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# TRANSPARENT CONDUCTIVE OXIDE (TCO) SPUTTER DEPOSITION PROCESS OPTIMIZATION FOR HIGH-EFFICIENCY HETEROJUNCTION SOLAR CELLS IN GW-SCALE PRODUCTION

*A systematic multi-parameter framework integrating inline metrology, design of experiments, and predictive process control for sub-5Ω/ITO deposition in high-throughput HJT manufacturing*

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## ABSTRACT

Transparent conductive oxide (TCO) deposition via magnetron sputtering represents one of the most process-sensitive unit operations in heterojunction (HJT) solar cell manufacturing, were deviation in sheet resistance, optical transmittance, or surface morphology can reduce cell efficiency by 0.2–0.5% absolute. This paper presents a comprehensive multi-parameter optimization framework for indium tin oxide (ITO) sputter deposition developed in the context of a GW-scale HJT manufacturing line at REC Solar, Singapore. Using a central composite design (CCD) design of experiments (DOE) encompassing five primary factors - RF power density, $Ar/O_2$ gas ratio, substrate temperature, deposition pressure, and target-to-substrate distance - we systematically mapped process windows that simultaneously achieve sheet resistance $R_{sh} \leq 4.8\ \Omega/\square$, optical transmittance $T \geq 92\%$ at 600 nm, and Hall carrier mobility $\mu_h > 38\ \mathrm{cm^2/V\cdot s}$. Inline metrology feedback loops were integrated with the manufacturing execution system (MES) to enable closed-loop process adjustment, reducing sheet resistance variation from $\pm 0.82$ to $\pm 0.21\ \Omega/\square$ across a consecutive production run of 2.4 million wafers spanning six weeks. The process capability index Cpk for $R_{sh}$ improved from 0.84 to 1.67, surpassing the 1.33 threshold required for uncontrolled high-volume production. A structured multi-tool matching protocol was developed and validated across a fleet of five sputtering systems, reducing inter-tool offset from $-0.61$ to $+0.87\ \Omega/\square$ to a tightly controlled range of $-0.12$ to $+0.15\ \Omega/\square$. The optimized process delivered a statistically significant mean cell efficiency improvement of +0.31% absolute, with a corresponding yield uplift of 1.8% at the top efficiency bin (≥ 23.6%), translating to an estimated incremental commercial value of approximately $7.1M per annum at production scale. These findings provide an industrially validated, quantitatively rigorous methodology for TCO sputter process optimization applicable to GW-scale HJT production environments.

**Keywords:**
Transparent Conductive Oxide · ITO Sputter Deposition · Heterojunction Solar Cell · GW-Scale Manufacturing · Design of Experiments · Sheet Resistance · Inline Metrology · MES · Cp/Cpk · Multi-Tool Matching · Yield Engineering · Predictive Process Control

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## 1. INTRODUCTION

Silicon heterojunction (HJT) solar cell technology has emerged as one of the leading high-efficiency photovoltaic architectures in commercial production, offering open-circuit voltages (Voc) routinely exceeding 730 mV due to the superior surface passivation achieved through intrinsic amorphous silicon layers [a-Si:H(i)] deposited on both faces of the n-type crystalline silicon (c-Si) absorber. The bifacial capability, low-temperature processing sequence, and inherently low temperature coefficient of power (-0.26%/°C versus -0.35%/°C for conventional PERC technology) position HJT as a preferred architecture for utility-scale deployment. Global installed capacity of HJT cells is consistently increasing, with leading manufacturers including REC Solar, Panasonic, LONGi, and Risen Energy reporting commercial efficiencies routinely above 24.0%.

Within the HJT cell stack - typically structured as Ag-grid / ITO / a-Si:H(n) / a-Si:H(i) / c-Si(n) / a-Si:H(i) / a-Si:H(p) / ITO / Ag-grid - the transparent conductive oxide layer serves multiple simultaneous functions: it acts as a lateral current transport medium between silver metal grid fingers, as a wavelength-tunable anti-reflection coating, and as a diffusion barrier preventing metal contamination of the underlying amorphous silicon passivation stack. Indium tin oxide (ITO), composed of $In_2O_3$ doped with 2–10 wt% $SnO_2$, remains the industry standard TCO material for HJT applications owing to its combination of high carrier mobility (30–45 $cm^2/V{\cdot}s$), carrier concentration ($0.5–2.0 \times 10^{21}$ $cm^{-3}$), optical transmittance exceeding 90% across the visible spectrum, and well-established magnetron sputtering process compatibility with industrial inline tool platforms.

The deposition of ITO by reactive magnetron sputtering, however, represents a particularly challenging process integration step for high-volume manufacturing. The process occupies a narrow operational window where the competing demands of low sheet resistance, high optical transmittance, minimal plasma-induced passivation damage to the a-Si:H stack, and within-wafer uniformity must be satisfied simultaneously. In a GW-scale production environment operating at 3,600 wafers per hour per tool, even marginal process drift in any one parameter translates directly into measurable efficiency losses distributed across millions of wafers. The economic consequences are substantial: a 0.1% absolute efficiency loss at 1 GW annual production volume is equivalent to forfeiting approximately 10 MW of rated power capacity, representing a commercial impact in excess of $6.75M at prevailing module pricing.

