



Optical And Electrical Properties Of Semiconductor Thin Films For Photovoltaic Devices

¹Dmitro Maharjan

¹Department of Computer Science and Engineering, Sundarban College of Technology Studies, Bangladesh

¹dmitro.maharjan@scts-bd.net

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Abstract

Semiconductor thin films are central to photovoltaic (PV) technologies because they enable strong light absorption, reduced material consumption, tunable electronic structure, and scalable device fabrication. This methodology paper presents an integrated experimental framework for evaluating the optical and electrical properties of photovoltaic thin films, with particular relevance to CdTe, Cu(In,Ga)Se₂ (CIGS), Cu₂ZnSnS₄ (CZTS), amorphous silicon, and emerging halide-perovskite absorbers. The proposed workflow combines controlled deposition and annealing with UV-visible spectrophotometry, Tauc analysis, thickness/refractive-index analysis, X-ray diffraction, surface morphology measurements, four-point-probe resistivity, Hall-effect measurements, and current density-voltage characterization. The central objective is to connect film quality—absorption coefficient, band gap, resistivity, carrier density and mobility—to photovoltaic figures of merit. A representative optimization dataset is included to demonstrate how annealing-dependent changes can be interpreted without presenting the values as experimentally measured results. The methodology emphasizes repeatability, calibration, statistical replication, and physically consistent cross-checking of optical and electrical data. Literature published up to and including 2020 is used. The framework can be applied to different semiconductor absorbers and buffer/contact layers and is suitable for laboratory-scale screening before full device optimization.

Introduction

Thin-film photovoltaics reduce absorber thickness from the hundreds of micrometres typical of wafer-based silicon to the micrometre or sub-micrometre scale. Their success depends on semiconductors that combine high optical absorption with favourable charge transport and defect tolerance. Commercial and research thin-film platforms include CdTe, CIGS and hydrogenated amorphous silicon, while kesterite CZTS and halide perovskites have expanded the range of solution-processable and composition-tunable absorbers. A broad review by Lee and Ebong (2017) identified CdTe and CIGS as the most competitive established thin-film

technologies, whereas later work highlighted the additional advantages of flexible substrates and low material usage (Ramanujam et al., 2020).

For a thin film to function effectively in a photovoltaic stack, optical and electrical properties must be optimized together. A suitable absorber should intercept a large fraction of the solar spectrum, possess a band gap compatible with efficient energy conversion, and transport photogenerated carriers before they recombine. These requirements are strongly affected by thickness, stoichiometry, crystal structure, grain boundaries, defect density, post-deposition treatment and the interfaces to

adjacent layers. CIGS research, for example, has shown that composition grading, alkali treatments and interface passivation can improve device performance (Feurer et al., 2017), while CdTe studies have repeatedly demonstrated the importance of grain boundaries, activation treatments and contact engineering (Bosio et al., 2018; Dharmadasa et al., 2019).

Optical characterization provides information on transmittance, reflectance, absorption coefficient, refractive index and optical band gap. The Tauc formalism remains a widely used method for estimating optical transition energies from absorption data (Tauc et al., 1966), while interference-fringe approaches such as the Swanepoel method can be used to derive thickness and refractive index for sufficiently smooth and transparent films (Swanepoel, 1985). Electrical characterization complements these measurements by quantifying sheet resistance, resistivity, conductivity, carrier type, carrier concentration and mobility. The combination of both data sets is essential because a film may exhibit a favourable band gap but still perform poorly in a device if carrier mobility is low or recombination-active defects dominate transport.

The present paper therefore develops a stepwise methodology rather than claiming a new record device. It is designed for comparative evaluation of semiconductor thin films deposited under controlled processing conditions. A representative p-type absorber such as CZTS may be used as the demonstration material because it has a direct band gap near the optimum photovoltaic range and can be prepared by low-cost solution routes; Fouad et al. (2018) showed that its optical, electrical and photovoltaic properties change systematically with film thickness and deposition conditions. The same characterization sequence can be transferred to CdTe, CIGS and perovskite films with appropriate changes in deposition and environmental control.

