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Combinatorial Exploration of Novel Transparent Conducting Oxide Materials

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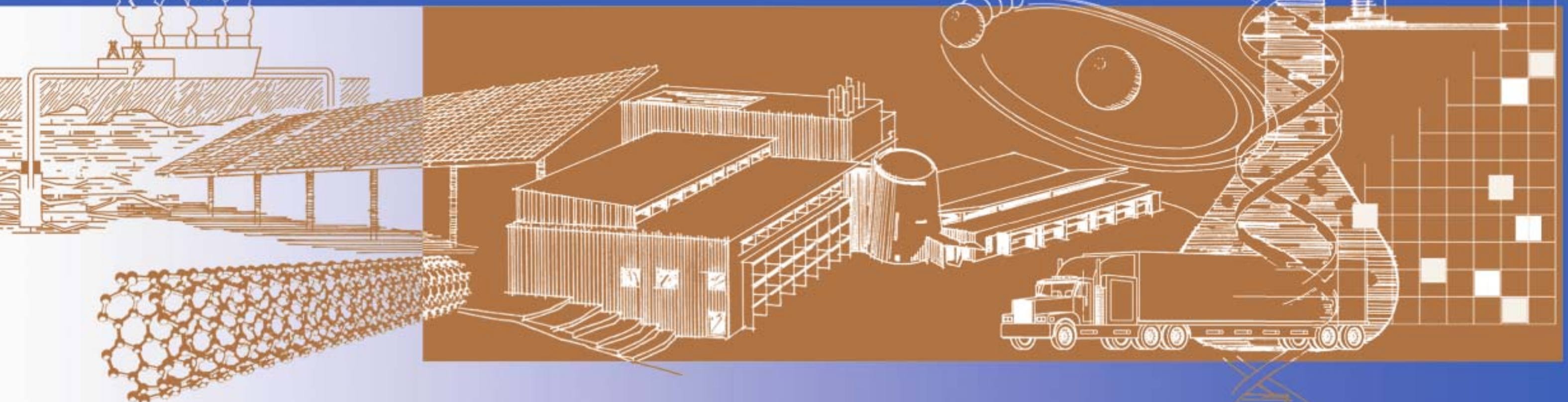

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Combinatorial Exploration of Novel Transparent Conducting Oxide Materials

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ABSTRACT

High-throughput combinatorial approaches have been used for the discovery and optimization of transparent conducting oxide (TCO) materials for PV applications. We report on current investigations in In-Zn-O, In-Ti-O and In-Mo-O systems. The InZnO system is shown to be amorphous in the best conducting range with a conductivity of ~ 3000 Ω-cm^{-1} for 50%-70% In/Zn. The amorphous InZnO films are very smooth (2 Å rms). In-Ti-O is found to be an excellent high-mobility TCO with mobilities of greater than 80 cm^2/v-sec and conductivities of more than 6000 Ω-cm^{-1} for sputtered thin film materials.

1. Technical Approach

The discovery and optimization of new materials and devices for photovoltaic applications is nominally a slow and time-consuming process. The advent of high-speed automated analysis and data-handling tools has enabled the use of combinatorial high-throughput approaches to photovoltaic materials. High-throughput combinatorial approaches have shown applicability in a wide range of materials areas including catalysis, inorganic synthesis, new materials discovery, device development, and organic synthesis. The advent of computer-automated deposition, analysis, and data-mining capabilities has enabled the broad application of these approaches. NREL has specifically worked for the past five years on the development of the appropriate tools for the discovery and optimization of optoelectronic materials and devices including TCOs and amorphous Si.

2. Results and Accomplishments

In the TCO area, we have developed a set of deposition tools (two systems) capable of depositing up to quartenary materials systems by sputter deposition with and without ion beam assist[2]. The ion-beam-assist mode is often helpful to optimize properties at lower deposition temperatures. A set of complementary analytical capabilities has been developed to examine the compositionally graded libraries. These are specifically tailored for TCO materials and all handle at least 2"x2" libraries. They include: a mapping x-ray diffraction system; a mapping simultaneous reflection transmission system (200nm-2000 nm); mapping FTIR; a four-probe system for mapping conductivity; mapping atomic-force, scanning-electron and EDS microscopy; a mapping micro-Raman system; mapping for corrosion analysis; and work function measurement by Kelvin probe. This core set of tools, coupled to appropriate data-basing and modeling, can rapidly evaluate very large phase spaces in weeks or months that would have taken years by conventional approaches.