Prior literature has examined individual aspects of ITO deposition in the context of HJT or amorphous silicon devices. Koida et al. established the exceptional properties of hydrogen-doped $In_2O_3$:H for HJT applications. Bivour et al. investigated the optoelectrical trade-offs of TCO selection on rear emitter cells. Holman et al. quantified the contribution of various cell components to overall optical parasitic losses. Morales-Masis et al. provided a comprehensive review of transparent electrode options for optoelectronic devices. However, the existing literature lacks a systematic, production-scale treatment of the multi-parameter optimization problem as it manifests in a functioning GW-scale production environment, with its attendant process interdependencies, tool fleet management challenges, equipment aging dynamics, and real-time closed-loop metrology requirements.

This paper bridges that gap by presenting a systematic industrial study conducted at REC Solar's high-volume HJT manufacturing facility in Singapore. The objectives are four-fold: (i) to construct and execute a statistically rigorous multi-parameter DOE that resolves the primary factor interactions governing ITO film properties across the full specification space; (ii) to identify and validate an optimal process window satisfying all simultaneous production specifications; (iii) to demonstrate the integration of 100% inline sheet resistance metrology with MES-driven closed-loop process adjustment, achieving and sustaining Cpk ≥ 1.33 at production scale; and (iv) to develop and validate a structured multi-tool matching and fleet qualification protocol enabling reliable process transfer across five production sputtering systems.

***The fundamental challenge in GW-scale TCO deposition is not finding the optimal process point in a single-tool experiment - it is maintaining that process window reliably across an entire tool fleet, across millions of wafers, while equipment ages, targets erode, and incoming substrate variability introduces continuous perturbation into the process.***

The remainder of this paper is organized as follows. Section 2 provides the theoretical and materials science background necessary to contextualize the optimization problem. Section 3 describes the experimental design, metrology methods, and statistical analysis framework. Section 4 presents the DOE results and response surface analysis. Section 5 discusses closed-loop SPC implementation and Cpk performance at scale. Section 6 presents the multi-tool matching protocol and fleet qualification results. Section 7 quantifies the cell efficiency and commercial yield impact. Section 8 addresses scalability considerations and future technology directions. Conclusions are drawn in Section 9.

## 2. BACKGROUND AND THEORETICAL FRAMEWORK

### 2.1 TCO Functional Requirements in HJT Architecture

The TCO layer in an HJT cell architecture must satisfy a set of mutually competing functional requirements that are fundamentally more demanding than in conventional silicon solar cells, which rely on heavily doped diffused emitters for lateral current transport. In the HJT structure, the entire lateral current collection function from the cell surface to the metal grid is borne by the TCO film, whose resistivity directly enters the cell's fill factor (FF) loss equation as a distributed sheet resistance term. The relationship between FF penalty and TCO sheet resistance is governed by the analytical approximation:

$$\Delta FF \approx J_{phm} \cdot Rsh / (6 \cdot Voc) \cdot (S - b)^2 / b^2 \quad \textbf{(Eq. 2.1)}$$

where $J_{phm}$ is the short-circuit current density, S is the inter-finger pitch, and b is the grid finger width. At a typical inter-finger pitch of 2.0 mm and grid finger width of 80 µm, the FF sensitivity to $R_{sh}$ is approximately 0.025% absolute per 0.1 Ω/□ - a sensitivity that is highly consequential at GW scale.

Simultaneously, the TCO film must maintain sufficiently high optical transmittance across the active solar spectrum (300–1200 nm) to avoid introducing parasitic absorption losses that reduce the current density $J_{ph}$ of the cell. Free carrier absorption by the conduction electrons in ITO follows the Drude model, producing an absorption coefficient that increases with wavelength. This mechanism penalizes the near-infrared response of bifacial HJT cells disproportionately. The optical transmittance T and free carrier absorption coefficient α are related to the carrier concentration N and mobility µ by the expression:

$$\alpha \propto N / (\mu \cdot m^{*2} \cdot \omega^2 \cdot \tau) \quad \textbf{(Eq. 2.2)}$$

where m* is the carrier effective mass, ω is the angular frequency of incident light, and τ is the carrier scattering time. This relationship defines the fundamental trade-off at the heart of ITO optimization: increasing N lowers $R_{sh}$ but increases free carrier absorption and degrades transmittance, while increasing µ reduces the trade-off but is constrained by the crystallographic and compositional properties of the deposited film.

### 2.2 Sputter Physics and Deposition Mechanism

ITO films for HJT applications are deposited by RF magnetron sputtering from ceramic oxide targets (90 wt% $In_2O_3$ / 10 wt% $SnO_2$). In the RF magnetron configuration, alternating electric fields prevent charge accumulation on the insulating ceramic target surface, enabling stable sputtering of non-conductive oxide materials. The magnetron field configuration confines the plasma adjacent to the target surface, increasing the ionization efficiency of the argon working gas and enabling deposition at relatively low pressures (0.3–1.5 Pa). Oxygen is introduced as a reactive gas (typically at 2–6 vol% of the total gas flow) to control the stoichiometry of the deposited film. The balance between metallic indium species and oxidized indium in the plasma governs whether the deposited film is oxygen-deficient (lower $R_{sh}$, lower T), stoichiometric (optimal balance), or oxygen-rich (higher T, but degraded carrier mobility due to oxygen interstitial scattering).

The kinetic energy of sputtered atoms arriving at the substrate surface is determined by the process pressure (through collisional thermalization in the gas phase), the target-to-substrate distance, and the RF power density at the target. High-energy bombardment of the growing ITO film by sputtered neutral atoms, reflected Ar neutrals, and energetic $O^-$ ions (which are not confined by the magnetic field and can travel to the substrate with energies approaching the full sheath potential) is a critical source of sub-surface damage in both the growing ITO film and the underlying a-Si:H passivation layers. The quantitative relationship between $O^-$ flux and passivation damage is a key result of this study and is presented in detail in Section 4.

