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Voltage waveform to achieve a desired ion energy distribution on a substrate in contact with plasma

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Abstract

A methodology is developed to determine the bias voltage waveform needed to achieve a desired (pre-selected) ion energy distribution (IED) on a substrate in contact with plasma. The approach is applicable to collisionless sheaths at all radio frequencies. It combines a circuit model with an equation for a 'damped' sheath potential to which ions respond. The methodology is demonstrated by computing the rf voltage waveform required to achieve a Gaussian IED with specified mean energy and energy spread on an electrode biased through a blocking capacitor. This *inverse* problem has multiple solutions, i.e. there exists a multitude of waveforms all producing the same IED.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Control of the energy of ions bombarding a substrate in contact with plasma is critical for plasma processing. For example, in reactive ion etching (RIE), the ion energy must be high enough to drive anisotropic etching, but not too high as to induce substrate damage and/or loss of selectivity. As device dimensions continue to shrink, precise control of the ion energy distribution (IED) becomes increasingly important. In atomic layer etching, for instance, a monoenergetic ion flux is needed, with a tightly controlled IED lying between the thresholds of chemical and physical sputtering. Thus, not only the mean energy but also the width of the IED function must be controlled.

Application of a bias voltage to the substrate is the most common approach to controlling the energy of bombarding ions. For substrates in contact with a high density plasma (collisionless sheath), application of a sinusoidal bias voltage results in a bimodal IED [1–4]. The controlling parameter is $\omega \tau_i$, with $\omega = 2\pi f$, f being the applied frequency, and τ_i being the ion transit time through the sheath. For low bias frequencies, $\omega \tau_i \ll 1$, ions respond to the instantaneous sheath voltage, and the IED is broad. For high bias frequencies, $\omega \tau_i \gg 1$, ions respond to a time-average sheath voltage, resulting in a narrow IED. The width of the distribution may be decreased by increasing $\omega \tau_i$.

Other researchers controlled the IED by applying a bias voltage to a separate electrode in contact with the plasma [5–7]. Xu et al [7] obtained nearly monoenergetic IEDs by the application of a dc bias to a 'boundary electrode'. They used a pulsed plasma and applied synchronous bias during the afterglow resulting in narrow IED (FWHM \sim few eV). Wendt and co-workers [8-10] controlled the IED by applying 'tailored' voltage waveforms primarily under the condition that ions respond fully to the instantaneous sheath voltage, i.e. $\omega \tau_i \ll 1$. Computations and experiments showed that both monoenergetic and two-peaked IEDs with controlled energies could be obtained. A similar approach was used in [11], where the effect of substrate charging on the required voltage waveform was addressed. Agarwal and Kushner [12] and Rauf [13] investigated computationally the effect of non-sinusoidal bias voltage waveforms on the IED. The etch selectivity could be controlled by adjusting the width and mean energy of the IED.

In this work, a general methodology is developed to determine the voltage waveform that must be applied to



Figure 1. Left: periodic sheath voltage profile $V(\omega t)$ given by equation (3). Right: resulting IED f(y) given by equation (4).

an electrode in contact with plasma to achieve a desired (pre-selected) IED. This is the *inverse* problem. Although the forward problem (that of finding the IED for given plasma conditions and applied rf voltage waveform) has been studied for the past several decades [1-4, 14-20], the inverse problem has come to the forefront only recently. The methodology developed here is applicable to both low ($\omega \tau_i \ll 1$) and high frequencies ($\omega \tau_i \gg 1$) of the applied rf voltage.

2. Ion energy distribution

When ions respond to the applied field ($\omega \tau_i \ll 1$), and there are no collisions in the sheath, the IED is found directly from the sheath voltage $V = V(\omega t)$ using equation (1), (see appendix A). Here f(y) is the IED as a function of ion energy, y.

$$f(y) = \frac{1}{2\pi} \sum_{\substack{\text{# of points in } 0 < \omega t < 2\pi \\ \text{ such that } V(\omega t) = y}} \frac{1}{\left|\frac{\mathrm{d}V}{\mathrm{d}(\omega t)}\right|}.$$
 (1)

This is a generalization of equation (31) in [1]. Eliminating the phase angle ωt in favor of y results

$$f(y) = \frac{1}{2\pi} \sum_{\substack{\text{\# of points in } 0 < \omega t < 2\pi \\ \text{such that } V(\omega t) = y}} \left| \frac{\mathrm{d} V^{-1}(y)}{\mathrm{d} y} \right|.$$
(2)

Here $V^{-1}(y)$ is the inverse function, i.e. $y = V(\omega t) \Rightarrow \omega t =$ $V^{-1}(y)$. If ions do not respond to the applied field, then $V(\omega t)$ in the expressions above is the sheath voltage 'seen' by the ions (hereafter referred to as 'damped' sheath voltage or 'damped' sheath potential). It is understood that the ion energy corresponding to voltage V (in volts) is in units of eV.

