

Plasma-Load-Adaptive LLC Bias Control for Energy-Resolved ICP Ion-Beam Polishing of Quartz

Lihong Zhu

qingwu5711@gmail.com

Southwestern Institute of Physics

Junwei Nie

Southwestern Institute of Physics

Yingrui Chu

The Engineering & Technical College of Chengdu University of Technology

Xuejing Han

The Engineering & Technical College of Chengdu University of Technology

Article

Keywords: gate voltage, ion energy distribution, ion-beam polishing, quartz, LLC resonant converter, power spectral density

Posted Date: June 29th, 2026

DOI: <https://doi.org/10.21203/rs.3.rs-10059384/v1>

License: © ⓘ This work is licensed under a Creative Commons Attribution 4.0 International License.
[Read Full License](#)

Additional Declarations: No competing interests reported.

Version of Record: A version of this preprint was published at Scientific Reports on September 26th, 2026. See the published version at <https://doi.org/10.1038/s41598-026-69064-7>.

Plasma-Load-Adaptive LLC Bias Control for Energy-Resolved ICP Ion-Beam Polishing of Quartz

Lihong Zhu,^{1,2,*} Junwei Nie,¹ Yingrui Chu,² and Xuejing Han²

¹*Plasma Engineering Research Center, Southwestern Institute of Physics, Chengdu 610041, China*

²*Department of Automation Engineering, The Engineering and Technical College of Chengdu University of Technology, Sichuan 614000, China*

(Dated: June 19, 2026)

Ion-beam polishing is often controlled through the extraction or gate voltage. The quartz surface, however, is modified by the ions that reach it, and these ions arrive with a finite energy distribution. This difference is important for optical quartz and fused silica because the final surface quality is governed not only by the root-mean-square roughness, but also by the power spectral density (PSD). In this work, we present a reduced simulation framework for ICP-extracted ion-beam polishing driven by a 2 kW LLC resonant DC bias supply. The framework connects the gate-voltage waveform, the plasma-loaded LLC response, the sheath-filtered ion energy distribution function (IEDF), and the PSD evolution of quartz. The results show that the IEDF, especially its mean energy and relative width, is a more direct polishing variable than the applied voltage alone. The simulations predict a finite smoothing window at intermediate ion energy and low IEDF width. Operation below this window gives weak removal, broad IEDFs promote mid-spatial-frequency roughening, and excessive ion energy increases damage risk. Robustness tests, surface simulations, inverse spectral design, waveform synthesis, and ablation studies support the use of gate voltage as a calibrated actuator for IEDF-resolved roughness-spectrum control. The study provides a testable design route for future experimental calibration of plasma-load-adaptive ion-beam polishing of quartz.

Keywords: gate voltage, ion energy distribution, ion-beam polishing, quartz, LLC resonant converter, power spectral density

I. INTRODUCTION

Quartz and fused silica are essential dielectric materials in precision optics, photonic components, plasma-facing parts, microfluidic devices, semiconductor processing systems, and high-stability mechanical assemblies. Their wide use comes from their high optical transparency, chemical stability, low thermal expansion, radiation tolerance, electrical insulation, and long-term dimensional reliability. These properties make them difficult to replace in applications where the surface must remain stable under optical, thermal, mechanical, or plasma exposure. In such systems, however, surface quality cannot be judged only by the root-mean-square roughness, R_q . A surface may show a small R_q value but still contain mid-spatial-frequency features that increase optical scatter, distort transmitted or reflected wavefronts, produce diffraction artifacts, or become more harmful after coating and lithographic processing. For this reason, optical-surface evaluation often requires a spectral description rather than a single roughness number. The power spectral density, $S(k)$, is particularly useful because it separates low-frequency figure error, mid-spatial-frequency structure, and high-spatial-frequency roughness in a physically meaningful way [1, 2]. This means that polishing should not only reduce the total roughness level. It should reduce the correct spatial-frequency band while avoiding the transfer of roughness into a band that

is more damaging for the final optical function [3–5].

During the last several decades, ion-beam figuring, ion-beam polishing, plasma-assisted finishing, and energy-controlled plasma processing have become important tools for improving hard optical materials. Experiments have shown that ion-based finishing can be attractive because it is non-contact, deterministic, local, and suitable for materials that are difficult to polish by purely mechanical techniques [6, 7]. For fused silica and fused quartz, ion-beam polishing has also been investigated as a route toward super-smooth optical surfaces, especially where conventional polishing may leave residual mid-spatial-frequency error or subsurface damage [8, 9]. At the same time, theoretical and experimental studies have made it clear that ion bombardment is not automatically a smoothing process. Depending on ion energy, incidence angle, surface relaxation, sputtering yield, collisional broadening, and ion-induced redistribution, the same process may smooth the surface, amplify roughness, or create damage-related features. On the plasma side, studies of RF sheaths, inductively coupled plasmas, pulsed biasing, and tailored ion energy distributions have shown that the ion energy distribution function can be modified by the bias waveform, plasma potential, pressure, sheath dynamics, and ion transit time [10, 11]. These studies support a central point of the present work: the quartz surface does not respond directly to the voltage setting of the power supply, but to the distribution of ions that finally reaches the surface [12, 13].

The specific problem addressed in this paper lies at the intersection of ion-induced surface evolution, IEDF-controlled plasma processing, and resonant gate-bias de-

* Corresponding Author: qingwu5711@gmail.com

livery. The historical foundation of ion-induced surface modification is commonly traced to Sigmund’s sputtering theory, which described how energetic ions deposit energy near a solid surface and remove material through collision cascades [14]. Sigmund later discussed mechanisms of ion-bombardment-induced micro-roughening, showing that ion irradiation could also destabilize a surface under certain conditions [15]. Building on this physical picture, Bradley and Harper developed a linear theory for ripple formation under ion bombardment, which became one of the classical models for understanding ion-induced surface morphology [16]. Later work expanded this view by including dynamic scaling, nonlinear morphology evolution, mass redistribution, viscous relaxation, and surface-transport effects [17, 18]. These developments are highly relevant for quartz polishing because useful processing must remain inside a regime where removal and smoothing dominate over roughening and damage. However, most existing studies treat only one part of the complete chain. Surface-evolution models usually start from the ion energy or ion flux and do not describe how the gate waveform, converter dynamics, and plasma load create that ion state. Plasma-processing studies show that the IEDF can be tailored or measured, but they do not usually connect the resulting distribution to the band-resolved PSD evolution of quartz [19, 20]. Power-electronics studies describe resonant converters and LLC behavior, but they are rarely connected to the final roughness spectrum of an optical surface [21, 22]. Therefore, the main research gap is the absence of a direct theoretical link from the LLC gate-voltage waveform, through the ICP extraction plasma and sheath, to the IEDF and finally to the PSD evolution of quartz.

In this work, we address this gap by treating the gate voltage as an upstream actuator rather than as the final polishing coordinate. The complete model used here was not invented as a single historical theory by one author; instead, it combines several well-established ideas from sputtering physics, plasma processing, PSD-based surface metrology, and resonant power conversion. Its physical roots come from Sigmund’s ion-energy-deposition theory and the Bradley–Harper description of ion-induced roughening, while its practical control meaning comes from modern IEDF tailoring and resonant bias delivery [14, 16]. The key point is that a polishing condition should be described by the ion state seen by the surface, especially the mean ion energy, $\langle E \rangle$, and the relative IEDF width, $\chi_E = \sigma_E / \langle E \rangle$. This distinction is important because two gate-voltage waveforms can have the same mean value but still produce different energy spreads, different mid-spatial-frequency roughening tendencies, and different final PSD responses. A narrow IEDF can behave like a well-defined polishing tool because most ions arrive inside a useful energy range. A broad IEDF can be harmful because weak, useful, and damaging ion impacts may occur at the same nominal voltage setting. Experimentally, the model can be pre-

pared and calibrated in an ICP ion-beam polishing system by applying controlled gate-bias waveforms through an LLC resonant DC supply and measuring the resulting IEDF using an energy analyzer or retarding-field diagnostic near the substrate position [13]. Once this calibration is available, the voltage is no longer used as a blind control knob; it becomes a calibrated actuator for producing a desired IEDF state and, through it, a desired roughness-spectrum response.

The theoretical chain considered in this paper is written as $V_g(t) \rightarrow T_{CP}(\omega) \rightarrow f_i(E, \theta, t) \rightarrow K_{QS}(E, \theta, k) \rightarrow S(k, t)$. Here, $V_g(t)$ is the applied gate-voltage waveform, $T_{CP}(\omega)$ is the reduced converter–plasma transfer response, $f_i(E, \theta, t)$ is the ion distribution reaching the quartz surface, $K_{QS}(E, \theta, k)$ is the reduced quartz surface-response kernel, and $S(k, t)$ is the evolving roughness PSD. We do not attempt to replace switching-level LLC simulations, kinetic plasma models, or atomistic sputtering calculations. Instead, we use a reduced framework that keeps the control physics visible and testable. The LLC stage restricts which harmonic components can reach the extraction gate, and the sheath response filters the voltage modulation before it appears as ion-energy modulation [23, 24]. The IEDF moments then determine whether the surface lies in a weak-sputtering region, a stable smoothing region, a broad-IEDF roughening region, or a high-energy damage-risk region. In this way, we solve a specific practical problem: how to identify and synthesize a gate-waveform condition that suppresses high-spatial-frequency roughness without creating unwanted mid-spatial-frequency amplification. The answer is not simply to increase the gate voltage. The answer is to find the IEDF state that gives the required PSD gain while keeping the energy spread and high-energy risk under control.

The motivation of this paper is both physical and practical. Physically, we aim to clarify why voltage-only control is insufficient for quartz ion-beam polishing and why the IEDF is a more meaningful state variable for predicting surface evolution. Practically, we aim to provide a design route for plasma-load-adaptive polishing systems in which the bias supply, plasma sheath, IEDF, and surface PSD are treated as parts of one control problem. This is important because optical-quality quartz processing cannot be evaluated only through removal rate or R_q . A condition that removes high-frequency roughness but creates mid-spatial-frequency structure may still degrade the final optical performance. For this reason, the present work focuses on band-resolved smoothing rather than only average roughness reduction. The proposed framework is also designed to be experimentally testable. If the predicted smoothing window is correct, then surfaces processed under narrow-IEDF, intermediate-energy conditions should show reduced high-frequency PSD without a strong MSF penalty. In contrast, broad-IEDF or high-energy conditions should show stronger MSF amplification or damage risk. To make this prediction useful for design, we also include inverse spectral design, uncer-

tainty analysis, and waveform synthesis using standard optimization and robustness concepts [25–27].

The rest of the article is organized as follows. Section II presents the theoretical framework used throughout the paper. It introduces the gate-voltage decomposition, the reduced LLC plasma-load constraint, the sheath-filtered IEDF model, the PSD gain, the smoothing score, and the mid-spatial-frequency roughening order parameter. Section III presents the main results. First, the smoothing-roughening phase map is constructed in the $(\langle E \rangle, \chi_E)$ plane. Then, a reduced IEDF-control coordinate is introduced and compared with voltage-only and mean-energy-only descriptions. After that, inverse spectral design is used to find the ion-energy state required for a target PSD response. The robustness of the smoothing window is tested under parameter uncertainty, and end-to-end surface-evolution simulations are used to show how different control states modify the same initial quartz height field. The section then closes the control loop by synthesizing a feasible gate waveform for target PSD control and by performing ablation tests to identify the physical ingredients that are necessary for prediction. Section IV discusses the physical meaning, experimental implications, and practical limits of the model. Section V summarizes the main conclusions and outlines future directions, including experimental calibration, full energy-angle IEDF measurements, more detailed plasma-sheath modeling, and validation on real quartz and fused-silica surfaces.

II. THEORETICAL FRAMEWORK

This section describes the reduced model used in the study. The purpose is not to build a full device-level simulation of the ICP source, LLC converter, plasma sheath, and quartz surface. That type of model would require many tool-specific inputs and would make the main control idea harder to see. We therefore use a compact framework that keeps each physical step clear. The gate voltage is treated as the electrical actuator. The converter, plasma load, and sheath transform this actuator into an ion energy distribution. The quartz surface then responds through a PSD gain that depends on spatial frequency. This separation follows the same modelling logic used in plasma processing, ion-beam finishing, and optical surface metrology [4, 5, 10, 11, 28].

A. Gate voltage, plasma load, and IEDF transfer

We first separate the measured gate voltage into a mean part and a time-varying part:

$$V_g(t) = \bar{V}_g + \tilde{V}_g(t), \quad (1)$$

where $\bar{V}_g$ is the time-averaged gate voltage and $\tilde{V}_g(t)$ is the part that varies in time. The time-varying part may

come from converter ripple, plasma-load changes, sheath motion, or a deliberately applied waveform. The separation in Eq. (1) is useful because two waveforms can have the same mean voltage but different ripple amplitudes and different frequency content. They can therefore produce different ion energy distributions, even when the nominal voltage setting is unchanged.

In a simple collisionless picture, a singly charged ion gains energy from the sheath voltage drop. The instantaneous ion energy can therefore be estimated as

$$E_i(t) \simeq e [V_p(t) - V_g(t)] - \Delta E_{\text{loss}}, \quad (2)$$

where e is the elementary charge, $V_p(t)$ is the plasma potential, and ΔE_{loss} represents energy lost through collisions, charge exchange, and transport before the ion reaches the surface. Equation (2) should not be read as a complete sheath model. It only states the basic energy balance. In real ICP extraction, the plasma potential, sheath impedance, pressure, ion transit time, and bias waveform all affect the final ion energy distribution [10, 13, 19]. For this reason, a polishing condition cannot be described reliably by voltage alone.

