**Transparent conductive Cu diffusion barriers: A 2-dimensional combinatorial screening study on the In-Zn-O system**

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Metallization costs can account for a significant proportion of the total processing cost of optoelectronic devices – for silicon solar cells up to 20-30%[1]. This high cost combined with supply-chain concerns motivate the substitution of costly contact materials such as silver by more abundant and less expensive metals like copper. However, the utilization of Cu gives rise to the issue of its high mobility, which potentially compromises device performance due to copper ingress into the Si wafer. Consequently, a diffusion barrier is required between the Cu contact and the active material. The employment of a transparent electrode that is capable of performing this additional function would result in a reduction of both processing time and costs.

Since amorphous thin films are reported to possess superior diffusion barrier performance compared to polycrystalline thin films[2], amorphous In-Zn-O (a-IZO) is a promising candidate for such a multifunctional transparent conductive Cu diffusion barrier.

In this study, we perform an accelerated co-optimization of electrical conductivity, optical transmission in the UV-Vis-NIR range and Cu diffusion barrier performance of the In-Zn-O material system. To accelerate this process, we combine high-throughput synthesis of materials libraries by combinatorial magnetron co-sputtering and high-throughput characterization procedures of XRF, XRD, Four-Point-Probe electrical conductivity measurements and UV-vis-NIR photospectroscopy. Due to the strong influence of even subtle changes in the oxygen content of the IZO films on the electrical and optical properties, materials libraries were deposited with 2-dimensional composition gradients covering the cation concentration (i.e. In/Zn) as well as the oxygen content.

The application of this approach enables the assessment of compositional limits of applicability as transparent conductive materials on a single material library. The electrical conductivity varies over several orders of magnitude with a maximum of 2.4 · 103 S/cm in the center of the library for a room temperature deposition. Simultaneously, the low oxygen content region of the library exhibits a substantial increase in absorptance up to 26%, averaged between 350 and 1100 nm, indicating a compositional limit of the applicability as transparent electrode. To screen the Cu diffusion barrier performance, thin materials libraries (23±1 and 8±1 nm) are reproduced on silicon wafers, covered with 100 nm Cu and heated in vacuum. The formation of Cu silicides for different cation and anion compositions is monitored by XRD and compared to the response of Cu films deposited directly on Si wafers without an IZO barrier. The diffusion behavior in selected samples is further investigated by means of XPS and ToF-SIMS measurements.

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[2] D. Gupta, *Diffusion Processes in Advanced Technological Materials* (Springer Berlin Heidelberg, Berlin, Heidelberg, 2005).