2.1. The forward problem

The forward problem consists of determining the IED for given plasma and boundary conditions. For example, what is the IED on a substrate on which a given voltage waveform $V_{\rm rf}$ is applied? To solve this problem, one has to determine the sheath voltage waveform 'seen' by the ions, before using equation (1) to find the IED. A way to find the damped sheath voltage is described later in the paper.

As an example, let us assume that an applied $V_{\rm rf}$ results in a damped sheath voltage waveform (not necessarily the actual sheath voltage), given by

$$V(\omega t) = V_{\rm m} + V_0 \sin \omega t,$$

$$|V_{\rm m}| > V_0, \quad V_{\rm m} < 0, \quad 0 < \omega t < 2\pi$$
(3)

where $V_{\rm m}$ is the average (mean) voltage, and V_0 is the amplitude of the sinusoidal term.

Direct application of equation (2) yields

$$f(y) = \frac{1}{2\pi} \sum_{\substack{\text{# of points in } 0 < \omega t < 2\pi \\ \text{ such that } V(\omega t) = y}} \left| \frac{d \sin^{-1}[(y - |V_m|)/V_0]}{dy} \right|$$
or

$$f(y) = \frac{1}{\pi} \frac{1}{V_0 \sqrt{1 - \left(\frac{y - |V_m|}{V_0}\right)^2}}.$$
 (4)

One can verify that the integral over the distribution given by equation (4) is unity, i.e. f(y) is normalized. The sheath voltage and the resulting IED are shown in figure 1. The IED displays the characteristic bimodal shape [1-4]. It should be noted that measured IEDs have 'smeared' peaks because of limited resolution of the ion energy analyzer and/or a distribution of energies of ions entering the sheath.

2.2. The inverse problem

The inverse problem is the following: given a desired IED (e.g. a Gaussian IED with prescribed mean energy and FWHM), determine the voltage waveform $V_{\rm rf}$ that must be applied to yield that IED. To solve this problem, one would first use equation (2) to solve for $V(\omega t)$ based on the given IED, f(y); see examples 1 and 2. This would be the sheath voltage to which ions respond. Then, one would need to determine the actual sheath voltage, and finally the required $V_{\rm rf}$, as detailed later in this paper.



Figure 2. Family of voltage waveforms parametrized by x (0 < x < 1) that result in the IED of equation (4). For the waveforms shown, x = 0.1 (solid line), 0.4 (dashed line) and 0.7 (dotted line). The voltage waveform of figure 1 (left), shifted by 1/4 phase, is recovered for x = 0.5.

Example 1. As an example, consider the IED of equation (4). The sheath voltage that ions must 'see' to yield this IED is (see appendix B)

$$V(\omega t) = V_0 \sin\left(\frac{1}{2x}\omega t - \frac{\pi}{2}\right) + V_{\rm m}$$
(5)

for $0 < \omega t < 2x\pi$, and

$$V(\omega t) = V_0 \sin\left(\frac{-1}{2(1-x)}\omega t + \frac{\pi(1+x)}{2(1-x)}\right) + V_m \quad (6)$$

for $2x\pi < \omega t < 2\pi$ where x is a parameter 0 < x < 1. Figure 2 shows a family of voltage waveforms each resulting in the IED of figure 1. Clearly the inverse problem has multiple solutions, i.e. there is a multitude of voltage waveforms all resulting in the same IED.

 $V(\omega t)$ in equations (5) and (6) is the sheath potential that would result in the IED of equation (4), if ions were to respond fully to the applied rf.