Unless otherwise stated, the numerical examples below assume near-normal incidence and a small angular spread. Under this assumption, the angular part of $f_i(E, \theta, t)$ is absorbed into a reduced energy distribution, so the working equations use $f_i(E, t)$ or $f_i(E)$. This choice keeps the study focused on energy-resolved control. Oblique incidence, angular broadening, and full energy-angle distributions are important extensions, especially for ripple formation and anisotropic polishing, but they are outside the reduced examples considered here [16, 18, 29].

For the control model, we write the ion-energy modulation in a reduced form,

$$E_i(t) = \langle E \rangle + H_{\text{EP}} [V_g(t) - \bar{V}_g] + \delta E_{\text{coll}}(t). \quad (3)$$

Here $\langle E \rangle$ is the mean ion energy produced by the mean bias condition. The coefficient H_{EP} is an effective converter-plasma-sheath transfer coefficient. It measures how strongly a small gate-voltage change is transferred into ion-energy modulation at the surface. The final term, $\delta E_{\text{coll}}(t)$, represents residual broadening from collisions, plasma fluctuations, and diagnostic or numerical smoothing.

The coefficient H_{EP} is not treated as a universal constant. It is a local transfer parameter for a given operating condition. In practice, it would depend on pressure, source power, extraction geometry, sheath impedance, ion transit time, and the frequency content of the waveform. A low-frequency voltage variation may be transferred to the ion energy more efficiently than a high-frequency variation if the ions average over the sheath motion during transit. This type of frequency-dependent response is well known in RF and pulsed plasma biasing, where the ion energy distribution depends not only on the bias amplitude but also on the waveform and plasma response time [12, 20, 30–32].

The resulting IEDF is modeled as

$$f_i(E) = \frac{1}{T} \int_0^T \delta[E - E_i(t)] dt * G(E; \sigma_{\text{coll}}), \quad (4)$$

where T is the averaging time, $\delta[\cdot]$ maps the time-dependent ion energy into an energy histogram, and $G(E; \sigma_{\text{coll}})$ is a Gaussian broadening kernel with width σ_{coll} . The convolution symbol $*$ means that the ideal energy histogram is smoothed by collisional and instrumental broadening. This expression is deliberately simple. It highlights the control point: the waveform does not act directly on the quartz surface. It first creates a distribution of ion energies.

The mean energy and energy spread are then defined by

$$\langle E \rangle = \int_0^\infty E f_i(E) dE, \quad (5)$$

$$\sigma_E = \left[\int_0^\infty (E - \langle E \rangle)^2 f_i(E) dE \right]^{1/2}, \quad (6)$$

and the relative width is

$$\chi_E = \frac{\sigma_E}{\langle E \rangle}. \quad (7)$$

The relative width χ_E is one of the central variables in this paper. If the beam is small (small χ_E), most ions possess a similar energy, and the beam is more akin to a controlled polishing tool. A large χ_E indicates that weak, useful and harmful ion impacts may take place at the same setting. In surface-evolution language, a wide IEDF implies a greater likelihood of the activation of both smoothing and roughening mechanisms. This is the reason for the inclusion of both $\langle E \rangle$ and χ_E in the model, not just the mean energy of the particle [16, 17, 33, 34].

Eqs. (1)–(7) show that the voltage setting and the ion state are not the same quantity. The gate voltage is an upstream electrical input. The IEDF is the state that the surface actually sees. The rest of the model is built around this distinction.

B. Reduced LLC plasma-load constraint

The waveform used for ion-energy control must also be compatible with the resonant bias supply and the plasma load. For this reason, we include a reduced small-signal description of the LLC stage coupled to the plasma sheath. This subsection does not attempt to give a complete switching-level model of the power converter. Instead, it defines the frequency-domain constraints that limit which voltage components can be delivered to the extraction gate after filtering by the resonant tank, transformer, plasma load, and sheath. This level of description is sufficient for the present control framework because the main objective is to connect waveform feasibility to IEDF formation and quartz PSD response, rather than

to optimize the detailed hardware design of the converter [21–24, 35].

In the simplified LLC representation, the resonant stage contains a resonant inductor L_r , a resonant capacitor C_r , a magnetizing inductance L_m , and a transformer with effective turns ratio n_t . The plasma and sheath are represented by a load impedance $Z_{\text{ps}}(\omega)$. This impedance is not fixed, because the plasma load can change with pressure, plasma density, sheath voltage, extraction current, and operating frequency. The resonant branch and magnetizing branch are written as

$$Z_r(\omega) = i\omega L_r + \frac{1}{i\omega C_r}, \quad Z_m(\omega) = i\omega L_m. \quad (8)$$

Here $Z_r(\omega)$ describes the series resonant path, while $Z_m(\omega)$ represents the magnetizing branch of the transformer. These two impedances determine how strongly different frequency components of the commanded waveform can pass through the resonant stage.

The plasma-sheath load is reflected through the transformer and combined with the magnetizing branch as

$$Z_{\text{eq}}(\omega) = \left[Z_m^{-1}(\omega) + (n_t^2 Z_{\text{ps}}(\omega))^{-1} \right]^{-1}. \quad (9)$$

This equivalent impedance is important because it makes the plasma part of the electrical response of the bias supply. If $Z_{\text{ps}}(\omega)$ changes, the delivered gate waveform can change even when the converter command is the same. This is the reduced sense in which the bias control is plasma-load adaptive in the present model.

The voltage-transfer factor from the resonant stage to the extraction gate is then approximated by

$$G_{\text{LLC}}(\omega) = \frac{n_t Z_{\text{eq}}(\omega)}{Z_r(\omega) + Z_{\text{eq}}(\omega)}. \quad (10)$$

This transfer function behaves as a frequency-dependent filter. Near favorable parts of the LLC response, a voltage component can be delivered efficiently. Away from those regions, the resonant tank and load reduce the amplitude and shift the phase. The exact response would depend on the hardware design and operating point, but Eq. (10) captures the constraint needed for waveform-level control.

The sheath adds a second filtering step between gate-voltage ripple and ion-energy modulation. We represent this step by a sheath response factor $H_{\text{sh}}(\omega)$. The converter–plasma transfer function used in the control chain is therefore

$$\mathcal{T}_{\text{CP}}(\omega) = G_{\text{LLC}}(\omega) H_{\text{sh}}(\omega). \quad (11)$$

A simple form for the sheath response is

$$H_{\text{sh}}(\omega) = \frac{\eta_{\text{sh}}}{1 + i\omega\tau_{\text{ion}}}, \quad (12)$$

where η_{sh} is the low-frequency sheath coupling factor and τ_{ion} is an effective ion transit time. This expression is not

intended as a universal sheath law. It is used to represent a common physical trend: slow voltage variations are transferred more directly to the ion energy, while fast variations are partly averaged by sheath motion and ion transit [12, 30, 32].

In the inverse-waveform calculation, each harmonic component is constrained by the magnitude and phase of $\mathcal{T}_{\text{CP}}(\omega)$. For a harmonic at frequency f_n , the delivered amplitude and phase are written as

$$A_n \leq A_{n,\text{max}} |\mathcal{T}_{\text{CP}}(2\pi f_n)|, \quad (13)$$

$$\phi_n = \phi_{n,0} + \arg \mathcal{T}_{\text{CP}}(2\pi f_n), \quad (14)$$

together with limits on total voltage, ripple, and slew rate. Here $A_{n,\text{max}}$ and $\phi_{n,0}$ denote the command-side amplitude limit and reference phase, while A_n and ϕ_n denote the harmonic component that reaches the extraction gate after filtering by the resonant supply and plasma-sheath load.

This reduced constraint connects waveform synthesis to the physical bias system without turning the paper into a full power-electronics design study. The inverse design is therefore not allowed to choose arbitrary voltage waveforms. It can only choose waveforms that remain compatible with the LLC transfer response, the changing plasma load, the sheath response, and the imposed voltage limits. In this way, the electrical model supplies the admissible gate-waveform space, while the IEDF and PSD models determine which admissible waveform gives the desired polishing response.

C. Reduced surface-response picture

The next step is to connect the IEDF to the surface PSD. The full microscopic problem is complex. Ion impacts may remove atoms, redistribute material, create defects, relax local curvature, or amplify selected surface modes. A complete treatment can be achieved with atomistic simulation or a detailed continuum equation. For the present control study, we use a reduced spectral response model. It keeps the key trade-off: useful smoothing at high spatial frequency and possible amplification in the mid-spatial-frequency band.

The starting point is the common linearized surface-evolution idea used in ion-bombardment theory. A Fourier component of the surface height, $h_{\mathbf{k}}$, can be written in the schematic form

$$\frac{dh_{\mathbf{k}}}{dt} = -\Gamma_{\text{sm}}(E, \chi_E, k) h_{\mathbf{k}} + \Gamma_{\text{r}}(E, \chi_E, k) h_{\mathbf{k}} + \eta_{\mathbf{k}}(t), \quad (15)$$

where Γ_{sm} is the smoothing rate, Γ_{r} is the roughening or amplification rate, and $\eta_{\mathbf{k}}(t)$ represents stochastic ion-impact noise. This equation is not a replacement for Bradley-Harper, Kuramoto-Sivashinsky, or redistribution-based surface models. It is a compact way to represent their shared message: smoothing and roughening compete, and the sign of the net rate depends on

ion energy, incidence conditions, relaxation, and redistribution [16–18, 33, 36].

In PSD form, the reduced model is expressed through the gain

$$G(k; \langle E \rangle, \chi_E) = \exp[-2\Gamma_{\text{sm}}(\langle E \rangle, k)t_p + \mathcal{D}], \quad (16)$$

where t_p and $\mathcal{D} = 2\Gamma_{\text{MSF}}(\langle E \rangle, \chi_E, k)t_p + 2\Gamma_{\text{hi}}(\langle E \rangle, k)t_p$ is the polishing time. The first term reduces the PSD and represents useful smoothing. The second term produces an MSF amplification peak when the IEDF becomes broad. The third term represents high-energy roughening or damage risk. In the simulations, the MSF term is centered in the MSF band and grows with χ_E . This implements the physical idea that a broad distribution mixes different sputtering and redistribution regimes in one exposure, making the surface response less selective.

A simple form used to generate the MSF roughening contribution is

$$\Gamma_{\text{MSF}}(\langle E \rangle, \chi_E, k) = \Gamma_0 \mathcal{B}_{\chi}(\chi_E) \mathcal{W}_{\text{MSF}}(\langle E \rangle) \exp[\mathcal{Y}]. \quad (17)$$

Here k_{MSF} is the center of the MSF response and $\mathcal{Y} = -\frac{(\log k - \log k_{\text{MSF}})^2}{2\sigma_{\text{MSF}}^2}$, σ_{MSF} controls its spectral width, and $\mathcal{B}_{\chi}(\chi_E)$ increases as the IEDF becomes broader. This form is phenomenological, but it is not arbitrary. It encodes the experimentally important observation that a polishing process can reduce fine roughness while still creating structure at intermediate spatial frequencies [4, 5, 8, 9, 37]. The analytical kernels employed in the figures are listed in Appendix A and therefore the phase maps and inverse-design calculations can be reproduced.

D. PSD response, smoothing score, and roughening order parameter

For a surface height map $h(x, y)$ over area A , the two-dimensional PSD is written as

$$S(k_x, k_y) = \frac{1}{A} |\mathcal{F}\{h(x, y) - \bar{h}\}|^2, \quad (18)$$

and the radially averaged PSD is

$$S(k) = \langle S(k_x, k_y) \rangle_{k=(k_x^2+k_y^2)^{1/2}}. \quad (19)$$

Here $h(x, y)$ is the measured or simulated surface height, $\bar{h}$ is its mean value, and $\mathcal{F}$ denotes the two-dimensional Fourier transform. The radial average converts the two-dimensional PSD into a one-dimensional curve when the response is treated as approximately isotropic. This is the form used in the figures. If the process produces strong directional ripples, the full two-dimensional PSD should be retained instead.

The spectral gain after polishing is

$$G(k) = \frac{S_f(k)}{S_0(k)}, \quad (20)$$

where $S_0(k)$ and $S_f(k)$ are the initial and final PSDs. Values $G(k) < 1$ indicate smoothing at spatial frequency k , while values $G(k) > 1$ indicate roughness amplification. This band-resolved view is essential because high-frequency smoothing and mid-spatial-frequency roughening can occur at the same time [5, 8, 37].

In the numerical examples, the mid-spatial-frequency band is taken as

$$k \in [0.07, 0.80] \text{ } \mu\text{m}^{-1}, \quad (21)$$

and the high-frequency band is taken as

$$k \in [0.80, 4.00] \text{ } \mu\text{m}^{-1}. \quad (22)$$

When k is interpreted as spatial frequency in cycles per micrometer, these ranges correspond approximately to wavelengths of 14–1.25 μm and 1.25–0.25 μm , respectively. These cutoffs are not universal. They can be changed to match a given optical specification, metrology tool, or polishing target. They are stated here so that the terms MSF and HF have a clear numerical meaning throughout the paper.

To classify the spectral response, we introduce a PSD-control score,

$$\begin{aligned} \mathcal{Q}_{\text{PSD}} = & A_{\text{sm}} \mathcal{S}_{\text{on}}(\langle E \rangle) \mathcal{W}_E(\langle E \rangle) [1 - \alpha_\chi \mathcal{B}_\chi(\chi_E)] \\ & - A_\chi \mathcal{B}_\chi(\chi_E) - A_{\text{hi}} \mathcal{D}_{\text{hi}}(\langle E \rangle) - A_{\text{lo}} [1 - \mathcal{S}_{\text{on}}(\langle E \rangle)]. \end{aligned} \quad (23)$$

The first line represents useful smoothing. It becomes large only when sputtering has turned on, the mean energy is near the useful polishing window, and the IEDF is not too broad. The second line contains penalty terms. The term with $\mathcal{B}_\chi$ penalizes broad IEDFs. The term with $\mathcal{D}_{\text{hi}}$ penalizes high-energy operation, where damage or roughening becomes more likely. The last term penalizes operation below sputtering onset, where removal is too weak to produce useful smoothing.

