Single-Step Non-Reactive Magnetron Sputtering of Copper Iodide (CuI) Thin Films for p-type Transparent Electrodes in Photovoltaic Heterojunction Architectures

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Abstract

Achieving efficient p-type transparent conductors is a key challenge in developing high-performance heterojunction photovoltaic (PV) devices. Copper Iodide (CuI), with its high optical transparency, wide direct bandgap (approx. 2.9-3.1 eV) and intrinsic p-type conductivity, has emerged as a viable option for its integration into next-generation solar cells. In the present work, we report deposition of γ-phase CuI thin films via a single-step, non-reactive magnetron sputtering technique. The applied technique eliminates the need of reactive gasses or post-deposition iodination, offering a scalable and controllable synthesis route suitable for large-area PV manufacturing.

In the context of magnetron sputtering, a ceramic CuI target (99.99% purity) in argon atmosphere was sputtered at room temperature on silicon, silica and textured silicon substrates using Advanced Energy Pinnacle+ pulsed-DC power supply. Prior to deposition, the chamber was evacuated to a base pressure of 10^{-6} mbar. The Ar flow rate was set at (30 sccm) with a working pressure ranging from 0.5 Pa to 1.5 Pa. The deposition conditions included a fixed applied voltage of 250 V with a pulsing frequency of 150 kHz and 2.6 µs off-time. The synthesized samples were characterized without annealing or post-iodination.

A cubic single-phase γ-CuI with [111] preferred orientation was confirmed via X-ray diffraction (XRD). Scanning electron microscopy (SEM) demonstrated columnar growth and uniform grain coverage. High-resolution transmission electron microscopy (HR-TEM) and selected area electron diffraction (SAED) validated the cubic structure oriented along [111], and grain twinning, backing consistent charge transport and vertical conductivity in heterojunction solar cell integration. Ellipsometry, UV-visible spectroscopy, and photoluminescence (PL) analysis consistently determined a direct optical bandgap between 2.87–2.99 eV, with a strong optical transmittance ($T > 80\%$) and sharp absorption onset near 2.95 eV, qualifying these films ideal for high-transparency top contacts in tandem solar cells. The extracted dielectric function and refractive index dispersion ($n \approx 2.29$ at 633 nm) coincide closely with known values for transparent semiconductors. Electrical measurements offer key pointers of PV suitability: Hall effect measurements confirms p-type conductivity, with a resistivity ranging 10^{-2} Ω·cm, hole mobility between 7-10 $cm^2 \cdot V^{-1} \cdot s^{-1}$, and carrier concentrations on the order of 10^{19} cm^{-3}, demonstrating a favorable balance between transparency and conductivity, important for lessening series resistance in functional devices. The acquired work function values (4.97–5.20 eV) are aligned with common absorber layers like silicon and perovskite, promoting effective hole extraction at the heterojunction interface.

These features altogether highlight the viability of a simplified non-reactive magnetron sputtering for producing CuI-based transparent electrode, particularly to use as hole transport layers or transparent back contacts in heterojunction, tandem, and Si solar cells**.** The strong agreement between structural, optical, and electronic data emphasizes the potential of CuI thin films for next-generation multi-junction PV architectures which demand both high performance and sustainability.

Keywords: CuI thin films, p-type semiconductor, non-reactive magnetron sputtering, transparent semiconductors, photovoltaics, heterojunctions.

References:

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