Example 2. As another example of solving the inverse problem, consider the bell-shaped (truncated Gaussian) IED,

$$f(y) = c \exp\left[-\frac{(y - |V_{\rm m}|)^2}{2\sigma^2}\right],$$

$$|V_{\rm m}| - V_0 < y < |V_{\rm m}| + V_0, \quad |V_{\rm m}| > V_0,$$

$$V_{\rm m} < 0, \quad 0 < \omega t < 2\pi$$
(7)

where the normalization factor, c, is

$$c = \frac{2}{\sigma\sqrt{2\pi} \operatorname{erf}\left[-\frac{V_0}{\sigma\sqrt{2}}, \frac{V_0}{\sigma\sqrt{2}}\right]}$$

and the error function is defined in a standard way as

$$\operatorname{erf}[z_1, z_2] = \frac{2}{\sqrt{\pi}} \int_{z_1}^{z_2} \exp[-t^2] dt.$$

Here $|V_{\rm m}|$ is the mean energy and σ is the standard deviation of the Gaussian.

Then, as in the previous example, with parameter 0 < x < 1, one obtains (see appendix C)

$$V(\omega t) = V_{\rm m} + \sigma \sqrt{2} {\rm erf}^{-1} \left[\frac{\omega t}{2\pi x} {\rm erf} \left[-\frac{V_0}{\sigma \sqrt{2}}, \frac{V_0}{\sigma \sqrt{2}} \right] + {\rm erf} \left[-\frac{V_0}{\sigma \sqrt{2}} \right] \right]$$
(8)

for $0 < \omega t < 2x\pi$, and

$$V(\omega t) = V_{\rm m} + \sigma \sqrt{2} {\rm erf}^{-1} \left[\frac{2\pi - \omega t}{2\pi (1 - x)} {\rm erf} \left[-\frac{V_0}{\sigma \sqrt{2}}, \frac{V_0}{\sigma \sqrt{2}} \right] + {\rm erf} \left[-\frac{V_0}{\sigma \sqrt{2}} \right] \right]$$
(9)

for $2x\pi < \omega t < 2\pi$.

 $V(\omega t)$ in equations (8) and (9) is the sheath potential that would result in the IED of equation (7), if ions were to respond fully to the applied rf. Equations (8) and (9) are plotted in figure 3. The shape of $V(\omega t)$ is intuitively understood by the fact that the voltage must remain around V_m most of the time, and spend relatively little time around $V_m - V_0$ or $V_m + V_0$. Again, the inverse problem has multiple solutions since *x* can take any value between 0 and 1. Note that for large values of the ratio σ/V_0 , the IED tends to be uniform, and this requires a linear variation of the voltage $V(\omega t)$. Note also that very narrow distributions with energy around $|V_m|$ (figure 3, left) may be difficult to realize, as voltage peaks of very low duration may be required (figure 3, right).

3. The 'damped' sheath potential

Ions, in general, do not respond to the instantaneous sheath potential, but to a 'damped' potential $V_d(x, t)$ found from the following equation [1–3],

$$\frac{dV_{d}(x,t)}{dt} = -\frac{V_{d}(x,t) - V(x,t)}{\tau_{i}}$$
(10)

where V(x, t) is the (actual) sheath potential as a function of position and time and τ_i is the ion transit time through the sheath. This is often approximated by the inverse of the ion plasma frequency, $1/\omega_{pi}$ [1–3]. This differential equation applies at any position in the sheath, including the electrode. When applied to the target electrode this equation becomes (omitting the independent variables for simplicity)

$$\frac{\mathrm{d}V_{\mathrm{d}}}{\mathrm{d}t} = -\frac{V_{\mathrm{d}} - (V_{\mathrm{T}} - V_{\mathrm{p}})}{\tau_{\mathrm{i}}}.$$
(11)

Since ions respond to the damped potential, the energy distribution of ions striking the target is a direct reflection of the damped voltage of the sheath over the target [1,4]. In equation (11), $V_{\rm T} - V_{\rm p}$ is the actual sheath voltage at the target electrode, i.e. the difference between the target potential $V_{\rm T}$ and the plasma potential $V_{\rm p}$.

Equation (11) can also be written as

$$\omega \tau_{\rm i} \frac{\mathrm{d}V_{\rm d}}{\mathrm{d}(\omega t)} + V_{\rm d}(\omega t) = V_{\rm T} - V_{\rm p} \tag{12}$$



Figure 3. Family of IED curves, equation (7) (left) and the voltage profiles that generate them, equations (8) and (9) (right). The IED curves and voltage profiles correspond to values of $\sigma/V_0 = 0.1$ (solid line), 0.2 (dashed line), 0.5 (dashed-dotted line) and 1 (dotted line). Parameter *x* can take any value in the interval 0 < x < 1. The value x = 0.3 was used for the plot on the right.