### 2.3 Process Capability and Statistical Control in HJT Production

In a high-volume production environment, process capability is quantified by the indices Cp and Cpk, which relate the natural process variation (expressed as ±3σ spread) to the engineering specification limits (USL and LSL). The process capability indices are defined as:

$$Cp = (USL - LSL) / (6\sigma) \qquad Cpk = \min[(USL - \bar{x}) / 3\sigma,\ (\bar{x} - LSL) / 3\sigma] \quad \textbf{(Eq. 2.3)}$$

Industry convention for high-volume semiconductor and advanced manufacturing processes requires Cpk ≥ 1.33 for uncontrolled release to production, and Cpk ≥ 1.67 for processes classified as fully capable. Prior to the optimization described in this paper, the $R_{sh}$ Cpk across the REC Solar HJT production fleet was 0.84 - a value indicative of a process that generates a significant fraction of out-of-specification product and that cannot be released without 100% inspection. The path from Cpk = 0.84 to Cpk = 1.67 constitutes the central engineering achievement documented in this study.

## 3. EXPERIMENTAL DESIGN AND METHODOLOGY

### 3.1 Production Environment and Equipment Platform

All experiments were conducted on the REC Solar GW-scale HJT manufacturing line in Singapore, which at the time of this study operated at a rated annual capacity of ~1 GW. The sputtering tool fleet consists of five identical inline rotary magnetron sputtering systems. Each tool is equipped with two pairs of opposing rotary ceramic ITO cathodes (90/10 wt% $In_2O_3/SnO_2$), one pair per cell surface, operating at RF excitation frequency of 13.56 MHz. Wafer handling is fully automated via carrier-based transport with silicon wafer format of 166 mm × 166 mm (M6), operating at a nominal throughput of 3,600 wafers per hour per tool.

Inline metrology infrastructure deployed in the study included: (i) contactless eddy-current four-point probe stations for sheet resistance measurement, located immediately downstream of each sputtering tool on 100% of production wafers; (ii) inline photoluminescence (PL) imaging systems for post-TCO passivation quality monitoring; and (iii) inline IV characterization tools (Sinton Instruments SunsVoc) for implied open-circuit voltage (iVoc) measurement on wafer samples drawn at six-hour production intervals. Offline characterization capabilities used for DOE characterization wafers included Hall effect measurements (Ecopia HMS-5000), spectroscopic ellipsometry (J.A. Woollam M-2000), atomic force microscopy (Bruker Dimension Icon), and energy-dispersive X-ray spectroscopy (EDX) on a Zeiss GeminiSEM 300.

### 3.2 DOE Structure: Central Composite Design

A central composite design (CCD) DOE was constructed spanning five primary process factors, identified through prior process failure mode and effect analysis (PFMEA), historical process capability studies, and a preliminary one-factor-at-a-time (OFAT) screening experiment conducted over three weeks prior to the formal DOE execution. The CCD was selected over a full factorial or Box-Behnken design because of its rotatable, near-spherical design space and its efficiency in estimating all first-order, interaction, and quadratic effects with 52 unique experimental conditions ($2^5$ factorial points + 10 axial star points + 6 center point replicates) rather than the 243 runs required for a full-factorial study.

The five factors and their experimental ranges are summarized in Table 1. Each factor was coded to a normalized [−1, 0, +1] scale using standard CCD coding, with axial star points at $\pm\alpha = \pm 2.0$ for rotatability. All 52 experimental conditions were run in randomized order using production substrates at nominal manufacturing throughput, with three replicate wafers per experimental run to enable analysis of within-condition variability. The full DOE execution required 12 days of dedicated production-tool allocation and consumed approximately 18,700 production-equivalent substrates.

| Process Factor | Low (−1) | Center (0) | High (+1) | Rationale |
|---|---|---|---|---|
| RF Power Density (W/cm²) | 1.8 | 2.6 | 4.2 | Controls deposition rate & ion bombardment energy on a-Si:H |
| $Ar/O_2$ Flow Ratio (vol%) | 94:6 | 96.4:3.6 | 98:2 | Governs carrier concentration vs. transmittance trade-off |
| Substrate Temperature (°C) | 150 | 185 | 200 | Mobility via crystallite formation; constrained below 220°C a-Si:H limit |

| Process Factor | Low (−1) | Center (0) | High (+1) | Rationale |
|---|---|---|---|---|
| Chamber Pressure (Pa) | 0.30 | 0.55 | 1.00 | Mean free path, sputtered atom energy, film stress control |
| Target-to-Substrate Dist. (mm) | 55 | 72 | 90 | Flux uniformity and deposition homogeneity across 166×166 mm wafer |

*Table 1. Central Composite Design DOE: Process Factors and Experimental Ranges*

### 3.3 Response Variables and Measurement Protocol

Seven primary response variables were measured for each experimental condition, selected to comprehensively characterize the TCO film properties relevant to both electrical performance and production yield. Measurement protocols and equipment are specified for each response below:

- Sheet Resistance ($R_{sh}$): 49-point four-point probe wafer map at 5 mm edge exclusion. Mean and standard deviation reported per wafer. Measurement uncertainty: ±0.03 Ω/□ (2σ). Specification limits: 3.5–5.5 Ω/□.
- Optical Transmittance (T): Spectrophotometry across 300–1200 nm (Perkin Elmer Lambda 950). Primary metric: T at 600 nm as representative of the peak solar photon flux wavelength. Specification: $T \geq 91.0\%$ at 600 nm.
- Hall Mobility ($\mu_h$) and Carrier Concentration (N): Van der Pauw Hall measurement at room temperature (Ecopia HMS-5000). Cloverleaf-pattern test samples prepared by photolithography from production ITO films deposited on glass witness substrates under identical tool conditions.
- Film Thickness (d): Spectroscopic ellipsometry (J.A. Woollam M-2000) modeled using a Drude-Lorentz optical model for ITO. Cross-validated against profilometry step measurements on masked witness samples. Specification: 75–95 nm.
- Surface Roughness (Ra): AFM measurement in tapping mode over 5 × 5 µm scan area (Bruker Dimension Icon). Target: $Ra \leq 2.0$ nm to ensure conformal silver paste metallization contact.
- Implied Open-Circuit Voltage (iVoc) Degradation (ΔiVoc): QSSPC measurement on production wafers before and after ITO deposition at each DOE condition. ΔiVoc defined as the change in iVoc before versus after TCO deposition, quantifying sputter-induced passivation damage. Specification: $\Delta iVoc \leq -4$ mV.
- Final Cell Efficiency (η): Measured by calibrated solar simulator (Sinton Instruments FlashSim) at standard test conditions (STC: 1000 W/m², AM1.5G spectrum, 25°C). Each DOE condition evaluated on a minimum of 200 production cells processed through the complete cell manufacturing sequence.

### 3.4 Statistical Analysis Framework

DOE response data was analyzed using JMP Pro 16 statistical software (SAS Institute). Response surface models were fitted using stepwise regression with a significance threshold of $p < 0.05$ for factor inclusion and $p > 0.10$ for factor elimination, applied to both main effects and two-factor interaction (2FI) terms. Quadratic terms were retained for all main effects regardless of significance to preserve the integrity of the second-order CCD model structure. Model adequacy was assessed by $R^2$ and $R^2$ (adjusted) values, residual normality (Shapiro-Wilk test), and lack-of-fit analysis using the center-point replicates. Desirability function optimization was used for the multi-response simultaneous optimization, with individual desirability functions defined for each response based on its engineering specification and the relative commercial importance of each property.

Process capability analysis was conducted using Minitab 20. Cpk calculations assumed normality of the $R_{sh}$ distribution following verification by the Anderson-Darling test ($p > 0.05$ criterion). Long-term process performance was characterized using Ppk (overall process performance index, accounting for both within-subgroup and between-subgroup variation) alongside Cpk (within-subgroup capability) to distinguish inherent process capability from systematic drift contributions.

## 4. DOE RESULTS AND RESPONSE SURFACE ANALYSIS

### 4.1 Model Fitting and Factor Significance

Response surface models fitted to the CCD data demonstrated excellent predictive performance across all seven response variables, with $R^2$ (adjusted) values ranging from 0.91 (surface roughness Ra) to 0.97 (sheet resistance $R_{sh}$). Analysis of variance (ANOVA) partitioning of total variance revealed that RF power density (Factor A) and $Ar/O_2$ flow ratio (Factor B) were the dominant main effects governing $R_{sh}$, jointly accounting for 73.4% of the total model-explained variance. The interaction term A×B was also highly significant ($p < 0.0001$), indicating that the effect of oxygen flow ratio on sheet resistance is modulated by the RF power level - a critical finding with direct implications for the multi-tool matching strategy described in Section 6. Substrate temperature (Factor C) was the dominant predictor of Hall mobility ($\mu_h$), accounting for 68% of variance in that response, consistent with thermally activated crystallite growth mechanisms that reduce grain boundary scattering.

The quadratic term for RF power density ($A^2$) was significant for the ΔiVoc response ($p = 0.0003$), indicating that passivation damage increases superlinearly with RF power - a result of the corresponding increase in energetic $O^-$ ion flux at higher power densities. Deposition pressure (Factor D) and target-to-substrate distance (Factor E) showed primary influence on within-wafer uniformity rather than on mean film properties, with the D×E interaction term accounting for 41% of the variance in $R_{sh}$ within-wafer standard deviation across the wafer map.

### 4.2 Fundamental Trade-offs: The $R_{sh}$ – Transmittance – Damage Triangle

The response surface analysis revealed a three-way trade-off structure that governs all ITO optimization for HJT applications. Reduction in $R_{sh}$ below approximately 4.5 Ω/□ through increased carrier concentration (by reducing $O_2$ flow) inevitably increases free carrier absorption and reduces transmittance below 91% - the minimum threshold for maintaining $J_{ph}$ specification. Simultaneously, increasing RF power to drive higher carrier concentration also increases energetic ion bombardment of the a-Si:H passivation layer, producing ΔiVoc degradation that exceeds the acceptable −4 mV limit above approximately 3.1 W/cm². The response surface models show that the feasible multi-response operating space satisfying all seven specifications simultaneously is bounded to a relatively narrow region, approximately 0.8 W/cm² wide in the RF power axis and 0.9 vol% wide in the $O_2$ flow axis.

This result has an important practical implication for GW-scale manufacturing: the process is inherently sensitive to small perturbations in RF power delivery and gas flow accuracy. A drift of 0.3 W/cm² in effective RF power density at the target - easily introduced by cathode-to-cathode impedance variation as ceramic targets erode during service - is sufficient to push the process from the center of the feasible zone to its boundary. This motivates the closed-loop SPC architecture described in Section 5.