Positive $\mathcal{Q}_{\text{PSD}}$ denotes a smoothing-dominated response, while negative $\mathcal{Q}_{\text{PSD}}$ denotes weak-removal or roughening-dominated response. This score is not proposed as a new fundamental law of sputtering. It is used as a compact control metric. Its role is to summarize the conditions that must hold at the same time: sputtering must be active, the mean energy must be useful, the IEDF must remain narrow enough, and high-energy roughening must be avoided. The analytical forms of $\mathcal{S}_{\text{on}}$, $\mathcal{W}_E$, $\mathcal{B}_\chi$, and $\mathcal{D}_{\text{hi}}$, together with the nominal parameter values used in the figures, are given in Appendix A.

The mid-spatial-frequency roughening order parameter is defined as

$$\mathcal{R}_{\text{MSF}} = \int_{k_{\text{M},1}}^{k_{\text{M},2}} \max[0, G(k) - 1] d \log k. \quad (24)$$

This quantity measures only the part of the MSF gain that lies above unity. Thus $\mathcal{R}_{\text{MSF}} = 0$ means that the MSF band is not amplified, while $\mathcal{R}_{\text{MSF}} > 0$ marks the

appearance of MSF roughening. The definition is intentionally one-sided. It does not penalize smoothing in the MSF band. It only penalizes the creation of additional spectral power, because MSF structure is often difficult to remove in later finishing steps and can strongly affect optical performance [4, 5, 9].

The framework can therefore be summarized in three steps. First, the LLC-plasma system constrains which gate-voltage waveform can actually be delivered. Second, the delivered waveform produces an IEDF described mainly by $\langle E \rangle$ and χ_E . Third, the quartz surface responds through a PSD gain that can either suppress high-frequency roughness or amplify MSF structure. The next section uses this framework to construct the phase map, the reduced IEDF-control coordinate, and the inverse waveform design.

III. RESULTS

A. Theoretical phase map for IEDF-controlled smoothing

The first result is the predicted smoothing–roughening structure of quartz roughness evolution in the plane $(\langle E \rangle, \chi_E)$. Figure 1(a) shows three gate-voltage waveforms with the same mean value, $\bar{V}_g = 500 \text{ V}$, but different ripple-transfer states. The cases are labeled I, II, and III and represent narrow-, moderate-, and broad-IEDF transfer regimes. Figure 1(b) shows the corresponding IEDFs. Although the mean gate voltage is the same, the relative width changes from approximately 0.7% to 2.4% and 5.7%. This directly shows the main point: a nominal voltage does not uniquely define the ion state.

The main prediction is shown in Fig. 1(c). The color map gives $\mathcal{Q}_{\text{PSD}}$ in the plane $(\langle E \rangle, 100\chi_E)$, and the contour $\mathcal{Q}_{\text{PSD}} = 0$ separates smoothing-dominated and roughening-dominated response. Four regimes appear naturally. Region Ω_1 is a weak-sputtering regime, where the mean ion energy is too low for efficient removal. Region Ω_2 is the stable narrow-IEDF smoothing window. Region Ω_3 is a broad-IEDF roughening regime, where energy spread produces MSF amplification. Region Ω_4 is a high-energy damage-risk regime, where the smoothing benefit is overwhelmed by high-energy roughening penalties.

Figure 1(d) shows the associated transition in $\mathcal{R}_{\text{MSF}}$. At small χ_E , $\mathcal{R}_{\text{MSF}}$ remains nearly zero, indicating smoothing without MSF amplification. Above a critical relative width, $\mathcal{R}_{\text{MSF}}$ grows rapidly. The result is a theoretical smoothing-to-roughening transition controlled by the IEDF state. It is not controlled by $\bar{V}_g$ alone, but by the pair $(\langle E \rangle, \chi_E)$ generated by the converter–plasma–sheath transfer chain. This is consistent with the broader ion-bombardment literature, where surface smoothing and roughening depend on the balance between erosion, redistribution, relaxation, and instability mechanisms [29, 36, 38, 39].

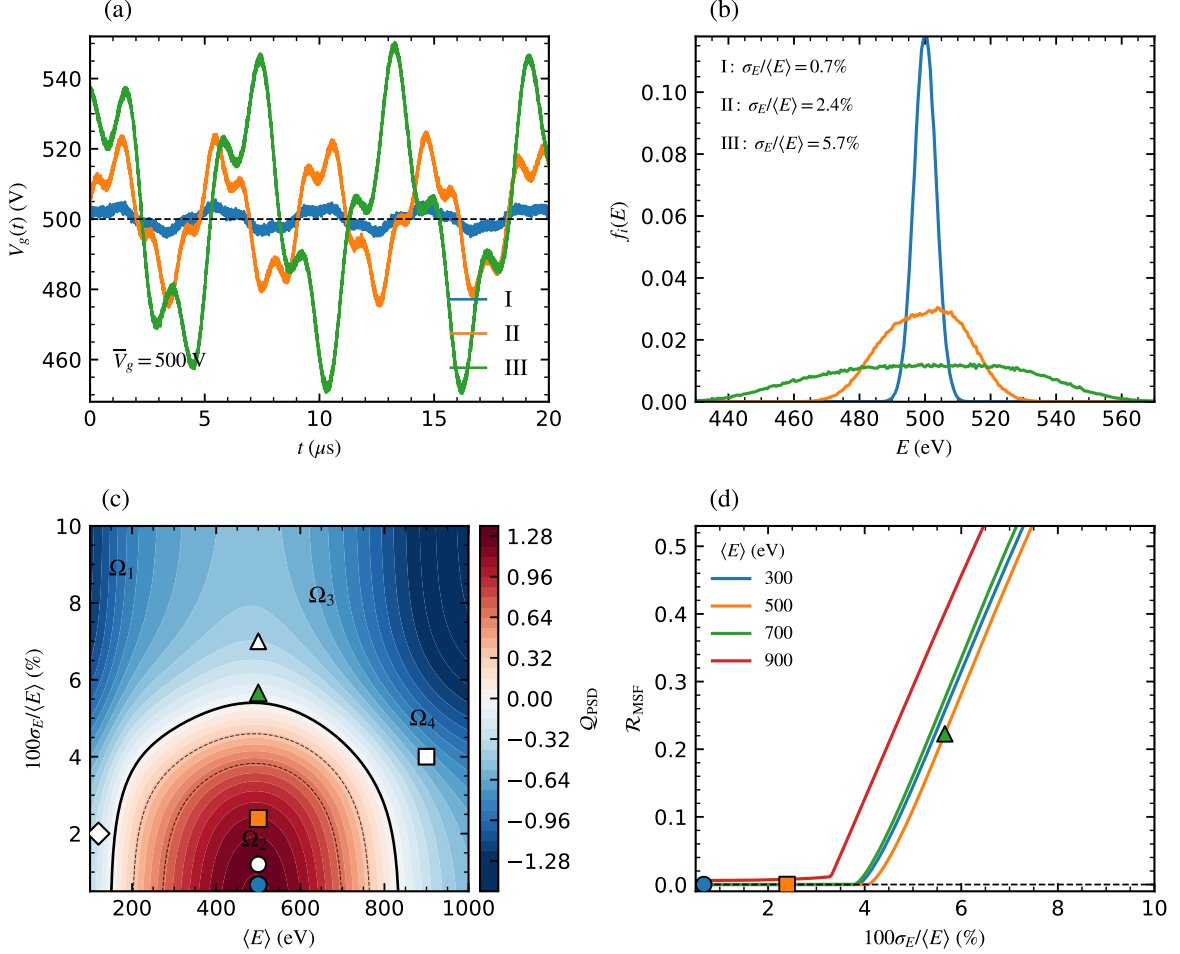


FIG. 1. Theoretical prediction of gate-voltage-resolved IEDF control of quartz roughness-spectrum evolution. (a) Gate-voltage waveforms with identical mean voltage, $\bar{V}_g = 500$ V, but different ripple-transfer conditions. (b) Corresponding ion energy distributions generated by the converter-plasma-sheath transfer model. (c) PSD-control phase map in the plane of mean ion energy and relative IEDF width. The contour $Q_{\text{PSD}} = 0$ separates smoothing-dominated and roughening-dominated regimes. The regions Ω_1 – Ω_4 denote weak sputtering, stable narrow-IEDF smoothing, broad-IEDF roughening, and high-energy damage risk. (d) Mid-spatial-frequency roughening order parameter R_{MSF} , showing the transition from stable smoothing to roughness amplification as the relative IEDF width increases.

B. Reduced IEDF-control law and inverse spectral design

The phase map shows that the polishing response depends on $(\langle E \rangle, \chi_E)$, but a useful control theory should also provide a compact coordinate for prediction and design. We therefore define the reduced IEDF-control coordinate

$$\Lambda_{\text{IEDF}} = \frac{\mathcal{S}_{\text{on}}(\langle E \rangle) \mathcal{W}_E(\langle E \rangle)}{1 + (\chi_E/\chi_c)^m + a_{\text{hi}} \mathcal{D}_{\text{hi}}(\langle E \rangle)}. \quad (25)$$

This quantity is large only when ions are above the sputtering onset, close to the useful smoothing-energy window, sufficiently narrow in energy spread, and not in the high-energy damage regime. It compresses the two most important IEDF moments into a coordinate that has direct control meaning.

The reduced prediction model is a low-order polynomial,

$$\hat{Q}_{\text{PSD}} = a_0 + a_1 \Lambda_{\text{IEDF}} + a_2 \Lambda_{\text{IEDF}}^2 + a_3 \Lambda_{\text{IEDF}}^3, \quad (26)$$

where the coefficients are fitted on a training set $\mathcal{D}_{\text{tr}}$. The model is evaluated on a held-out set $\mathcal{D}_{\text{te}}$ using

$$R^2 = 1 - \frac{\sum_{j \in \mathcal{D}_{\text{te}}} (Q_{\text{PSD},j} - \hat{Q}_{\text{PSD},j})^2}{\sum_{j \in \mathcal{D}_{\text{te}}} (Q_{\text{PSD},j} - \bar{Q}_{\text{PSD}})^2}. \quad (27)$$

A voltage-only fit, $Q_{\text{PSD}} \approx F(\bar{V}_g)$, is evaluated with the same held-out metric.

Figure 2(a) shows the voltage-only representation. The response is broad and multivalued because points with similar $\bar{V}_g$ can have different IEDF widths. The held-out

coefficient is only $R_V^2 = 0.58$. In contrast, Fig. 2(b) shows that the same operating points collapse onto a nearly single-valued relation when plotted against Λ_{IEDF} , with $R_A^2 = 0.97$. Figure 2(c) confirms the predictive character of the collapse with a parity plot between $\mathcal{Q}_{\text{PSD}}$ and $\hat{\mathcal{Q}}_{\text{PSD}}$. Both training and held-out points remain close to the ideal line. This result shows why the IEDF state is a more useful theoretical control coordinate than the mean gate voltage.

The last part of Fig. 2 performs inverse spectral design. Instead of predicting the surface response from a chosen voltage, we prescribe a target gain $G^*(k)$ and search for the ion-energy state that best reproduces it. The design objective is

$$\mathcal{J}(\langle E \rangle, \chi_E) = \int [\log G(k; \langle E \rangle, \chi_E) - \log G^*(k)]^2 d \log k + \mu \mathcal{R}_{\text{MSF}} + \zeta \mathcal{D}_{\text{hi}}(\langle E \rangle). \quad (28)$$

The inverse-designed state is

$$(\langle E \rangle^*, \chi_E^*) = \arg \min_{\langle E \rangle, \chi_E} \mathcal{J}(\langle E \rangle, \chi_E). \quad (29)$$

For the target spectrum in Fig. 2(d), the selected state is approximately

$$\langle E \rangle^* \simeq 398 \text{ eV}, \quad 100 \chi_E^* \simeq 3.8\%. \quad (30)$$

The corresponding $G_{\text{inv}}(k)$ approaches $G^*(k)$, whereas low-energy, high-energy, and broad-IEDF alternatives fail in different ways. The low-energy case does not remove enough high-frequency roughness; the high-energy and broad-IEDF cases produce MSF amplification. The model is therefore more than descriptive. It can also select an ion-energy state for a desired roughness-spectrum response.

C. Robustness of the IEDF-controlled smoothing window

The reduced-control result would be less useful if it depended on only one nominal parameter set. To test this, we perform a Monte Carlo uncertainty analysis over the reduced converter-plasma-surface model. The uncertain parameters are collected as

$$\xi = \{E_{\text{th}}, E_{\text{opt}}, \chi_c, E_{\text{hi}}, A_{\text{sm}}, A_{\chi}, A_{\text{hi}}, A_{\text{lo}}, k_{\text{sm}}, k_{\text{MSF}}\}, \quad (31)$$

where the entries control sputtering onset, the useful energy window, the IEDF-width threshold, high-energy damage, PSD-response amplitudes, and characteristic spatial frequencies. This is a reduced uncertainty model, but it follows the logic of robust design. A useful prediction should remain visible when plausible physical parameters are changed [26, 27].