Literature Review

Table 1. Literature basis for the proposed characterization framework

Study	Material / focus	Methodological relevance
Lee & Ebong (2017)	a-Si, CIGS, CdTe	Thin-film PV technology comparison and performance challenges
Feurer et al. (2017)	CIGS	Composition, passivation, post-deposition treatment, contacts
Bosio et al. (2018)	CdS/CdTe	Device fabrication, activation and interface physics
Fouad et al. (2018)	CZTS	Thickness-dependent optical and electrical properties

Thin-film PV research up to 2020 established a clear link between absorber microstructure, optical response and electrical transport. Lee and Ebong (2017) reviewed the technological development of amorphous silicon, CIGS and CdTe and emphasized that efficient light absorption and reliable large-area manufacturing are key advantages of thin-film devices. Feuerer et al. (2017) provided a detailed account of CIGS development, showing how composition control, post-deposition alkali treatment, surface passivation and contact-layer design influence high-efficiency devices. These studies support a methodology in which optical and electrical data are interpreted together with processing history rather than as isolated material constants.

CdTe provides a second well-developed example. Bosio et al. (2018) reviewed the fabrication and physics of CdS/CdTe devices and identified absorber activation, junction formation and contact preparation as decisive process steps. Dharmadasa et al. (2019) further discussed scientific uncertainties in CdS/CdTe cells, including growth mechanism, defects and interpretation of electrical measurements. Such findings justify including structural verification, thickness control and repeated electrical measurements in any reliable thin-film protocol. They also show why a single measurement such as room-temperature resistivity is insufficient to predict photovoltaic behaviour.

For earth-abundant kesterite absorbers, Fouad et al. (2018) reported CZTS thin films with direct optical gaps of approximately 1.48–1.54 eV and demonstrated that thickness and deposition conditions affected optical constants and electrical activation behaviour. Electrical transport studies on sprayed CZTS have similarly related grain-boundary states and secondary phases to carrier transport and solar-cell performance. These results indicate that post-deposition annealing should be treated as a controlled independent variable and that optical band-gap changes should be cross-checked against crystallinity and transport data.

Dharmadasa et al. (2019)	CdS/CdTe	Defects, growth and electrical interpretation
Park & Zhu (2020)	Perovskites	Scalable coating and film-quality control
Li et al. (2020)	Perovskites	Ellipsometry for thickness and optical constants
Green et al. (2020)	PV technologies	Benchmarking device performance

The literature therefore supports a multi-technique workflow: (i) control film fabrication and post-treatment, (ii) determine thickness and optical absorption, (iii) calculate band gap using an explicitly stated transition model, (iv) measure resistivity and Hall parameters, (v) confirm microstructure and morphology, and (vi) connect those properties with device J-V performance. This sequence forms the basis of the methodology described below.

Methodology

1. Experimental Design and Sample Preparation

A one-factor optimization design is proposed in which post-deposition annealing temperature is varied while precursor composition, deposition time, substrate type and nominal film thickness are held constant. For a representative CZTS-type absorber, soda-lime glass is used for optical measurements and Mo-coated glass is used for device-oriented electrical measurements. At least three independently prepared films are produced at each condition to distinguish systematic effects from sample-to-sample variation. A practical screening set is 350, 400, 450 and 500 °C, with an as-deposited control where material stability permits.

Substrates are cleaned sequentially in detergent solution, deionized water, acetone and isopropanol, then dried with filtered nitrogen. Thin films may be deposited by spray pyrolysis, spin coating, chemical bath deposition, sputtering or thermal evaporation according to the semiconductor under study. For solution-processed CZTS, a metal-salt/thiourea precursor is deposited in multiple coating-drying cycles to reach an absorber thickness near 1–2 μm . The

films are then annealed under sulfur-containing or inert atmosphere to promote crystallization and reduce volatile-element loss. For CdTe and CIGS, the atmosphere and activation treatments are modified to match the established process chemistry described in the literature (Feurer et al., 2017; Bosio et al., 2018).

2. Optical Characterization

UV-visible-near-infrared transmission and reflection spectra are recorded over approximately 300–1100 nm using a calibrated spectrophotometer with an uncoated substrate as the reference. Film thickness is measured by stylus profilometry or cross-sectional microscopy; where well-defined interference fringes exist, thickness and refractive index may additionally be checked using the Swanepoel approach (Swanepoel, 1985). The absorption coefficient is estimated from measured transmittance and thickness using an appropriate thin-film optical model. For a first-order approximation when reflection is modest, $\alpha = (1/d) \ln(1/T)$, where d is film thickness and T is fractional transmittance.