Figure 4. Sheath voltage at the target electrode that produces the voltage of equations (8) and (9) (figure 3 (right), for x = 0.5), which in turn would yield the Gaussian IED of figure 3 (left). For $\omega \tau_i = 0.1$, ions respond, and the required sheath voltage is almost identical to that in figure 3. For $\omega \tau_i \ge 1$, the amplitude of the sheath voltage must be increased and the waveform becomes quite different than that in figure 3.

where $dV_d/d(\omega t)$ can be obtained from equations such as (5) and (6) or (8) and (9). Knowing $V_d(\omega t)$ and its derivative, equation (12) can now be solved for the actual sheath voltage, $V_T - V_p$. Applying equation (12) to *example 2*, above, results in

$$V_{\rm T} - V_{\rm p} = \omega \tau_{\rm i} \frac{1}{c2\pi x} \exp\left[\frac{(V_{\rm d}(\omega t) - V_{\rm m})^2}{2\sigma^2}\right] + V_{\rm d}(\omega t) \quad (13)$$

for $0 < \omega t < 2x\pi$, and,

$$V_{\rm T} - V_{\rm p} = \omega \tau_{\rm i} \frac{1}{c 2\pi (x - 1)} \exp\left[\frac{(V_{\rm d}(\omega t) - V_{\rm m})^2}{2\sigma^2}\right] + V_{\rm d}(\omega t)$$
(14)

for $2x\pi < \omega t < 2\pi$, where V_d is the voltage in equations (8) and (9). Note the amplification of $V_T - V_p$ as $\omega \tau_i$ increases (figure 4).

4. Circuit model

A circuit model is used to relate the externally applied rf voltage, $V_{\rm rf}$, to the resulting target and plasma potentials, for a set of plasma and electrical characteristics of the system [1,21]. The substrate holding the wafer (target electrode) is in contact with a plasma with given (bulk) plasma density, n_0 , and electron temperature, $T_{\rm e}$. A radio frequency voltage, $V_{\rm rf}$, is applied to the target through a blocking capacitor having



Figure 5. Equivalent circuit of the system under study. *I* is the sum of the ion and electron currents. The subscripts T and G refer to the target and 'grounded' electrode, respectively.

capacitance C_b (figure 5). A sheath forms naturally over the target accelerating ions toward the substrate. The goal is to determine the IED function at the substrate. The area of the substrate is A_T while the area of the 'counter-electrode' is A_G . Although the target bias voltage is assumed small enough not

to alter the bulk electron density or electron temperature, the plasma potential may be affected, depending on the area ratio, $A_{\rm G}/A_{\rm T}$. For large values of this ratio, the plasma potential will be near ground. A collisionless sheath and a single ionic species are assumed throughout.

The sheath is modeled as a capacitor in parallel with a current source and a diode. The current source represents the ion current and the diode represents the electron current. Subscripts T and G denote the target electrode (holding the wafer) and the 'ground' electrode, respectively. V_p is the plasma potential. The sheath capacitance is a non-linear function of the sheath potential (equation (18)).

Applying Kirchhoff's law to this circuit yields

$$C_{\rm b} \frac{\rm d}{{\rm d}t} (V_{\rm rf} - V_{\rm T}) + C_{\rm T} \frac{\rm d}{{\rm d}t} (V_{\rm p} - V_{\rm T}) + I_{\rm T} = 0$$

$$C_{\rm T} \frac{\rm d}{{\rm d}t} (V_{\rm p} - V_{\rm T}) + C_{\rm G} \frac{\rm d}{{\rm d}t} V_{\rm p} + I_{\rm T} + I_{\rm G} = 0$$
(15)

where V, C and I are voltage, sheath capacitance and total particle current to an electrode, respectively. The particle current is the sum of the ion and electron currents. The former is given by the Bohm flux, while the latter is found from the thermal electron flux at the wall,

$$I_{\rm T} = A_{\rm T}(J_{\rm i} + J_{\rm e}) = A_{\rm T}en_0 \left[0.605u_{\rm B} - \frac{1}{4}u_{\rm e}\exp\left(e\frac{V_{\rm T} - V_{\rm p}}{kT_{\rm e}}\right) \right]$$
(16)

where $A_{\rm T}$ is the area of the target electrode, $u_{\rm B}$ is the Bohm speed ($u_{\rm B} = \sqrt{kT_{\rm e}/M}$), M is the ion mass, $u_{\rm e}$ is the electron thermal speed, ($u_{\rm e} = \sqrt{8kT_{\rm e}/\pi m}$), and m is the electron mass. The factor 0.605 accounts for the drop off in plasma density from the bulk plasma to the plasma–sheath interface.