For each draw $m = 1, \dots, N_\xi$, the model evaluates

$$\mathcal{Q}_{\text{PSD}}^{(m)} = \mathcal{Q}_{\text{PSD}}(\langle E \rangle, \chi_E; \xi^{(m)}). \quad (32)$$

The smoothing probability is

$$P_{\text{sm}}(\langle E \rangle, \chi_E) = \frac{1}{N_\xi} \sum_{m=1}^{N_\xi} \Theta \left[\mathcal{Q}_{\text{PSD}}^{(m)}(\langle E \rangle, \chi_E) \right], \quad (33)$$

where $\Theta(x)$ is the Heaviside function. Thus $P_{\text{sm}} = 1$ means that all perturbed models predict smoothing, while $P_{\text{sm}} = 0$ means that all perturbed models predict weak-removal or roughening.

To define a conservative robust-design region, we also use the ensemble mean and standard deviation,

$$\bar{\mathcal{Q}}_{\text{PSD}} = \frac{1}{N_\xi} \sum_{m=1}^{N_\xi} \mathcal{Q}_{\text{PSD}}^{(m)}, \quad (34)$$

$$\sigma_{\mathcal{Q}} = \left[\frac{1}{N_\xi} \sum_{m=1}^{N_\xi} \left(\mathcal{Q}_{\text{PSD}}^{(m)} - \bar{\mathcal{Q}}_{\text{PSD}} \right)^2 \right]^{1/2}. \quad (35)$$

The robust smoothing set is

$\Omega_{\text{rob}} = \{(\langle E \rangle, \chi_E) : P_{\text{sm}} \geq P_0, \bar{\mathcal{Q}}_{\text{PSD}} \geq Q_0, \sigma_{\mathcal{Q}} \leq \sigma_0\}$. This condition is stricter than $\mathcal{Q}_{\text{PSD}} > 0$ because it requires the smoothing prediction to remain stable across the uncertainty ensemble.

Figure 3(a) maps P_{sm} in the $(\langle E \rangle, \chi_E)$ plane. The high-probability region remains concentrated at intermediate mean energy and low relative IEDF width. The star marks the median inverse-designed operating point across the uncertain model ensemble. Figure 3(b) shows the uncertainty of the smoothing-roughening boundary. Each gray curve is a perturbed boundary $\partial\Omega$, while the black curve is the nominal boundary $\partial\Omega_0$. The boundary shifts, but the same qualitative structure is preserved: weak sputtering at low energy, broad-IEDF roughening at high χ_E , and high-energy risk at large $\langle E \rangle$.

We also compare candidate control choices. For a design $\mathcal{C}_j = (\langle E \rangle_j, \chi_{E,j})$, the smoothing probability is

$$P_{\text{sm}}(\mathcal{C}_j) = \frac{1}{N_\xi} \sum_{m=1}^{N_\xi} \Theta \left[\mathcal{Q}_{\text{PSD}}(\mathcal{C}_j; \xi^{(m)}) \right], \quad (36)$$

and the probability of MSF roughening is

$$P_{\text{MSF}}(\mathcal{C}_j) = \frac{1}{N_\xi} \sum_{m=1}^{N_\xi} \Theta \left[\mathcal{R}_{\text{MSF}}(\mathcal{C}_j; \xi^{(m)}) - R_0 \right]. \quad (37)$$

Figure 3(c) shows that the robust IEDF-aware choice maintains high smoothing probability while suppressing MSF amplification. Finally, Fig. 3(d) shows that inverse-designed operating points cluster around a finite intermediate-energy, low- χ_E region rather than moving toward the highest ion energy. The median design is near

$$\text{med}(\langle E \rangle^*) \approx 367 \text{ eV}, \quad 100 \text{ med}(\chi_E^*) \approx 3.5\%. \quad (38)$$

The narrow-IEDF smoothing window is therefore a robust feature of the model, not an artifact of one parameter choice.

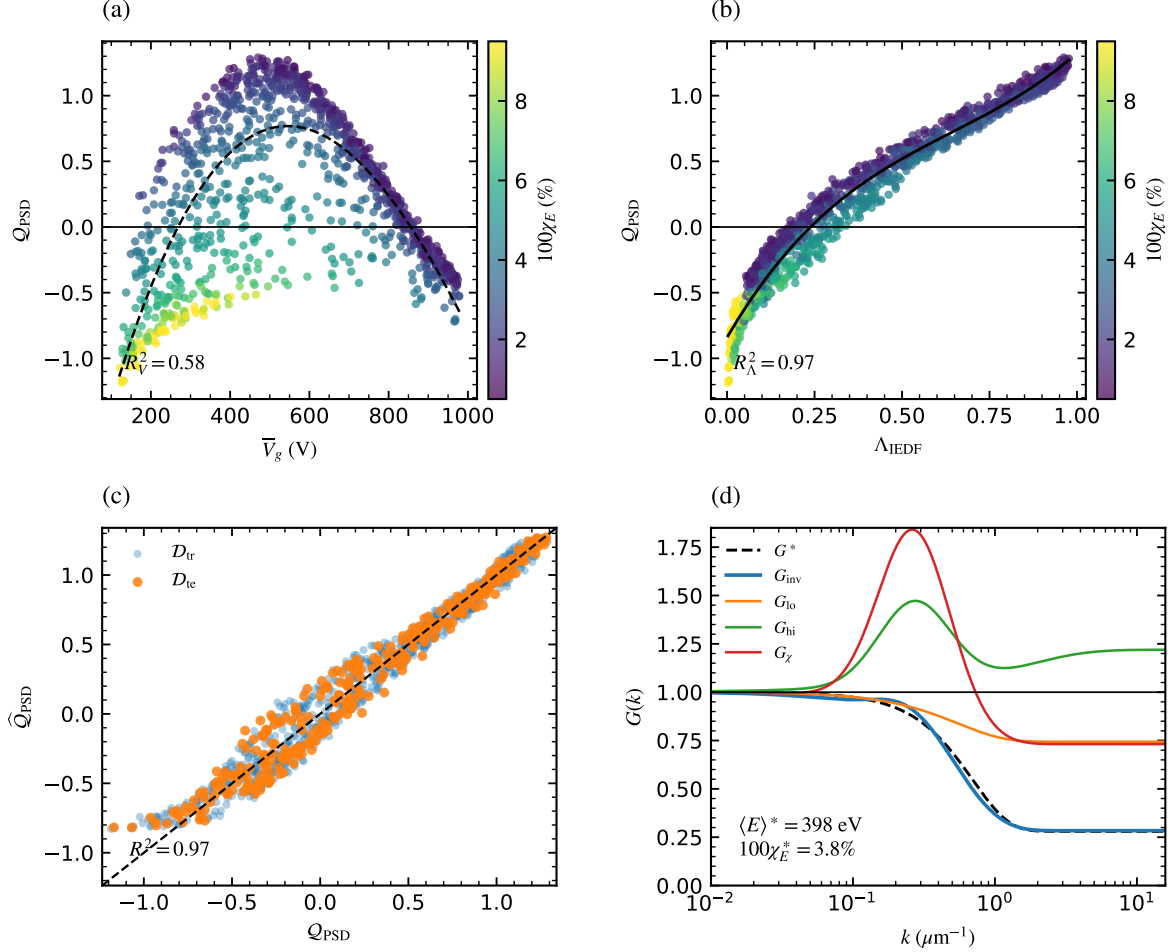


FIG. 2. Reduced IEDF-control law and inverse spectral design. (a) Voltage-only representation of the PSD smoothing score. The broad scatter and low R_V^2 show that $\bar{V}_g$ is not a sufficient control variable. (b) Collapse of the same operating points using the IEDF-control coordinate Λ_{IEDF} , giving a much stronger held-out prediction. (c) Parity plot comparing model-evaluated and reduced-law-predicted Q_{PSD} for the training set $\mathcal{D}_{\text{tr}}$ and held-out set $\mathcal{D}_{\text{te}}$. (d) Inverse spectral design. The target PSD gain $G^*(k)$ is approached by the inverse-designed response $G_{\text{inv}}(k)$, while low-energy, high-energy, and broad-IEDF alternatives fail to reproduce the desired spectral response.

D. End-to-end roughness-spectrum control of quartz

The previous results establish the main control principle. The phase map shows where smoothing is possible. The reduced coordinate gives a compact prediction rule. The uncertainty analysis shows that the window is not tied to one parameter set. We now apply the model to an explicit quartz height field to show what these ideas mean for a surface morphology. Starting from the same initial roughness spectrum, we ask whether IEDF-aware control produces a different final morphology from high-voltage or broad-IEDF control.

The surface-evolution step is phenomenological, but its structure is explicit. We assume that the height perturbations remain small enough for each spatial-frequency component to evolve independently to first order. This

is the same linearized spirit used in many ion-induced morphology models before nonlinear pattern growth becomes dominant. In Fourier space, the model can be viewed as $\partial_t \hat{h}(k, t) = \Gamma(k; \langle E \rangle, \chi_E) \hat{h}(k, t) + \eta(k, t)$, where Γ is a net smoothing or roughening rate and η represents weak stochastic forcing. Narrow IEDFs make the high-frequency part of Γ more negative, which gives smoothing. Broad IEDFs add a positive contribution centered in the MSF band, which produces the roughening peak. The explicit gain functions used to generate the figures are listed in Appendix B.

The initial synthetic quartz surface $h_0(x, y)$ is generated from a broadband roughness spectrum containing low-frequency figure content, MSF structure, and high-frequency roughness. The initial PSD is $S_0(k)$. Three control states are applied to the same surface,

$$\mathcal{V}_{\text{hi}}, \quad \mathcal{I}_{\text{inv}}, \quad \mathcal{I}_\chi. \quad (39)$$

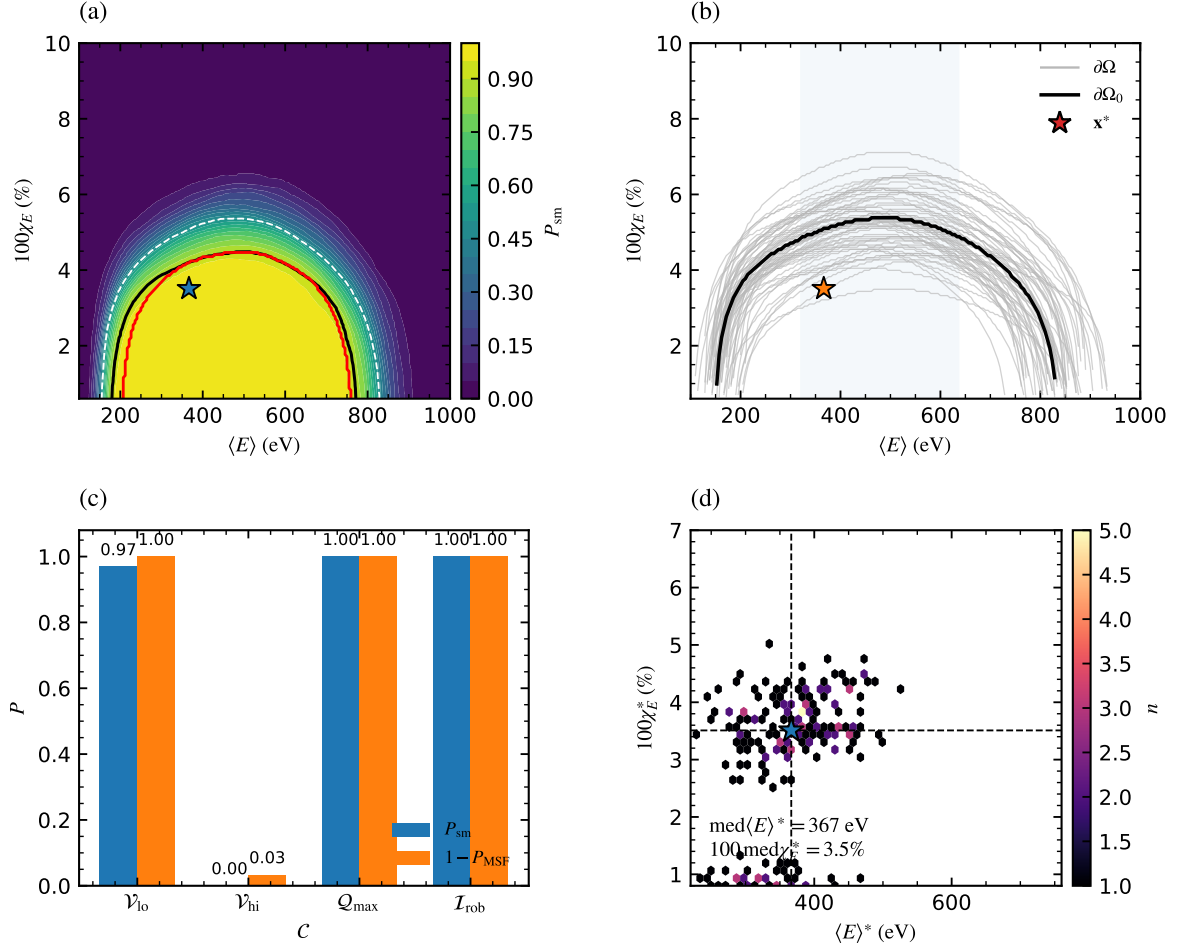


FIG. 3. Robustness of the IEDF-controlled smoothing window under model uncertainty. (a) Smoothing probability P_{sm} in the $(\langle E \rangle, \chi_E)$ plane, computed over an ensemble of perturbed sputtering, broadening, and damage parameters. (b) Uncertainty of the smoothing-roughening boundary. Gray curves show perturbed boundaries $\partial\Omega$, while the black curve shows the nominal boundary $\partial\Omega_0$. (c) Comparison of candidate control strategies. The IEDF-aware robust design maintains high smoothing probability while suppressing MSF amplification. (d) Distribution of inverse-designed operating points under parameter uncertainty. The solutions concentrate in a finite low- χ_E region rather than at the highest ion energy.