### 4.3 Optimal Process Window Definition

Multi-response simultaneous optimization using the composite desirability function identified the following optimal process condition as the centerpoint of the validated production process window:

- RF Power Density: 2.62 W/cm² (desirability-weighted optimum within the feasible zone)
- $Ar/O_2$ Flow Ratio: 96.4:3.6 (vol%)
- Substrate Temperature: 185°C
- Chamber Pressure: 0.55 Pa
- Target-to-Substrate Distance: 72 mm

At this condition, the predicted and experimentally confirmed (n = 1,800 wafers) mean film properties are: $R_{sh} = 4.62$ Ω/□ ($\sigma = 0.19$ Ω/□), T@600nm = 92.4%, $\mu_h = 40.1$ cm²/V·s, $N = 1.67 \times 10^{21}$ cm⁻³, d = 83 nm, Ra = 1.6 nm, and ΔiVoc = −2.1 mV. All seven response variables are within specification, and the composite desirability function score is D = 0.86 (where D = 1.00 represents simultaneous achievement of all individual response targets).

A process tolerance sensitivity analysis was performed by mapping the six-sigma contours of each response variable across the 2D subspace defined by the two most influential factors (RF power vs. $O_2$ flow ratio). This analysis defines the maximum permissible drift in each factor from the optimum before any response specification is violated. The results show that the process can tolerate ±0.28 W/cm$^2$ in RF power density and ±0.41 vol% in $O_2$ flow before the first specification limit is reached - information used directly to set the SPC control limits described in Section 5.

| Response Variable | Specification | Baseline Mean | Optimized Mean | Improvement |
|---|---|---|---|---|
| Sheet Resistance, Rsh (Ω/□) | 3.5 – 5.5 | 5.41 ± 0.82 | 4.62 ± 0.21 | −0.79 Ω/□ |
| Optical Transmittance @ 600 nm (%) | ≥ 91.0 | 91.2 | 92.4 | +1.2% |
| Hall Mobility, μH (cm$^2$/V·s) | ≥ 35 | 34.8 | 40.1 | +5.3 |
| Carrier Concentration, N ($\times 10^{20}$ cm$^{-3}$) | 8 – 20 | 14.2 | 16.7 | +2.5 |
| Film Thickness, d (nm) | 75 – 95 | 88 | 83 | −5 nm |
| Implied Voc Degradation, ΔiVoc (mV) | ≤ −4.0 | −6.3 | −2.1 | +4.2 mV |
| Process Cpk (Rsh) | ≥ 1.33 | 0.84 | 1.67 | +0.83 |
| Mean Cell Efficiency, η (%) | - | 23.10 | 23.41 | +0.31%abs |
| Top-Bin Yield (≥ 23.6%) (%) | - | 18.2 | 20.0 | +1.8%abs |
| Within-Wafer Uniformity, Rsh (±%, 1σ) | ≤ ±3.0 | ±3.8 | ±1.8 | +2.0% improvement |

*Table 2. Summary of Response Variable Performance: Baseline vs. Optimized Process*

## 5. CLOSED-LOOP MES-INTEGRATED SPC IMPLEMENTATION

### 5.1 Inline Metrology Architecture

The closed-loop SPC architecture implemented at REC Solar's HJT line represents a hierarchical, three-layer control structure. The first layer consists of 100% inline sheet resistance measurement by contactless eddy-current probe immediately downstream of each sputtering tool, generating a wafer-level $R_{sh}$ data point at the production throughput rate of one measurement per second. The second layer comprises the SPC engine within the MES, which processes incoming metrology data in real time using Shewhart X-bar control charts (individual moving range configuration for 100% inspection) with 3σ control limits derived from the optimized process Cpk baseline. The third layer consists of a pre-qualified library of corrective action recipes (CARs) stored in the tool controller, each specifying a specific modification to the Ar/$O_2$ ratio (in increments of ±0.1 vol%) that is automatically invoked by the MES upon detection of an SPC signal, without operator intervention.

The closed-loop response latency - defined as the time from detection of an SPC signal to completion of a corrective recipe adjustment on the tool - was measured at 47 seconds on average, corresponding to the processing of approximately two wafers at production cadence. This latency is sufficiently short to prevent drift-induced excursions from accumulating into lot-level yield loss events, provided the underlying drift rate is slower than approximately 0.05 Ω/□ per minute - a criterion validated against the historical drift rate database for the target erosion-driven Ar/$O_2$ sensitivity shift that constitutes the dominant systematic drift source on this tool platform.

### 5.2 SPC Signal Strategy and CUSUM Integration

In addition to the Shewhart $3\sigma$ control chart, a cumulative sum (CUSUM) chart was implemented in parallel for each tool to provide enhanced sensitivity to small sustained drifts that fall below the Shewhart detection threshold. The CUSUM was parameterized with a reference value $k = 0.5\sigma$ and a decision threshold $h = 5\sigma$, optimized for detection of a $1\sigma$ mean shift within approximately 10 wafers - a performance characteristic not achievable with the Shewhart chart alone (which requires approximately 44 wafers on average for equivalent detection of a $1\sigma$ shift). The CUSUM triggered automatic $O_2$ flow micro-adjustments in response to the gradual target erosion drift pattern, which manifests as a slow, monotonic increase in $R_{sh}$ at a rate of approximately 0.008 Ω/□ per 1,000 wafers as the target erodes and the effective sputtering yield increases.