When applied to the ground electrode, the particle current reads

$$I_{\rm G} = A_{\rm G}(J_{\rm i} + J_{\rm e}) = A_{\rm G}en_0 \left[0.605u_{\rm B} - \frac{1}{4}u_{\rm e}\exp\left(-e\frac{V_{\rm p}}{kT_{\rm e}}\right) \right].$$
(17)

The sheath capacitance is given by

$$C_{\rm s} = -\varepsilon_0 A \frac{\partial E}{\partial V_{\rm s}} \tag{18}$$

where the electric field at the wall is [2]

$$E = -\sqrt{\frac{2n_s k T_e}{\varepsilon_0}} \times \left(\frac{(\tilde{u}-1)}{\tilde{\chi}}(1+\chi-e^{\chi})\right)^{1/2} \quad \text{for} \quad -\infty < V_s(t) < V_1$$

$$\chi = e(V_s - V_1)/k T_e$$

$$\bar{\chi} = e(V_d - V_1)/k T_e$$

$$\bar{u} = (1-2\bar{\chi})^{1/2} \quad (19)$$

E = 0 for $V_1 \leq V_s(t) \leq 0$.

Here $V_{\rm s} (\leq 0)$ is the sheath voltage, ε_0 is the permittivity of free space, $n_{\rm s}$ is the electron (ion) density at the sheath edge ($n_{\rm s} = 0.605n_0$) and V_1 is the potential at the sheath edge relative to the plasma potential. When the plasma potential is set arbitrarily to zero, then $V_1 = -(kT_{\rm e}/2e)$ (see figure 6) [22, p 170].



Figure 6. Schematic of the sheath and pre-sheath over an electrode. Ions accelerate from the bulk plasma to acquire the Bohm speed at the sheath/pre-sheath interface where the potential is V_1 (with respect to the bulk). The target electrode potential is V_T . The electron, ion and displacement currents are also shown.

The circuit model can be used in two ways (see figure 7):

- (a) In solving the *forward* problem one would use $V_{\rm rf}$ as input to equations (15) to find the target $V_{\rm T}$ and plasma $V_{\rm p}$ potential, thus the (actual) sheath voltage ($V_{\rm T} V_{\rm p}$). The latter would then be used in equation (11) to find the damped sheath voltage to which ions respond. Finally, the damped sheath voltage would be used in equation (1) or equation (2) to find the IED.
- (b) In solving the *inverse* problem, the reverse procedure would be followed. One would first solve equation (2) for (what would be the damped) sheath voltage, then insert this into equation (12) to find the actual sheath voltage $(V_{\rm T} V_{\rm p})$, then use the circuit model (equation (15)) to find the required $V_{\rm rf}$ ($V_{\rm p}$ would also be found as part of the solution).

If the desired IED can be expressed as an analytic function, the procedure for solving the inverse problem is applied directly. If the IED is known only at discrete points, then a continuous (or piecewise continuous) IED can be determined via either regression or interpolation through the given points, before the required voltage $V_{\rm rf}$ is finally computed. For IED points known with little noise, interpolation can be done fairly safely, without introducing significant noise-driven artifacts to the continuous IED. If the discrete IED points are noisy, standard filtering can be applied to generate the approximate continuous IED, f(y). Representative results in solving the inverse problem are shown next. The example problem is to find the required $V_{\rm rf}$ that results in the IED shown in figure 8. The IED specified in this example is a Gaussian with energy equal to $|V_m| = 123 \text{ eV}$, $\sigma = 2 \text{ eV}$ and $V_0 = 10.9 \text{ eV}$. In equation form, the desired IED is (see also equation (7))

$$f(V) = c \exp\left[-\frac{(V - |V_{\rm m}|)^2}{2\sigma^2}\right] + \delta,$$



Figure 7. Methodology to solve the forward and inverse problems of IEDs on a substrate. Top: ions respond to the applied frequency, $\omega \tau_i < 1$. Bottom: ions do not respond to the applied frequency, $\omega \tau_i > 1$. V_p , V_T , V_{rf} and V_d are plasma potential, target electrode potential (facing the plasma), applied rf potential and damped sheath potential, respectively (see also figure 5). $V = V_T - V_p$ is the sheath potential over the target electrode.