Here $\mathcal{V}_{hi}$ represents high-voltage control, $\mathcal{I}_{inv}$ represents inverse IEDF control, and $\mathcal{I}_\chi$ represents a broad-IEDF state at a similar mean energy to the inverse-designed case.

For each control state $\mathcal{C}$, the final PSD is written as

$$S_f(k; \mathcal{C}) = G(k; \mathcal{C}) S_0(k), \quad (40)$$

where

$$G(k; \mathcal{C}) = \frac{S_f(k; \mathcal{C})}{S_0(k)} \quad (41)$$

is the PSD gain. To make the spectral response visible in real space, the gain is applied to the Fourier amplitudes of the initial surface. A weak anisotropic MSF component is added when the control state has high ripple-risk or broad IEDF width. This produces model-generated final height maps $h_f(x, y; \mathcal{C})$.

The band power in a spatial-frequency interval is

$$\mathcal{B}_\mathcal{K}[S] = \int_{k_{\mathcal{K},1}}^{k_{\mathcal{K},2}} S(k) d \log k, \quad \mathcal{K} \in \{\text{MSF}, \text{HF}\}. \quad (42)$$

The high-frequency reduction is

$$\mathcal{M}_{\text{HF}} = 1 - \frac{\mathcal{B}_{\text{HF}}[S_f]}{\mathcal{B}_{\text{HF}}[S_0]}, \quad (43)$$

and the MSF gain is

$$\mathcal{M}_{\text{MSF}} = \frac{\mathcal{B}_{\text{MSF}}[S_f]}{\mathcal{B}_{\text{MSF}}[S_0]}. \quad (44)$$

A desirable polishing condition has $\mathcal{M}_{\text{HF}} > 0$ and $\mathcal{M}_{\text{MSF}} \leq 1$: it removes high-frequency roughness without creating an MSF penalty.

Figure 4(a) shows the initial surface, with $R_q = 1.20$ nm. Figures 4(b)–4(d) show the final surfaces produced from the same initial morphology. The high-voltage and broad-IEDF cases increase the final roughness to $R_q = 1.45$ nm and $R_q = 1.40$ nm, while the inverse-designed IEDF condition reduces the roughness to $R_q = 0.93$ nm. The scalar roughness shows the difference, while the PSD explains why it occurs.

Figure 4(e) shows the radially averaged PSDs, and Fig. 4(f) shows the corresponding gain $G(k)$. The high-voltage state $\mathcal{V}_{hi}$ and the broad-IEDF state $\mathcal{I}_\chi$ both generate strong MSF amplification, visible as $G(k) > 1$ in the MSF band. In contrast, $\mathcal{I}_{inv}$ suppresses the high-frequency PSD while keeping the MSF gain close to unity. This is the desired spectral behavior: the model reduces the roughness band of interest without transferring error into a more damaging band.

Figure 4(g) tracks the normalized band powers during polishing. The inverse-designed condition steadily reduces the high-frequency band power while leaving the MSF band nearly unchanged. The high-voltage case produces a negative high-frequency reduction, meaning net high-frequency amplification, and it also increases the MSF band. The broad-IEDF case gives some high-frequency reduction, but at the cost of a large MSF penalty. The summary metrics in Fig. 4(h) make the tradeoff explicit. Only the inverse-designed state combines strong high-frequency reduction with no meaningful MSF amplification,

$$\mathcal{M}_{HF} = 0.68, \quad \mathcal{M}_{MSF} = 0.98. \quad (45)$$

The same initial quartz surface therefore does not have a unique outcome under a voltage scale. The final morphology is determined by the PSD gain imposed by the IEDF state.

E. Inverse gate-waveform synthesis for target PSD control

The previous sections show that the quartz roughness response is controlled more directly by the IEDF than by the mean gate voltage alone. We now close the theoretical control loop by asking the inverse question: given a desired roughness-spectrum response, can the model synthesize a gate-voltage waveform that produces the required IEDF and drives the surface toward the target PSD? This step moves the framework from interpretation toward design. The model does not only identify a favorable ion-energy window. It also computes a gate-voltage waveform, within the imposed constraints, that can produce the desired spectral response.

The gate waveform is parameterized as a mean bias plus a finite set of harmonic components,

$$V_g(t; \mathbf{u}) = \bar{V}_g + \sum_{n=1}^{N_h} A_n \sin(2\pi f_n t + \phi_n), \quad (46)$$

where

$$\mathbf{u} = \{\bar{V}_g, A_1, \dots, A_{N_h}, \phi_1, \dots, \phi_{N_h}\}. \quad (47)$$

The frequencies f_n represent waveform components allowed by the bias-supply bandwidth and converter-plasma transfer response. The amplitudes and phases are optimized subject to voltage, ripple, and slew-rate constraints so that the waveform remains physically meaningful for an LLC-biased extraction system. The optimization is not intended to replace power-electronics design; it defines what spectral information the voltage waveform should carry [25, 40, 41].

For each candidate waveform, the converter-plasma-sheath transfer model maps $V_g(t; \mathbf{u})$ to $f_i(E; \mathbf{u})$. The corresponding mean energy and relative width are

$$\langle E \rangle(\mathbf{u}) = \int_0^\infty E f_i(E; \mathbf{u}) dE, \quad \chi_E(\mathbf{u}) = \frac{\sigma_E(\mathbf{u})}{\langle E \rangle(\mathbf{u})}. \quad (48)$$

The predicted PSD gain is

$$G(k; \mathbf{u}) = \frac{S_f(k; \mathbf{u})}{S_0(k)}. \quad (49)$$

The waveform is chosen by minimizing

$$\begin{aligned} \mathcal{J}(\mathbf{u}) = & \int [\log G(k; \mathbf{u}) - \log G^*(k)]^2 d \log k \\ & + \lambda_{MSF} \mathcal{R}_{MSF}(\mathbf{u}) + \lambda_\chi [\chi_E(\mathbf{u}) - \chi_E^*]^2 \\ & + \lambda_V \left(\frac{V_{rms}(\mathbf{u})}{\bar{V}_g(\mathbf{u})} \right)^2 + \lambda_{lim} \mathcal{P}_{lim}(\mathbf{u}). \end{aligned} \quad (50)$$

The first term enforces spectral tracking. The second penalizes MSF amplification. The third keeps the IEDF width near the desired value. The fourth discourages excessive ripple, and $\mathcal{P}_{lim}$ is a soft penalty for voltage and slew-rate violations. The optimized waveform is

$$\mathbf{u}^* = \arg \min_{\mathbf{u}} \mathcal{J}(\mathbf{u}). \quad (51)$$

Figure 5(a) defines the spectral task by comparing $S_0(k)$ with the desired target spectrum $S^*(k)$. The target is not a uniform reduction; it suppresses high-spatial-frequency roughness while avoiding unwanted MSF amplification. Figure 5(b) shows the synthesized waveform $V_g^*(t)$, compared with a DC waveform V_{dc} and an uncontrolled ripple waveform V_{rip} . The optimized waveform remains within a moderate voltage window,

$$\bar{V}_g^* \approx 380 \text{ V}, \quad V_{rms}^* \approx 17.3 \text{ V}. \quad (52)$$

The corresponding IEDFs are shown in Fig. 5(c). The optimized waveform produces an ion-energy state close to the desired smoothing window,

$$\langle E \rangle^* \approx 383 \text{ eV}, \quad 100\chi_E^* \approx 3.6\%. \quad (53)$$

The DC waveform is narrower but less properly placed, while the uncontrolled ripple waveform broadens the

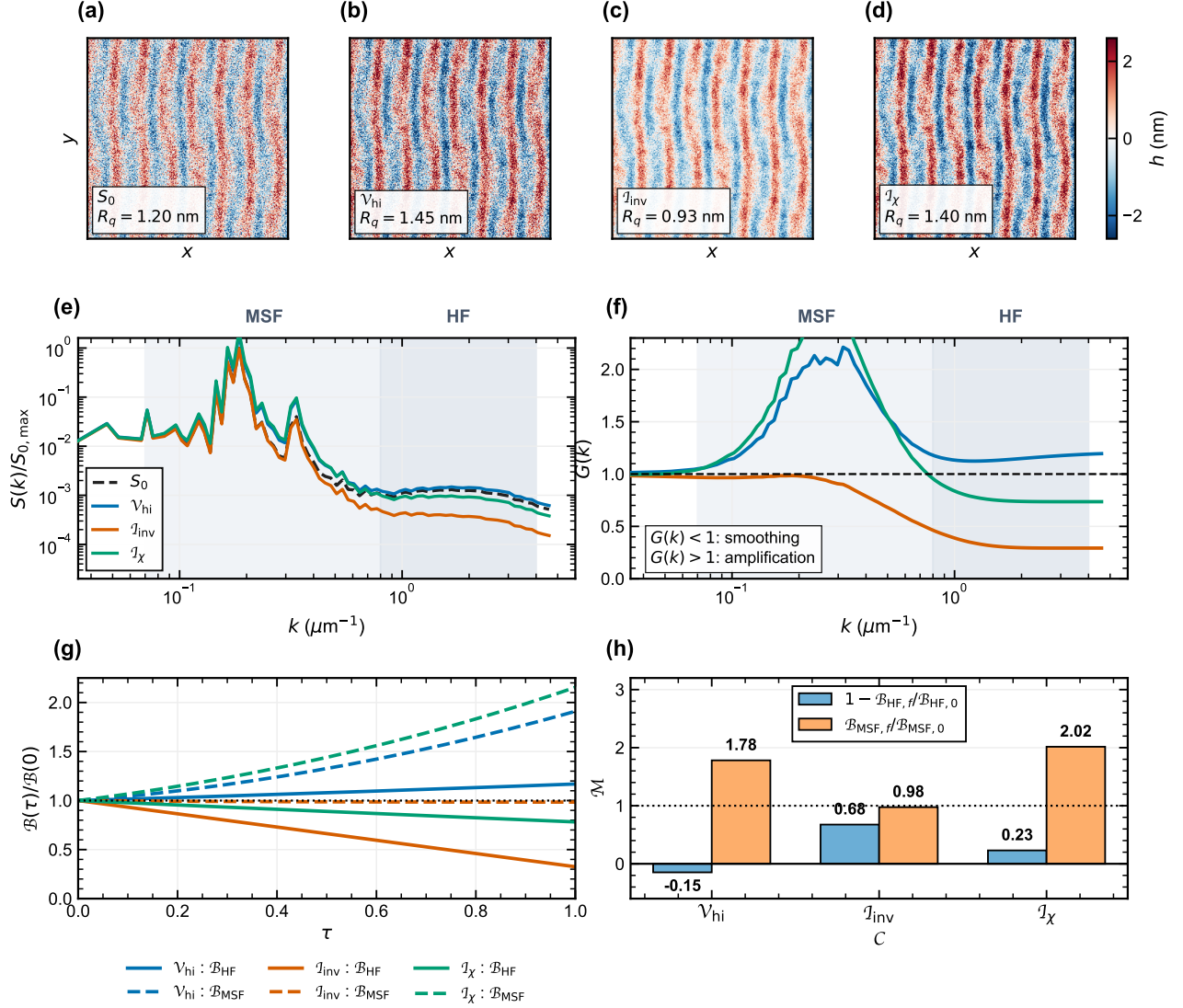


FIG. 4. End-to-end roughness-spectrum control of quartz by IEDF-controlled ion-beam polishing. (a) Initial synthetic quartz surface generated from a broadband roughness spectrum. (b)–(d) Final surfaces obtained from the same initial morphology under high-voltage control V_{hi} , inverse IEDF control I_{inv} , and broad-IEDF control I_χ . (e) Radially averaged PSDs before and after polishing. (f) PSD gain $G(k) = S_f(k)/S_0(k)$, showing that inverse IEDF control suppresses high-spatial-frequency roughness without the MSF amplification produced by high-voltage or broad-IEDF conditions. (g) Evolution of normalized high-frequency and MSF band powers. (h) Summary of high-frequency reduction and MSF penalty for the competing control strategies.

IEDF and increases the risk of MSF roughening. Figure 5(d) shows convergence of the inverse-design objective toward $\mathcal{J}_{min} \approx 1.76 \times 10^{-2}$. The main result is shown in Fig. 5(e): the optimized gain $G(k; V_g^*)$ follows the target $G^*(k)$ closely, whereas V_{dc} misses the target and V_{rip} produces an MSF amplification peak. Figure 5(f) summarizes the control performance. The optimized waveform gives the smallest PSD error and suppresses $\mathcal{R}_{MSF}$.

