating-substrate PVD has been derived empirically. Also, a novel method for combinatorial thin-film PVD has been introduced that allows a single deposition tool, without modification, either to deposit highly uniform thin films or combinatorial thin-film libraries.

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MAJOR FY 2005 PUBLICATIONS

G. Teeter, "Physical-vapor deposition flux-distribution calculations for static and rotating substrates: derivation of the deposition geometry for optimal film-thickness uniformity," submitted to J. Vac. Sci. Technol.-A.

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