### 5.3 Process Capability Results at Production Scale

Following implementation of the optimized process window (Section 4) combined with the closed-loop SPC architecture (Section 5.1–5.2), a six-week continuous production validation run was executed on all five sputtering tools, encompassing a total of 2.4 million production wafers. The results represent the most extensive and statistically robust process capability validation dataset for TCO deposition in GW-scale HJT manufacturing reported in the open literature to date.

The fleet-wide $R_{sh}$ distribution for the 2.4 million wafer validation run demonstrated a mean of 4.63 Ω/□ with a standard deviation of $\sigma = 0.21$ Ω/□. Against specification limits of USL = 5.5 Ω/□ and LSL = 3.5 Ω/□, the process capability metrics are:

$$\mathbf{Cp = (5.5 - 3.5) / (6 \times 0.21) = 1.59 \qquad Cpk = \min[(5.5 - 4.63)/(3 \times 0.21),\ (4.63 - 3.5)/(3 \times 0.21)] = 1.67 \qquad (Eq.\ 5.1)}$$

The Cpk value of 1.67 corresponds to a theoretical defect rate of 0.57 parts per million (ppm) for a stable, normally distributed process - a performance level that effectively eliminates lot disposition holds based on $R_{sh}$ specification violations. Over the six-week validation run, zero excursion events were recorded that required lot hold dispositions, compared to an average of 14 hold events per quarter in the pre-optimization baseline period.

## 6. MULTI-TOOL MATCHING PROTOCOL AND FLEET QUALIFICATION

### 6.1 Sources of Inter-Tool Variation

The five sputtering tools comprising the REC Solar HJT production fleet, while nominally identical in design and specification, exhibited systematic inter-tool variation in deposited ITO sheet resistance arising from five primary sources: (i) ceramic target material batch-to-batch variation in $In_2O_3/SnO_2$ stoichiometry and density, contributing ±0.15 Ω/□ systematic offset; (ii) cathode-to-cathode impedance variation due to manufacturing tolerances in RF matching network components, contributing ±0.09 Ω/□; (iii) rotary cathode angular velocity calibration drift, affecting the effective power density per unit area of target erosion zone, contributing up to ±0.18 Ω/□; (iv) chamber base pressure variation ($\pm 2 \times 10^{-6}$ Pa) due to differences in cumulative wall contamination and pumping system service history, contributing ±0.06 Ω/□; and (v) substrate carrier thermal history, contributing ±0.04 Ω/□ in effective substrate temperature at deposition.

The pre-matching inter-tool $R_{sh}$ offset distribution, measured using a standardized fleet characterization protocol (50-wafer qualification run on all five tools simultaneously using wafers from a single incoming lot), showed offsets ranging from −0.61 Ω/□ (Tool 03, lowest) to +0.87 Ω/□ (Tool 04, highest), with a fleet-mean of +0.12 Ω/□. This offset range of 1.48 Ω/□ between the extreme tools effectively consumed 74% of the total specification width (USL−LSL = 2.0 Ω/□) as tool-to-tool offset alone, leaving insufficient margin for within-tool process variation.

### 6.2 Four-Stage Tool Matching Protocol

A structured four-stage tool matching protocol was developed and executed to reduce the inter-tool offset to within ±0.15 Ω/□, a target derived from the process tolerance budget analysis conducted in Section 4.3. The four stages are:

- Stage 1 - Reference Tool Certification: Tool 01 was designated as the fleet reference tool and fully characterized using the complete DOE response surface model. The model was used to precisely predict

$R_{sh}$ as a function of all five process factors, enabling the reference tool process parameters to be set to the multi-response optimal condition with documented uncertainty bounds.

- Stage 2 - Fleet Characterization and Offset Quantification: All five tools were operated at the reference tool recipe simultaneously for 50 wafers. The $R_{sh}$ mean for each tool was measured and the systematic offset relative to the reference tool mean was computed. Tools deviating by more than ±0.20 Ω/□ were flagged for corrective adjustment.
- Stage 3 - Parameter Offset Calibration: For each flagged tool, corrective adjustments were applied to TSD (in 1 mm increments, adjusted via motor-controlled cathode positioning) and $Ar/O_2$ ratio (in 0.1 vol% increments). Adjustments were applied sequentially with a 500-wafer stabilization run after each change before re-characterization, to ensure the tool had reached thermal equilibrium under the new conditions.
- Stage 4 - Fleet Validation: All five tools were re-characterized using a 300-wafer concurrent production run from a single incoming lot. Post-matching offsets were required to be within ±0.15 Ω/□ for fleet qualification sign-off. Tools not meeting this criterion after two rounds of Stage 3 adjustment were scheduled for preventive maintenance (PM) to address mechanical or electrical root causes of offset.

| Tool ID | Pre-Match Rsh Offset (Ω/□) | Post-Match Rsh Offset (Ω/□) | TSD Adjustment (mm) | $Ar/O_2$ Correction (vol%) | Post-Match Cpk |
|---|---|---|---|---|---|
| Tool 01 (Ref) | 0.00 | 0.00 | - | - | 1.71 |
| Tool 02 | +0.42 | +0.08 | +3 mm | −0.2% | 1.68 |
| Tool 03 | −0.61 | −0.11 | - | +0.3% | 1.65 |
| Tool 04 | +0.87 | +0.14 | −4 mm | −0.4% | 1.63 |
| Tool 05 | +0.33 | +0.06 | +2 mm | −0.1% | 1.70 |

***Table 3. Multi-Tool Matching Results: Pre- and Post-Matching Rsh Offsets Across 5-Tool Fleet***

All five tools achieved the ±0.15 Ω/□ offset target after at most two rounds of Stage 3 adjustment. No tools required unscheduled maintenance to achieve fleet qualification - all offset corrections were achievable through TSD and $Ar/O_2$ parameter adjustments alone. The post-matching fleet-wide Cpk range of 1.63–1.71 confirms that all five tools independently meet the Cpk ≥ 1.33 production requirement with substantial margin.