This result gives the clearest expression of gate-voltage-resolved control. The model treats the voltage waveform as a design object whose purpose is to generate an IEDF that produces a prescribed roughness-spectrum

transformation:

$$S^*(k) \longrightarrow V_g^*(t) \longrightarrow f_i^*(E) \longrightarrow G(k) \approx G^*(k). \quad (54)$$

F. Ablation tests and physical necessity of IEDF control

The preceding sections show that the IEDF-resolved model predicts a smoothing–roughening transition, collapses the PSD response, remains robust under uncertainty, and synthesizes a gate-voltage waveform for a pre-

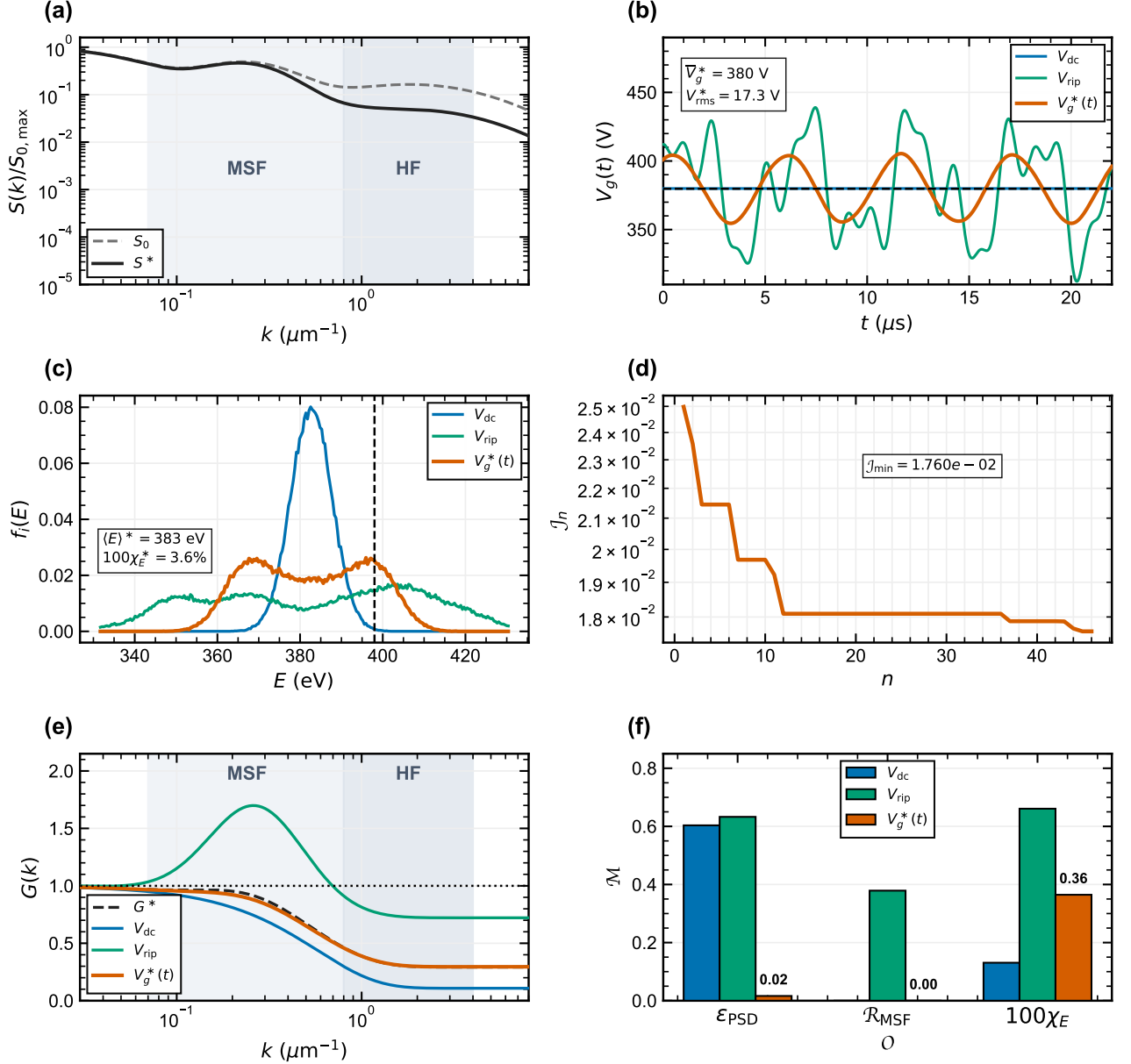


FIG. 5. Inverse gate-waveform synthesis for target quartz PSD control. (a) Initial roughness spectrum $S_0(k)$ and prescribed target spectrum $S^*(k)$. (b) Optimized gate-voltage waveform $V_g^*(t)$, compared with a DC waveform V_{dc} and an uncontrolled ripple waveform V_{rip} . (c) Ion energy distributions generated by the three waveforms. The optimized waveform produces an IEDF near the desired smoothing window. (d) Convergence of the waveform-design objective J_n . (e) PSD gain comparison. The optimized waveform closely follows the target gain $G^*(k)$, while the uncontrolled ripple waveform produces MSF amplification. (f) Summary of PSD tracking error, MSF roughening, and relative IEDF width for the competing waveform controls.

scribed target. A final question is whether these conclusions truly require IEDF physics, or whether a simpler voltage-only or mean-energy-only description would give the same result. To address this, we remove key physical ingredients one at a time and determine whether the predictive structure survives.

We compare five descriptions of the same operating ensemble. The first two are scalar controls based only on the mean gate voltage and mean ion energy, $\bar{V}_g$ and

$\langle E \rangle$. The remaining three are reduced IEDF-based coordinates. The first removes explicit relative-width dependence and is denoted by $\Lambda_{-\chi}$. The second removes the high-energy penalty and is denoted by $\Lambda_{-E_{hi}}$. The last is the full IEDF coordinate Λ_{IEDF} . If voltage alone were sufficient, $\bar{V}_g$ would predict the PSD response. If the energy scale alone were sufficient, $\langle E \rangle$ would perform comparably to the full model. If IEDF physics is necessary, the best prediction should require both the mean

energy and the distribution width.

For each model $\mathcal{M}$, a reduced predictor is fitted on a training set and evaluated on a held-out set. The held-out coefficient of determination is

$$R_{\text{te}}^2(\mathcal{M}) = 1 - \frac{\sum_{j \in \mathcal{D}_{\text{te}}} [\mathcal{Q}_{\text{PSD},j} - \hat{\mathcal{Q}}_{\text{PSD},j}^{(\mathcal{M})}]^2}{\sum_{j \in \mathcal{D}_{\text{te}}} [\mathcal{Q}_{\text{PSD},j} - \bar{\mathcal{Q}}_{\text{PSD}}]^2}. \quad (55)$$

Figure 6(a) shows that voltage-only and mean-energy-only predictors give moderate performance,

$$R_{\text{te}}^2(\bar{V}_g) \simeq 0.60, \quad R_{\text{te}}^2(\langle E \rangle) \simeq 0.61, \quad (56)$$

whereas the full IEDF coordinate reaches $R_{\text{te}}^2(\Lambda_{\text{IEDF}}) \simeq 0.98$. Removing the width term weakens prediction, while the high-energy-aware coordinate remains close to the full model. Thus the response cannot be reduced to voltage or energy alone.

The second ablation test examines the phase boundary. We compare the full model $\mathcal{M}_{\text{full}}$ with three leave-one-physics-out variants,

$$\mathcal{M}_{\neg \chi_E}, \quad \mathcal{M}_{\neg E_{\text{hi}}}, \quad \mathcal{M}_{\neg \text{MSF}}. \quad (57)$$

Each model produces a boundary

$$\partial \Omega_{\mathcal{M}} = \left\{ (\langle E \rangle, \chi_E) : \mathcal{Q}_{\text{PSD}}^{(\mathcal{M})}(\langle E \rangle, \chi_E) = 0 \right\}. \quad (58)$$

Figure 6(b) shows that removing the IEDF-width, high-energy, or MSF-roughening terms distorts the smoothing-roughening boundary. The finite window in the full model is therefore not created by the plotting coordinates alone. It depends on physical terms that describe the distribution width and the roughening channels activated by it.

The third test asks whether inverse design is target-specific. We generate a family of target gains $G_i^*(k)$ and compare voltage-only, mean-energy-only, and full IEDF design descriptions. For each target, the PSD tracking error is

$$\epsilon_{\text{PSD}} = \left[\frac{1}{N_k} \sum_{\ell=1}^{N_k} (\log G(k_\ell) - \log G^*(k_\ell))^2 \right]^{1/2}. \quad (59)$$

Figure 6(c) shows that voltage-only design sometimes reaches the target but has a broad error distribution. Mean-energy-only design is less reliable because it cannot adjust IEDF width independently. Full IEDF design gives the smallest and narrowest error distribution.

Finally, a design is counted as successful if it satisfies

$$\epsilon_{\text{PSD}} < \epsilon_0, \quad \mathcal{R}_{\text{MSF}} < R_0, \quad \chi_E < \chi_0. \quad (60)$$

The corresponding pass probability is

$$P_{\text{pass}}(\mathcal{D}) = \frac{1}{N_{\text{tar}}} \sum_{i=1}^{N_{\text{tar}}} \Theta[\epsilon_0 - \epsilon_{\text{PSD},i}] \Theta[R_0 - \mathcal{R}_{\text{MSF},i}] \Theta[\chi_0 - \chi_{E,i}]. \quad (61)$$

Figure 6(d) shows that voltage-only design is partially useful but unreliable: it passes the combined criterion for about 47% of target spectra. Mean-energy-only design passes about 6%. The full IEDF-control design passes all criteria across this simulated target ensemble. This gives the falsification test a clear interpretation: voltage may occasionally land in a useful region, but only IEDF-resolved design systematically controls the PSD response while avoiding MSF amplification.

Taken together, the ablation tests support the central claim. The smoothing window, predictive collapse, many-target inverse design, and waveform-control result are not consequences of a voltage-only correlation or a flexible curve fit. They require the physical content of the IEDF state, especially the relative width and roughening channels that it activates.

IV. METHODS AND REPRODUCIBILITY

This work uses a reduced theoretical and numerical workflow. No experimental polishing data are fitted in the main simulations. Each operating point is defined first by a gate-voltage waveform and the reduced converter-plasma-sheath transfer response. The resulting waveform is mapped to an ion energy distribution, from which the mean energy $\langle E \rangle$ and the relative width χ_E are calculated. These IEDF moments are then passed to the PSD-response model to obtain the smoothing score, the roughening order parameter, and the spectral gain. For the end-to-end height-field tests, the same gain is applied to the Fourier components of a synthetic quartz surface so that the final PSD and morphology can be compared across control strategies.

The kernel definitions, nominal parameter values, and surface-evolution procedure are given in Appendices A and B. The purpose of placing these expressions explicitly in the manuscript is to make the phase maps, inverse-design calculations, uncertainty tests, and ablation studies reproducible. The numerical values should not be interpreted as universal constants for quartz polishing. For a specific ICP source, gas chemistry, extraction geometry, incidence angle, or metrology bandwidth, the onset energy, useful-energy window, high-energy penalty, and MSF-response kernel should be calibrated against measured IEDFs and measured PSD gains.

The robustness analysis perturbs the reduced sputtering, broadening, damage, and spectral-response parameters and then recomputes the smoothing probability and the uncertainty of the smoothing-roughening boundary. The inverse-design tests use the same forward model, but solve the reverse problem: a target PSD gain is prescribed, and the model searches for an IEDF state and an admissible gate waveform that reproduce that target while penalizing MSF amplification and excessive voltage ripple. This makes the framework testable. If measured surfaces are predicted equally well by nominal voltage or mean energy alone, the IEDF-control description is un-

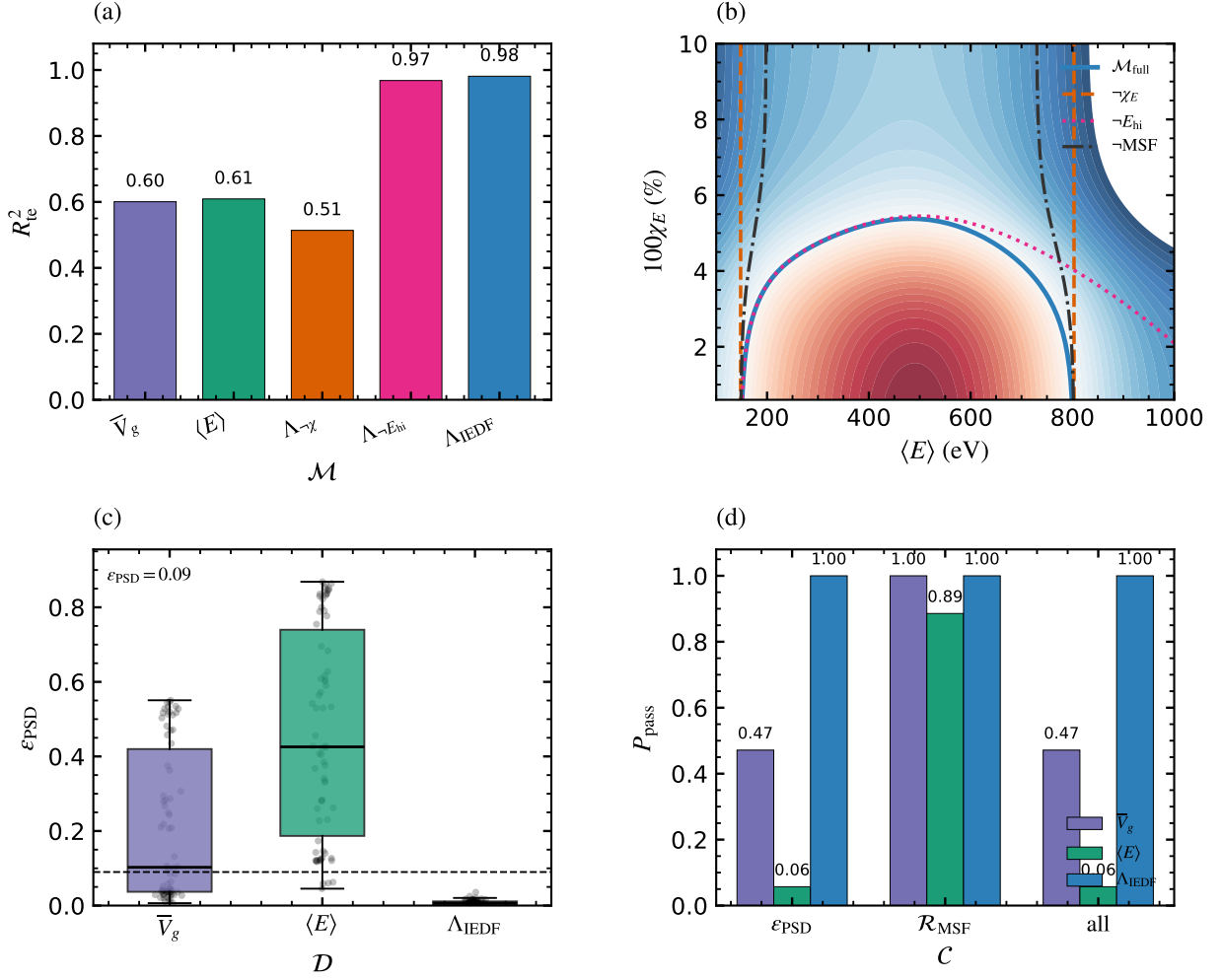


FIG. 6. Ablation and falsification tests for the IEDF-control theory. (a) Held-out prediction performance for voltage-only, mean-energy-only, ablated, and full IEDF-control descriptions. The full coordinate Λ_{IEDF} gives the strongest held-out prediction. (b) Leave-one-physics-out phase boundaries. Removing the IEDF-width, high-energy, or MSF-roughening terms distorts the smoothing-roughening boundary relative to the full model. (c) Many-target inverse-design test. The PSD tracking error ϵ_{PSD} is smallest and most concentrated for the full IEDF-control design. (d) Pass probability for PSD tracking, MSF suppression, and the combined criterion. Voltage-only control is partially successful but unreliable, while IEDF-resolved design passes all criteria in this simulated target ensemble.

necessary. If measured PSD gains collapse more reliably with the IEDF coordinate, the model provides a practical basis for waveform-level control.