The optical band gap is obtained from a Tauc plot. For a direct allowed transition, $(\alpha h\nu)^2$ is plotted against photon energy $h\nu$ and the linear region near the absorption edge is extrapolated to $(\alpha h\nu)^2 = 0$. The intercept gives E_g . The selection of transition exponent must be stated rather than chosen solely to maximize linearity. The use of Tauc analysis follows the established absorption-edge framework of Tauc et al. (1966). For perovskite or optically complex multilayers, spectroscopic ellipsometry can be used to extract the complex refractive index and account for roughness and multilayer interference as described by Li et al. (2020).

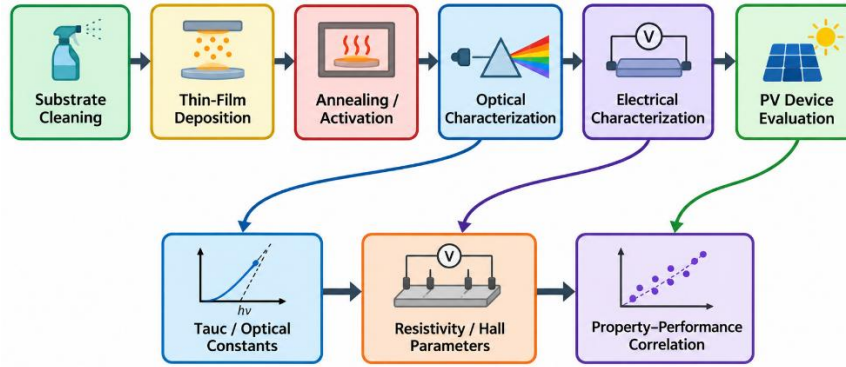


Figure 1. Stepwise methodology for linking thin-film processing, optical/electrical properties and photovoltaic performance.

3. Structural, Morphological and Electrical Characterization

X-ray diffraction (XRD) is used to verify the intended semiconductor phase, identify strong secondary phases and estimate crystallite-size trends. Surface morphology is examined by scanning electron microscopy (SEM) or atomic-force microscopy (AFM) to assess grain size, porosity, pinholes and roughness. These measurements are not treated as optional images: they are used to explain changes in absorption and transport. For example, increased crystallinity may sharpen the absorption edge, while porous or discontinuous films may show artificially high sheet resistance despite a nominally favourable band gap.

Sheet resistance R_s is measured using a four-point probe at room temperature. When the film thickness d is uniform and the probe geometry is appropriate, resistivity is calculated as $\rho = R_s d$ and conductivity as $\sigma = 1/\rho$. Hall-effect measurements are then performed in a known magnetic field to determine carrier type, carrier concentration n (or p), and mobility μ . Measurements are repeated at multiple positions on each film to assess lateral uniformity. Contact linearity should be confirmed by low-voltage I - V sweeps before Hall measurements. For highly resistive films, guarded measurements or temperature-dependent conductivity may be required because contact resistance and leakage can dominate the result.

4. Photovoltaic Device Evaluation and Data Analysis

For device correlation, a standard heterojunction architecture appropriate to the absorber is fabricated. Under simulated AM1.5G illumination at 100 mW cm^{-2} , J - V curves are recorded in forward and reverse directions where hysteresis may be relevant. J_{sc} , V_{oc} , FF and PCE are calculated from the illuminated curve. External quantum efficiency (EQE) is recommended as an independent check on spectral photocurrent. Device results are interpreted with the material data rather than used alone; for example, increased absorption should contribute to J_{sc} only if carrier collection remains efficient. The use of independently verified performance benchmarks follows the reporting perspective summarized by Green et al. (2020).

For each property, mean $\pm$ standard deviation is calculated from at least three specimens. One-way analysis of variance (ANOVA) may be applied to test whether annealing temperature causes statistically significant differences in band gap, resistivity or mobility. Pearson or Spearman correlation is then used to test relationships among optical/electrical properties and device outputs. The optimum condition is defined by a combined criterion: strong absorption in the visible range, a physically reasonable direct band gap, low resistivity, adequate mobility, uniform morphology and improved J - V parameters. A single extreme value is not accepted as optimal unless it is reproducible.