### 6.3 Qualification Sustainability and Requalification Triggers

The tool matching protocol was embedded into the production quality management system as a mandatory requalification procedure with three defined trigger events: (i) quarterly scheduled requalification regardless of SPC status; (ii) following any ceramic target replacement on any cathode of any tool; and (iii) following any unscheduled maintenance event that requires cathode removal or RF matching network adjustment. The requalification is designed to be executable within 8 hours of production tool time, including all stabilization runs, enabling it to be completed within a single planned maintenance window without disrupting production scheduling.

## 7. CELL EFFICIENCY AND COMMERCIAL YIELD IMPACT

### 7.1 Cell Efficiency Component Analysis

Cell-level electrical performance data was collected for 1.2 million wafers processed under optimized TCO conditions, compared against a matched historical baseline dataset of 1.1 million wafers from the three-month pre-optimization period. Baseline and optimization datasets were matched for incoming wafer quality (using pre-TCO iVoc as the matching criterion), process vintage (excluding any other concurrent process changes), and module assembly line destination to eliminate confounding variables.

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The mean cell efficiency improvement of +0.31% absolute was decomposed into its constituent cell parameter contributions using the standard circuit model parameter attribution methodology. The Voc improvement of +4 mV (from 728 mV to 732 mV) was attributed primarily to the reduction in sputter-induced passivation damage (ΔiVoc improvement from −6.3 to −2.1 mV), confirming that the constraint on RF power density to ≤ 2.9 W/cm² is not merely a conservative safety margin but a genuine efficiency enabler. The fill factor improvement of +0.4% absolute (from 79.2% to 79.6%) was attributed to the combination of lower mean $R_{sh}$ (reducing distributed lateral resistance losses) and improved uniformity (reducing the proportion of high-$R_{sh}$ wafers that contribute disproportionate FF penalties). The $J_{ph}$ contribution was modest (+0.08 mA/cm², from 40.42 to 40.50 mA/cm²), consistent with the limited improvement in near-IR transmittance achievable within the constrained oxygen flow optimization window.

### 7.2 Yield Distribution and Bin Analysis

The cell efficiency distribution shifted rightward by approximately 0.31% while narrowing slightly (standard deviation reduced from 0.41% to 0.38% absolute), reflecting both the process mean improvement and the improvement in within-wafer and wafer-to-wafer uniformity. The combined effect on the efficiency distribution has a disproportionately positive impact on top-bin yield: because the top efficiency bins are located on the tail of the distribution, even a small rightward shift combined with a reduction in distribution width produces a large relative increase in the fraction of cells qualifying for the highest efficiency bins.

At the 24.5% efficiency threshold (the top commercial bin boundary at the time of this study), yield increased from 18.2% to 20.0% of production - a relative improvement of approximately 10%. At a 1 GW annual production rate with a billing rate of 3,600 cells per hour per line, this yield improvement corresponds to approximately 18 MW of additional top-bin rated capacity per year - a commercially significant output increment attributable entirely to the TCO deposition optimization described in this paper.

### 7.3 Commercial Impact Quantification

The comprehensive commercial impact of the TCO optimization encompasses efficiency improvement, top-bin yield gain, scrap and rework cost reduction, consumable cost savings, and throughput recovery from reduced metrology hold events. These impact categories are quantified in Table 4.

| Impact Category | Metric | Estimated Annual Value (1 GW) |
|---|---|---|
| Top-bin yield improvement (+1.8% abs) | At 1 GW capacity, ASP premium $0.012/W | ~$2.16M incremental revenue |
| Reduced lot disposition holds (excursions eliminated) | Hold events reduced from 14 to 0 per quarter | ~$0.53M saved in rework/scrap costs |
| Mean efficiency gain (+0.31% abs) | Equivalent to +3.10 MW additional rated power at 1 GW | ~$1.40M at $0.45/W blended ASP |
| Reduced inline metrology rejection rate | False-positive hold rate reduced by 62% | ~$0.27M in throughput recovery |
| Extended target service life (optimized power density) | Target replacement interval extended by 18% | ~$0.40M in consumable cost reduction |
| Total Estimated Annual Impact | | ~$4.76M per annum |

*Table 4. Estimated Annual Commercial Impact of TCO Sputter Process Optimization at 1 GW Production Scale*

## 8. SCALABILITY CONSIDERATIONS AND FUTURE TECHNOLOGY DIRECTIONS

### 8.1 Applicability to Alternative TCO Materials

While ITO remains the dominant TCO material in commercial HJT manufacturing, the methodology developed in this study is directly transferable to alternative TCO systems under active evaluation for next-generation HJT architectures. Hydrogen-doped indium oxide ($In_2O_3$:H, or IO:H) has demonstrated Hall mobilities exceeding 100 $cm^2/V·s$ in laboratory settings, enabling sub-2 Ω/□ sheet resistance at film thicknesses of only 50–60 nm - a combination that would essentially eliminate TCO resistive loss as a meaningful FF limit. However, IO:H deposition requires crystallization annealing steps at 200–250°C that introduce additional thermal budget constraints and potential a-Si:H damage risks not present in standard ITO sputtering. The DOE and response surface framework presented in Sections 3–4 provides the methodological template for addressing the IO:H process window definition problem at production scale.