V. DISCUSSION

The results point to one main message: the useful polishing state is the IEDF, not the nominal gate voltage. The phase map shows a finite smoothing window in $(\langle E \rangle, \chi_E)$. The reduced-control result shows that the PSD response becomes easier to predict when it is described with an IEDF-based coordinate. The uncertainty analysis shows that the window is not simply the consequence of one selected parameter set. The surface-

evolution calculation shows how the same control idea changes the final morphology, while the inverse-waveform calculation closes the loop from a target PSD back to a gate waveform. The ablation tests support the same interpretation, because the predictive structure weakens when the IEDF width and roughening terms are removed.

This interpretation has a direct practical meaning. The mean gate voltage is an electrical setting at the power supply; it is not the quantity that directly acts on the quartz surface. It becomes useful only after the converter, plasma load, and sheath have converted it into $f_i(E, \theta)$. Raising the voltage can increase removal, but it can also increase roughening or damage. In the same way, ripple or pressure-driven broadening can leave the mean energy almost unchanged while moving the surface

response from stable smoothing to MSF amplification. The best operating point is therefore not necessarily the highest voltage. It is the condition in which the mean energy is high enough for useful removal, while the relative IEDF width remains low enough to avoid roughening.

The model also separates removal strength from polishing quality. A faster removal condition is not automatically the better optical-polishing condition. If it creates MSF structure, it may make later finishing more difficult even when the average roughness appears acceptable. A condition that reduces high-frequency roughness while leaving the middle of the PSD unchanged may be preferable, even if it removes material more slowly. This tradeoff is captured by the reduced coordinate Λ_{IEDF} and the roughening measure $\mathcal{R}_{\text{MSF}}$. Together they allow polishing conditions to be compared by their spectral consequence, not only by their removal power.

The energy scale predicted here should be treated as a calibrated model result, not as a universal polishing recipe. The inverse-designed points in this study cluster near $\langle E \rangle \approx 367\text{--}398$ eV with $100\chi_E \approx 3.5\text{--}3.8\%$. Published fused-silica ion-polishing studies often use higher Ar-ion energies, and some report their strongest smoothing near the 0.8–1.3 keV scale, with degradation appearing again at still higher energies [9]. Other ion-beam figuring and reactive ion-beam figuring studies also show that roughness response depends on material, chemistry, incidence angle, removed depth, and measured spatial-frequency band [8, 28, 37]. This comparison does not weaken the control idea. Rather, it shows how the present model should be used: the parameters E_{opt} and E_{hi} should be fitted to the specific tool, material, and process window under study. The main claim is not that one numerical energy is universal, but that the useful control variable is the IEDF state rather than the nominal voltage alone.

The proposed framework is written in terms of quantities that can be measured. The mean energy $\langle E \rangle$, energy spread σ_E , and IEDF shape can be measured or inferred using plasma diagnostics and energy analyzers. The PSD gain $G(k)$ can be measured by combining AFM, white-light interferometry, and optical-scattering measurements over the relevant spatial-frequency ranges [4, 5, 8]. A direct experimental test would hold the mean gate voltage fixed, change the ripple-transfer state, and measure whether both $f_i(E)$ and $S_f(k)/S_0(k)$ change. A second test would use an inverse-designed waveform and compare the measured PSD gain with the target gain. These tests would show whether voltage-only control is sufficient, or whether IEDF-resolved control is needed.

VI. LIMITATIONS AND OUTLOOK

This work is theoretical and should not be read as an experimental demonstration of a specific polishing tool. The numerical boundaries in the phase maps depend on the chosen sputtering-onset function, broadening model,

high-energy penalty, and PSD-response kernel. The main claim is therefore not the exact numerical position of the smoothing window. The main claim is that the reduced model predicts an IEDF-controlled smoothing–roughening transition, a compact IEDF-based response collapse, and a route for inverse spectral design that can be calibrated and tested experimentally.

A second limitation is the compact IEDF description. The present model uses mainly $\langle E \rangle$ and χ_E . This is useful for building a clear control picture, but real beams may require the full distribution $f_i(E, \theta)$. This will be especially important for oblique incidence, anisotropic ripple formation, or strongly collisional extraction. The same framework can be extended by replacing χ_E with higher moments, or by building Λ_{IEDF} from the full energy-angle distribution.

A third limitation is the reduced surface-evolution model. The height-field calculations are designed to show the spectral consequences of different IEDF states. They are not a substitute for atomistic simulations, detailed continuum models, or controlled polishing experiments. Future work should compare the predicted PSD gains with Monte Carlo ion-solid simulations, continuum evolution equations, and measured polishing data. The ablation tests make the theory testable. If future measurements show that PSD evolution is predicted equally well by $\bar{V}_g$ or $\langle E \rangle$ alone, then the IEDF-control description is not needed. If the measured response follows the IEDF coordinate more closely than nominal voltage, the framework will provide a practical path toward predictive waveform design.

VII. CONCLUSION

We developed a reduced theoretical framework for gate-voltage-resolved IEDF control in ICP-extracted ion-beam polishing of quartz using a 2 kW LLC resonant DC bias supply. The central result is that the mean gate voltage is not the most direct polishing coordinate. The more useful control state is the ion energy distribution generated by the coupled power-electronics, plasma-load, and sheath-transfer chain. Within the model, stable smoothing occurs in a finite region of the $(\langle E \rangle, \chi_E)$ plane. The process moves toward MSF roughening when the IEDF becomes too broad, and toward high-energy risk when the mean energy becomes too large.

A reduced IEDF-control coordinate collapses the simulated PSD response more effectively than voltage-only or mean-energy-only descriptions. It also supports inverse design of target roughness spectra. Robustness analysis, end-to-end surface evolution, inverse waveform synthesis, and ablation tests all support the same conclusion within the assumptions of the reduced model. Predictive quartz polishing should therefore be designed through the IEDF state, not through nominal voltage alone. In this view, the gate voltage is a machine actuator that must be calibrated through the plasma and sheath response before

it can be used for reliable roughness-spectrum control.

FUNDING DECLARATION

This work was supported by the Priority S & T Plan Project of Leshan of P.R. China (23GZD013)

COMPETING INTERESTS

The authors declare no competing interests.

DATA AVAILABILITY

No experimental datasets were used in this study. The numerical data shown in the figures are generated from the equations, kernel definitions, and parameter values reported in the main text and appendices. Additional numerical output files can be provided by the corresponding author upon reasonable request.

CODE AVAILABILITY

The scripts used to generate the phase maps, inverse-design calculations, robustness tests, ablation studies, and synthetic surface-evolution examples are available from the corresponding author upon reasonable request.

Appendix A: Kernel definitions and numerical parameters

This Appendix contains the analytical forms used for the reduced PSD-control score and the IEDF-control coordinate. The aim is to allow reproducibility of the phase maps, robustness tests, and inverse-design calculations. The kernels are not meant to be universal laws of matter. They are smooth phenomenological functions that incorporate the main physical requirements for ion-beam polishing: sputtering must be active, the mean energy must be in a useful range, the IEDF must be sufficiently narrow, and high-energy roughening must be avoided.

The sputtering-onset function is written as

$$\mathcal{S}_{\text{on}}(E) = \left[1 + \exp \left(-\frac{E - E_{\text{th}}}{\Delta E_{\text{th}}} \right) \right]^{-1}, \quad (\text{A1})$$

where E_{th} is the effective onset energy and ΔE_{th} controls how gradual the onset is. This smooth form avoids an artificial discontinuity at threshold while still representing the fact that very low-energy ions produce weak material removal.

The useful polishing-energy window is modeled as

$$\mathcal{W}_E(E) = \exp \left[-\frac{(E - E_{\text{opt}})^2}{2\sigma_E^{*2}} \right], \quad (\text{A2})$$

where E_{opt} is the center of the nominal smoothing window and σ_E^* controls its width. This term expresses the idea that the most useful polishing condition is not obtained at the highest energy, but in an intermediate region where removal is active without strong damage or roughening penalties.

The broad-IEDF penalty is written as

$$\mathcal{B}_\chi(\chi_E) = \left[1 + \exp \left(-\frac{\chi_E - \chi_c}{\Delta\chi} \right) \right]^{-1}. \quad (\text{A3})$$

Here χ_c is the relative-width scale where broadening begins to affect the surface response, and $\Delta\chi$ controls the sharpness of that transition. Thus $\mathcal{B}_\chi \approx 0$ for narrow IEDFs and $\mathcal{B}_\chi \approx 1$ for broad IEDFs.

The high-energy damage or roughening penalty is

$$\mathcal{D}_{\text{hi}}(E) = \left[1 + \exp \left(-\frac{E - E_{\text{hi}}}{\Delta E_{\text{hi}}} \right) \right]^{-1}, \quad (\text{A4})$$

where E_{hi} is the energy scale where high-energy damage or roughening becomes important. This term is included because a larger ion energy does not always improve polishing quality. At sufficiently high energy, the process can increase defect production, roughening, or subsurface modification.

Using these kernels, the PSD-control score used in the main text is

$$\begin{aligned} \mathcal{Q}_{\text{PSD}} = & A_{\text{sm}} \mathcal{S}_{\text{on}}(E) \mathcal{W}_E(E) [1 - \alpha_\chi \mathcal{B}_\chi(\chi_E)] \\ & - A_\chi \mathcal{B}_\chi(\chi_E) - A_{\text{hi}} \mathcal{D}_{\text{hi}}(E) - A_{\text{lo}} [1 - \mathcal{S}_{\text{on}}(E)]. \end{aligned} \quad (\text{A5})$$

The first term represents useful smoothing. The remaining terms penalize broad IEDFs, high-energy operation, and operation below sputtering onset.

The reduced IEDF-control coordinate is

$$\Lambda_{\text{IEDF}} = \frac{\mathcal{S}_{\text{on}}(E) \mathcal{W}_E(E)}{1 + (\chi_E / \chi_c)^m + a_{\text{hi}} \mathcal{D}_{\text{hi}}(E)}. \quad (\text{A6})$$

This coordinate becomes large only when the ion energy is in the useful smoothing range, the IEDF is narrow, and the high-energy penalty is small.

The nominal parameter values used in the numerical examples are listed in Table I. These values define the baseline model. In the uncertainty analysis, the same parameters are perturbed around their nominal values to test whether the smoothing window survives plausible model variation.

For the robustness calculations, the uncertain parameter vector is

$$\xi = \{E_{\text{th}}, E_{\text{opt}}, \chi_c, E_{\text{hi}}, A_{\text{sm}}, A_\chi, A_{\text{hi}}, A_{\text{lo}}, k_{\text{sm}}, k_{\text{MSF}}\}. \quad (\text{A7})$$

Unless otherwise stated, each parameter is varied independently around its nominal value using a bounded perturbation. In the present simulations, the energy scales and amplitude weights are varied by $\pm 15\%$, while the

TABLE I. Nominal reduced-model parameters used for the PSD-control score and IEDF-control coordinate. Energies are given in electronvolts, while χ_E is dimensionless. The values should be interpreted as calibration parameters for the reduced theoretical model rather than universal constants for quartz polishing.

Parameter	Nominal value	Meaning
E_{th}	135 eV	effective sputtering-onset energy
ΔE_{th}	25 eV	onset smoothness
E_{opt}	380 eV	center of useful polishing-energy window
σ_E^*	130 eV	width of useful energy window
E_{hi}	820 eV	high-energy roughening or damage scale
ΔE_{hi}	70 eV	high-energy transition width
χ_c	0.045	IEDF-width transition scale
$\Delta\chi$	0.008	IEDF-width transition smoothness
m	4	width penalty exponent in Λ_{IEDF}
A_{sm}	1.50	smoothing weight
A_χ	0.85	broad-IEDF penalty weight
A_{hi}	1.10	high-energy penalty weight
A_{lo}	0.90	low-energy penalty weight
α_χ	0.55	smoothing reduction caused by IEDF broadening
a_{hi}	1.00	high-energy penalty in Λ_{IEDF}

spatial-frequency centers are varied by $\pm 20\%$. These ranges are not meant to represent a specific experimental uncertainty budget. They are used to test whether the predicted smoothing region is structurally stable rather than tuned to one exact parameter set.