These tools have been applied to a number of relevant TCO systems including ZnSnO [3], InZnO [2,4], Mo:In_2O_3 and Ti: In_2O_3 [5]. In this paper, we discuss results on indium-oxide-based systems doped with Mo and Ti and substituted with Zn. The InZnO system is shown to be amorphous in the best conducting range (50%-70% In) as shown in Fig. 1 and films are deposited at room temperature and are very smooth (2 Å rms). In the amorphous range, films have a conductivity of 3000 Ω-cm^{-1} [2]. More interesting, as can be seen in Fig. 2, the amorphous phase is remarkably stable under thermal annealing (in this case Ar), showing no crystallization and very little conductivity change to 600°C over 10 hours of annealing. This indicates that amorphous TCOs may be well suited to OLED applications.

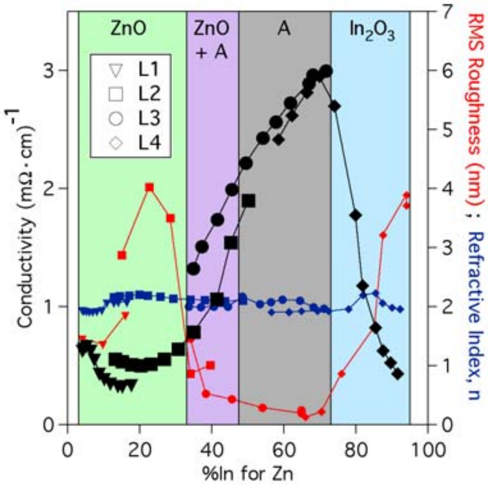

Fig. 1. Conductivity, RMS roughness, and refractive index and crystalline phase fields for as-deposited In-Zn-O.

The Mo- and Ti-doped materials we have explored by combinatorial approaches have demonstrated outstanding properties with mobilities of greater than 80 cm^2/v-sec and conductivities of greater than 6000

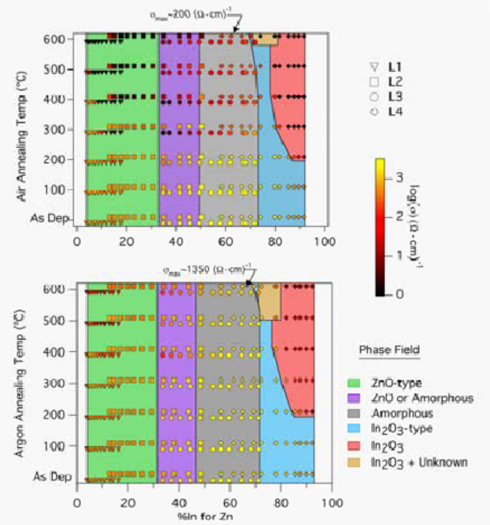

Fig. 2. Effect of annealing in air (top) and argon (bottom) on the conductivity and structure of In-Zn-O

Ω-cm^{-1} as shown in Fig. 3 for the Ti-doped In_2O_3 system [5]. However, their optimum process temperature is more than 400°C and thus they may not be optimal for organic applications. Note, however, that the work function (ie contact potential difference) varies by almost half a volt. It was only through the application of the high-throughput techniques that this range of compositions could be explored. Once interesting phase regions are identified, then single composition samples are evaluated by pulse laser deposition or sputtering using in-house target fabrication and deposition system capabilities [1].

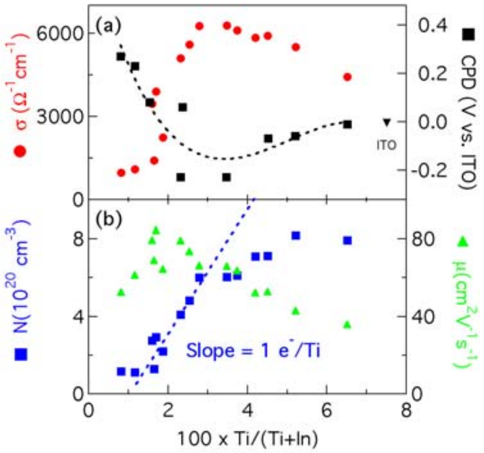

Fig. 3. Electrical properties and work function of Ti-doped In_2O_3.

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