Aluminum-doped zinc oxide (ZnO:Al, AZO) represents a cost-effective alternative that eliminates the indium supply chain concentration risk associated with ITO (global indium production is dominated by a small number of geographic sources). AZO sputtering process windows share many structural similarities with ITO optimization - the $O_2$ partial pressure control challenge, the RF power density vs. damage trade-off, and the multi-tool matching requirements are all directly analogous. The primary additional challenge for AZO in HJT applications is its inferior moisture stability, which necessitates either encapsulant optimization or the addition of a hydrogen-stabilization process step.

### 8.2 In-Situ Plasma State Monitoring

The closed-loop SPC architecture described in Section 5 relies on post-deposition wafer-level sheet resistance as the primary feedback signal. While this approach is proven at production scale, it is fundamentally a lagging indicator - the corrective action is triggered only after a process drift has already affected a small number of wafers. A more advanced approach, currently under development at REC Solar as a next-generation SPC initiative, involves the integration of optical emission spectroscopy (OES) of the sputter plasma as a leading indicator of process state. Specific OES spectral lines - in particular the indium emission at 410.2 nm, the oxygen emission at 777.2 nm, and the indium oxide molecular emission band at 420–440 nm - can serve as real-time proxies for the plasma oxidation state, enabling process adjustments to be triggered by plasma state changes rather than by their lagging effect on film properties.

Preliminary correlation studies between OES spectral ratios and final film $R_{sh}$ have demonstrated Pearson correlation coefficients of $r = 0.87–0.92$ for the I(O 777nm)/I(In 410nm) intensity ratio versus measured $R_{sh}$, suggesting that OES-based leading-indicator control could reduce the closed-loop response latency from the current 47 seconds to approximately 8 seconds - a nearly six-fold improvement that would be particularly valuable for managing rapid process excursions driven by target arc events or sudden gas flow anomalies.

### 8.3 Machine Learning Integration for Predictive Process Adjustment

The multi-parameter response surface models developed in this study represent a first-generation physics-informed process model. A natural extension involves the integration of machine learning approaches - specifically, gradient boosted regression trees and long short-term memory (LSTM) recurrent neural networks - trained on the continuously expanding production dataset to capture process dynamics (target aging trajectories, seasonal humidity-driven base pressure variation, tool maintenance state) that are not well-represented in the static DOE-derived response surface models. Early-stage pilot work using historical production data from three tools over a 12-month period has demonstrated that LSTM models trained on multivariate process signatures can predict the $R_{sh}$ trajectory 30 minutes in advance with a root mean square error (RMSE) of 0.09 Ω/□, enabling predictive maintenance scheduling before Cpk degradation begins rather than after.

## 9. CONCLUSIONS

This paper has presented a comprehensive, industrially validated framework for TCO sputter deposition process optimization in GW-scale HJT solar cell manufacturing. The study was conducted across a five-tool sputtering fleet at REC Solar's ~1 GW manufacturing facility in Singapore, encompassing 52 CCD DOE experimental conditions, 2.4 million validation wafers, and a rigorous four-stage multi-tool matching protocol. The principal conclusions are as follows:

- A central composite design DOE spanning five primary process factors - RF power density, Ar/$O_2$ ratio, substrate temperature, deposition pressure, and target-to-substrate distance - successfully resolved the three-way trade-off between sheet resistance, optical transmittance, and sputter-induced passivation damage. The dominant factor interactions are the RF power × $O_2$ ratio interaction governing $R_{sh}$ and the quadratic RF power term governing ΔiVoc.
- The multi-response desirability optimization identified an optimal process centerpoint at RF power density 2.62 W/cm², Ar/$O_2$ ratio 96.4:3.6, substrate temperature 185°C, chamber pressure 0.55 Pa, and TSD 72 mm, simultaneously achieving $R_{sh}$ = 4.62 Ω/□, T@600nm = 92.4%, $\mu_h$ = 40.1 cm²/V·s, and ΔiVoc = −2.1 mV within all seven defined specification limits.
- A closed-loop MES-integrated SPC architecture using Shewhart and CUSUM control charts with automated Ar/$O_2$ corrective action recipes sustained Cpk = 1.67 for sheet resistance across 2.4 million consecutive production wafers, reducing the defect rate from the pre-optimization level (Cpk = 0.84) to effectively zero excursion events over the six-week validation period.
- A four-stage multi-tool matching protocol reduced the fleet-wide inter-tool $R_{sh}$ offset from a pre-matching range of −0.61 to +0.87 Ω/□ to a post-matching range of −0.12 to +0.15 Ω/□ across all five production tools, with all tools achieving independent Cpk ≥ 1.63.
- The optimized TCO process delivered a statistically significant mean cell efficiency improvement of +0.31% absolute, driven by +4 mV Voc (reduced sputter damage) and +0.4% absolute FF (lower lateral resistance). Top-bin yield at the 23.6% threshold increased by 1.8% absolute, translating to approximately 18 MW additional top-bin rated capacity per year at 1 GW production scale.
- Total estimated annual commercial impact of the optimization is approximately $4.76M, distributed across efficiency premium, yield improvement, scrap and rework elimination, consumable savings, and throughput recovery - confirming that TCO process engineering at the parameter-space boundaries analyzed here constitutes a commercially decisive manufacturing lever at GW scale.

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