Appendix B: Reduced PSD-gain and surface-evolution model

This appendix gives the reduced surface-response model used to generate the PSD gains and height-field examples. The model is phenomenological, but it is written in a form that follows the usual linearized interpretation of ion-induced surface evolution. Each Fourier component of the surface is assumed to evolve under a competition between smoothing, roughening, and weak stochastic forcing.

For a Fourier component $\hat{h}_{\mathbf{k}}(t)$, the reduced evolution equation is written as

$$\frac{d\hat{h}_{\mathbf{k}}}{dt} = \Gamma_{\text{net}}(k; E, \chi_E) \hat{h}_{\mathbf{k}} + \eta_{\mathbf{k}}(t), \quad (\text{B1})$$

where Γ_{net} is the net spectral growth rate and $\eta_{\mathbf{k}}(t)$ represents weak stochastic forcing from ion-impact noise. A negative value of Γ_{net} gives smoothing, while a positive value gives amplification of that spatial-frequency component.

The net rate is decomposed as

$$\Gamma_{\text{net}}(k; E, \chi_E) = -\Gamma_{\text{sm}}(E, k) + \Gamma_{\text{MSF}}(E, \chi_E, k) + \Gamma_{\text{hi}}(E, k). \quad (\text{B2})$$

The first term is the useful smoothing contribution. The second term is the mid-spatial-frequency roughening contribution that grows when the IEDF becomes broad. The third term is a high-energy roughening contribution.

The smoothing term is modeled as

$$\Gamma_{\text{sm}}(E, k) = \Gamma_{\text{sm},0} \mathcal{S}_{\text{on}}(E) \mathcal{W}_E(E) \mathcal{H}_{\text{HF}}(k), \quad (\text{B3})$$

where $\Gamma_{\text{sm},0}$ is a smoothing-rate scale and $\mathcal{H}_{\text{HF}}(k)$ weights the high-frequency band. We use

$$\mathcal{H}_{\text{HF}}(k) = \left[1 + \exp \left(-\frac{\log k - \log k_{\text{HF},1}}{\Delta_{\text{HF}}} \right) \right]^{-1}, \quad (\text{B4})$$

so that smoothing acts most strongly above the lower edge of the high-frequency band.

The MSF roughening term is written as

$$\Gamma_{\text{MSF}}(E, \chi_E, k) = \Gamma_{\text{MSF},0} \mathcal{B}_\chi(\chi_E) \mathcal{W}_{\text{MSF}}(E) \exp \left[-\frac{(\log k - \log k_{\text{MSF}})^2}{2\sigma_{\text{MSF}}^2} \right]. \quad (\text{B5})$$

Here k_{MSF} is the center of the MSF response and σ_{MSF} controls its width in log-frequency space. The energy factor is

$$\mathcal{W}_{\text{MSF}}(E) = \exp \left[-\frac{(E - E_{\text{MSF}})^2}{2\sigma_{\text{MSF},E}^2} \right]. \quad (\text{B6})$$

This term implements the idea that broad IEDFs can mix different sputtering and redistribution regimes during the same exposure. The result can be an MSF amplification peak even when part of the high-frequency roughness is reduced.

The high-energy roughening term is

$$\Gamma_{\text{hi}}(E, k) = \Gamma_{\text{hi},0} \mathcal{D}_{\text{hi}}(E) \mathcal{H}_{\text{hi}}(k), \quad (\text{B7})$$

where

$$\mathcal{H}_{\text{hi}}(k) = \exp \left[-\frac{(\log k - \log k_{\text{hi}})^2}{2\sigma_{\text{hi}}^2} \right]. \quad (\text{B8})$$

This contribution is small at moderate energy and becomes important when E approaches the high-energy penalty region.

For a polishing time t_p , the PSD gain is then

$$G(k; E, \chi_E) = \exp[2\Gamma_{\text{net}}(k; E, \chi_E)t_p]. \quad (\text{B9})$$

The factor of two appears because the PSD is proportional to the squared Fourier amplitude. If the height amplitude changes as $\hat{h}_{\mathbf{k}} \rightarrow \hat{h}_{\mathbf{k}} \exp(\Gamma_{\text{net}}t_p)$, then the PSD changes as $S(k) \rightarrow S(k) \exp(2\Gamma_{\text{net}}t_p)$.

The final PSD used in the height-field examples is

$$S_f(k; \mathcal{C}) = G(k; \mathcal{C})S_0(k), \quad (\text{B10})$$

where $\mathcal{C}$ denotes the chosen control state. To construct a final height map, the Fourier amplitudes of the initial surface are multiplied by $G^{1/2}(k; \mathcal{C})$, while the phases are kept fixed except for a weak stochastic contribution. In cases with broad IEDF or high ripple-risk, a small anisotropic MSF component is added to make the MSF amplification visible in real space. This procedure is not a substitute for a kinetic surface simulation. It is used

only to show the spectral consequence of different IEDF states on the same initial surface.

The nominal surface-response parameters are listed in Table II. These values set the scale of the simulated PSD gains. They can be recalibrated when measured PSD data are available for a specific tool, material, gas species, and incidence geometry.

The MSF and HF band powers used in the main text are computed from

$$\mathcal{B}_{\mathcal{K}}[S] = \int_{k_{\mathcal{K},1}}^{k_{\mathcal{K},2}} S(k) d \log k, \quad \mathcal{K} \in \{\text{MSF}, \text{HF}\}. \quad (\text{B11})$$

The high-frequency reduction and MSF gain are

$$\mathcal{M}_{\text{HF}} = 1 - \frac{\mathcal{B}_{\text{HF}}[S_f]}{\mathcal{B}_{\text{HF}}[S_0]}, \quad \mathcal{M}_{\text{MSF}} = \frac{\mathcal{B}_{\text{MSF}}[S_f]}{\mathcal{B}_{\text{MSF}}[S_0]}. \quad (\text{B12})$$

A favorable polishing response has $\mathcal{M}_{\text{HF}} > 0$ and $\mathcal{M}_{\text{MSF}} \leq 1$. This means that high-frequency roughness is reduced without transferring error into the mid-spatial-frequency band.

-
- [1] E. L. Church, [Wear](#) **57**, 93 (1979).
 - [2] J. M. Elson and J. M. Bennett, [Applied Optics](#) **34**, 201 (1995).
 - [3] J. M. Bennett and L. Mattsson, *Introduction to Surface Roughness and Scattering* (Optical Society of America, Washington, DC, 1989).
 - [4] J. C. Stover, *Optical Scattering: Measurement and Analysis*, 2nd ed. (SPIE Press, Bellingham, 1995).
 - [5] A. Duparré, J. Ferré-Borrull, S. Gliech, G. Notni, J. Steinert, and J. M. Bennett, [Applied Optics](#) **41**, 154 (2002).
 - [6] L. N. Allen and H. W. Romig, in *Advanced Optical Manufacturing and Testing*, Proceedings of SPIE, Vol. 1333 (1990) pp. 22–34.
 - [7] T. W. Drueding, T. G. Bifano, S. C. Fawcett, and S. J. Waldman, [Optical Engineering](#) **34**, 3565 (1995).
 - [8] N. I. Chkhalo, S. A. Churin, A. E. Pestov, N. N. Salashchenko, Y. A. Vainer, and M. V. Zorina, [Optics Express](#) **22**, 20094 (2014).
 - [9] N. I. Chkhalo, S. A. Churin, M. S. Mikhaylenko, A. E. Pestov, V. N. Polkovnikov, N. N. Salashchenko, and M. V. Zorina, [Applied Optics](#) **55**, 1249 (2016).
 - [10] M. A. Lieberman and A. J. Lichtenberg, *Principles of Plasma Discharges and Materials Processing*, 2nd ed. (Wiley-Interscience, Hoboken, 2005).
 - [11] P. Chabert and N. Braithwaite, *Physics of Radio-Frequency Plasmas* (Cambridge University Press, Cambridge, 2011).
 - [12] E. Kawamura, V. Vahedi, M. A. Lieberman, and C. K. Birdsall, [Plasma Sources Science and Technology](#) **8**, R45 (1999).
 - [13] D. Gahan, B. Dolinaj, and M. B. Hopkins, [Review of Scientific Instruments](#) **79**, 033502 (2008).
 - [14] P. Sigmund, [Physical Review](#) **184**, 383 (1969).
 - [15] P. Sigmund, [Journal of Materials Science](#) **8**, 1545 (1973).
 - [16] R. M. Bradley and J. M. E. Harper, [Journal of Vacuum Science & Technology A](#) **6**, 2390 (1988).
 - [17] R. Cuerno and A.-L. Barabási, [Physical Review Letters](#) **74**, 4746 (1995).
 - [18] M. A. Makeev, R. Cuerno, and A.-L. Barabási, [Nuclear Instruments and Methods in Physics Research Section B](#) **197**, 185 (2002).
 - [19] D. J. Economou, [Journal of Vacuum Science & Technology A](#) **31**, 050823 (2013).
 - [20] E. Schüngel, Z. Donkó, P. Hartmann, A. Derzsi, I. Korolov, and J. Schulze, [Plasma Sources Science and Technology](#) **25**, 054002 (2016).
 - [21] M. K. Kazimierczuk and D. Czarkowski, *Resonant Power Converters*, 2nd ed. (Wiley, Hoboken, 2011).
 - [22] B. Yang, F. C. Lee, A. J. Zhang, and G. Huang, in *Proceedings of the Seventeenth Annual IEEE Applied Power Electronics Conference and Exposition*, APEC, Vol. 2 (2002) pp. 1108–1112.
 - [23] B. Lu, W. Liu, Y. Liang, F. C. Lee, and J. D. van Wyk, in *Proceedings of the Twenty-First Annual IEEE Applied Power Electronics Conference and Exposition*, APEC (2006) pp. 533–538.
 - [24] R. W. Erickson and D. Maksimović, *Fundamentals of Power Electronics*, 2nd ed. (Kluwer Academic Publishers, Boston, 2001).
 - [25] J. Nocedal and S. J. Wright, *Numerical Optimization*, 2nd ed. (Springer, New York, 2006).
 - [26] D. Bertsimas and M. Sim, [Operations Research](#) **52**, 35 (2004).
 - [27] A. Saltelli, M. Ratto, T. Andres, F. Campolongo, J. Cariboni, D. Gatelli, M. Saisana, and S. Tarantola, *Global Sensitivity Analysis: The Primer* (Wiley, Chichester, 2008).

TABLE II. Nominal parameters for the reduced PSD-gain model. The polishing time t_p is normalized, so the rate constants are dimensionless in the present simulations.

Parameter	Nominal value	Meaning
t_p	1	normalized polishing time
$\Gamma_{\text{sm},0}$	0.45	high-frequency smoothing-rate scale
$\Gamma_{\text{MSF},0}$	0.35	MSF roughening-rate scale
$\Gamma_{\text{hi},0}$	0.25	high-energy roughening-rate scale
$k_{\text{HF},1}$	$0.80 \mu\text{m}^{-1}$	lower edge of HF smoothing band
Δ_{HF}	0.25	smoothness of HF transition in $\log-k$
k_{MSF}	$0.25 \mu\text{m}^{-1}$	center of MSF roughening response
σ_{MSF}	0.45	width of MSF response in $\log-k$
E_{MSF}	430 eV	energy center of MSF roughening response
$\sigma_{\text{MSF},E}$	220 eV	energy width of MSF response
k_{hi}	$1.20 \mu\text{m}^{-1}$	center of high-energy roughening response
σ_{hi}	0.55	width of high-energy roughening response in $\log-k$

- [28] T. Arnold, G. Böhm, R. Fechner, J. Meister, A. Nickel, F. Frost, T. Hänsel, and A. Schindler, *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment* **616**, 147 (2010).
- [29] J. Muñoz-García, R. Cuerno, and M. Castro, *Current Opinion in Solid State and Materials Science* **18**, 323 (2014).
- [30] M. A. Lieberman, *IEEE Transactions on Plasma Science* **16**, 638 (1988).
- [31] A. Metze, D. W. Ernie, and H. J. Oskam, *Journal of Applied Physics* **60**, 3081 (1986).
- [32] Z. Donkó, J. Schulze, B. G. Heil, and U. Czarnetzki, *Journal of Physics D: Applied Physics* **42**, 025205 (2009).
- [33] G. Carter and V. Vishnyakov, *Physical Review B* **54**, 17647 (1996).
- [34] C. S. Madi, E. Anzenberg, K. F. Ludwig, and M. J. Aziz, *Physical Review Letters* **106**, 066101 (2011).
- [35] R. L. Steigerwald, *IEEE Transactions on Power Electronics* **3**, 174 (1988).
- [36] S. A. Norris, M. P. Brenner, and M. J. Aziz, *Journal of Physics: Condensed Matter* **23**, 335006 (2011).
- [37] F. Frost, R. Fechner, B. Ziberi, D. Flamm, and A. Schindler, *Journal of Physics: Condensed Matter* **21**, 224026 (2009).
- [38] C. C. Umbach, R. L. Headrick, and K.-C. Chang, *Physical Review Letters* **87**, 246104 (2001).
- [39] B. Davidovitch, M. J. Aziz, and M. P. Brenner, *Physical Review B* **76**, 205420 (2007).
- [40] S. Boyd and L. Vandenberghe, *Convex Optimization* (Cambridge University Press, Cambridge, 2004).
- [41] R. Y. Rubinstein, *Methodology and Computing in Applied Probability* **1**, 127 (1999).