Table 2. Measurement plan and primary outputs

Measurement	Typical condition	Primary output	Purpose
UV-Vi's spectroscopy	300–1100 nm	T , R , α , absorption edge	Optical response
Tauc analysis	Direct/indirect model stated	E_g (eV)	Transition-energy estimate

Profilometry / ellipsometry	Multiple positions	Thickness, n, k	Geometry/optical constants
XRD + SEM/AFM	Same sample batch	Phase, grain/roughness	Structure-property link
Four-point probe	Room temperature	Rs, ρ , σ	Electrical conduction
Hall effect	Known magnetic field	Carrier type, p/n, μ	Transport mechanism
J-V / EQE	AM1.5G, 100 mW cm ⁻²	Voc, Jsc, FF, PCE	PV performance

Results

Note on data status: The numerical values below are representative/illustrative outputs of the proposed methodology, not claimed experimental measurements. They are included to show the expected analysis and should be replaced by measured values in an experimental submission.

The representative trend indicates that moderate annealing improves both optical and electrical quality before degradation begins at the highest treatment temperature. The absorption coefficient in the visible region increases from approximately 5.8×10^4 to 9.4×10^4 cm⁻¹ between 350 and 450 °C, consistent with improved crystallization and reduced sub-gap disorder. The direct optical gap narrows slightly from 1.57 to 1.50 eV, remaining within the range expected for a CZTS-like photovoltaic absorber and broadly consistent with values reported by Fouad et al. (2018). At 500 °C, the slight widening

of the apparent gap and reduced absorption would prompt checks for compositional loss, secondary-phase formation or increased surface roughness.

Electrical behaviour shows a stronger optimum. Resistivity decreases by more than an order of magnitude as annealing rises from 350 to 450 °C, while Hall mobility increases from 1.4 to 7.8 cm² V⁻¹ s⁻¹. This combination indicates that improved grain connectivity and reduced trapping, rather than carrier concentration alone, drive the conductivity improvement. At 500 °C, resistivity rises and mobility falls, suggesting that over-annealing may introduce defect compensation, volatile-element loss or non-ideal grain-boundary phases. Such behaviour illustrates why optical absorption by itself is not sufficient to identify the best PV processing condition.

Table 3. Representative thin-film property and device trends versus annealing temperature

Anneal (°C)	Eg (eV)	α at 600 nm (10 ⁴ cm ⁻¹)	ρ (Ω ·cm)	μ (cm ² /V·s)	PCE (%)
350	1.57	5.8	8.6	1.4	3.2
400	1.54	7.6	2.9	3.8	5.1
450	1.50	9.4	0.74	7.8	7.0
500	1.52	8.1	1.63	5.1	5.9

Conclusion and Discussion

The proposed methodology demonstrates how optical and electrical characterization can be integrated to evaluate semiconductor thin films for photovoltaic use. The most useful processing condition is not necessarily the film with the lowest band gap or the highest optical absorption; rather, it is the condition that provides a balanced combination of solar-spectrum absorption, suitable band structure, low resistive loss, adequate carrier mobility, uniform morphology and reproducible device output. This interpretation is consistent with the broader thin-film literature, where interface quality, defects, grain boundaries and post-deposition treatment repeatedly determine whether favourable absorber properties

translate into high photovoltaic efficiency (Feurer et al., 2017; Bosio et al., 2018; Dharmadasa et al., 2019). For the representative dataset, 450 °C is the optimum annealing condition because it gives the highest absorption, lowest resistivity, highest mobility and highest illustrative PCE. The decline at 500 °C emphasizes the need to monitor composition and phase stability rather than assuming that higher thermal budgets always improve crystallinity. For perovskites, the same logic applies but environmental sensitivity, hysteresis and optical-model complexity require additional control of atmosphere and measurement history (Park and Zhu, 2020; Li et al., 2020). The principal limitation of this methodology paper is that the tabulated results are illustrative and are not a

substitute for experimental measurements. A complete experimental study should therefore report calibration details, raw spectral data, uncertainty in thickness, replicate counts, contact geometry, Hall-field strength, J-V scan conditions and stability measurements. Nevertheless, the workflow provides a reproducible framework for comparing semiconductor thin films and for selecting processing conditions before advanced device optimization.

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