Figure 8. A desired IED. The problem is to find the voltage waveform $V_{\rm rf}$ that will yield this pre-selected IED (inverse problem).

with
$$-\mathbf{V}_0 + |V_{\mathrm{m}}| < V < \mathbf{V}_0 + |V_{\mathrm{m}}|$$

$$c = \frac{2(1 - 2\delta V_0)}{\sigma \sqrt{2\pi} \operatorname{erf} \left[-\frac{V_0}{\sigma \sqrt{2}}, \frac{V_0}{\sigma \sqrt{2}} \right]}.$$

The addition of δ serves to alleviate numerical problems associated with exponentials having large positive arguments. The value of δ used was 0.001 eV^{-1} , too small on the *y*-axis scale of figure 8, to influence the final result. Other conditions were $C_b = 500 \text{ pF}$, $n_0 = 2 \times 10^{10} \text{ cm}^{-3}$, $T_e = 3 \text{ eV}$, M = 40 amu (argon discharge), and the area ratio $A_G/A_T = 20$. The applied frequency was such that $\omega \tau_i = 1$. Before applying the inverse problem procedure, ion energy E (abscissa in figure 8) was converted to voltage $V = E - T_e$ (all in units of volts), where T_e is an average energy ions gain in the pre-sheath. The resulting voltage waveforms are shown in figure 9. The required V_{rf} has a slope at the base, and the spikes are needed to neutralize the net particle current through the blocking capacitor. The slope of the V_{rf} waveform corresponds to charging of the capacitor [11]. The damped potential to which ions respond (dotted line) is almost constant, as required for a single-peaked IED with tight energy spread.

5. Summary

Control of the energy of ions bombarding a substrate is important for both plasma etching and plasma deposition. As device dimensions keep shrinking, requirements on selectivity and damage become ever more stringent. This imposes strict limits not only on the mean ion energy but also of the ion energy distribution (IED). The problem of determining the IED for given plasma conditions and applied rf bias voltage has been studied for decades. The *inverse problem*, that of determining the required rf bias waveform in order to achieve a desired IED, has been the subject of study only recently.

In this work, a general methodology was developed to determine the rf bias voltage waveform that must be



Figure 9. Voltage waveform $V_{\rm rf}$ (solid line) that must be applied before the blocking capacitor (see figure 5) to yield the IED shown in figure 8, when $\omega \tau_{\rm i} = 1$. The resulting target voltage $V_{\rm T}$ and damped sheath voltage $V_{\rm d}$ are also shown. Other conditions were $C_{\rm b} = 500 \,\mathrm{pF}$, $n_0 = 2 \times 10^{10} \,\mathrm{cm}^{-3}$, $T_{\rm e} = 3 \,\mathrm{eV}$, $M = 40 \,\mathrm{amu}$ (argon discharge) and the area ratio $A_{\rm G}/A_{\rm T} = 20$.

applied through a blocking capacitor to a substrate in contact with plasma, in order to achieve a desired (pre-selected) ion energy distribution (IED) bombarding the substrate. A circuit model was combined with an equation for a damped sheath potential to which ions respond. The approach is applicable to collisionless sheaths at all radio frequencies. Examples of applying this methodology are given including the case of determining the voltage waveform to achieve a single-peaked IED with specified mean energy and energy spread. The inverse problem has multiple solutions, i.e. there are many voltage waveforms all resulting in the same IED.

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Appendix A. Derivation of the IED

When ions respond to the applied field, and ion flow through the sheath is collisionless, the IED depends entirely on the sheath voltage waveform. Consider the sheath voltage over one dimensionless period, 2π . Ions entering the sheath at phase ωt bombard the electrode with energy corresponding to $V(\omega t)$. Now, partition the voltage (ion energy) range into equal segments of size dy.

The probability of V being between y and y + dy is

$$P[y \leqslant V(\omega t) \leqslant y + dy] = \frac{\text{support}(y, y + dy)}{2\pi}$$
(A1)



Figure A1. Definition of the support of a function.

where support (y, y+dy) is shown on the ωt axis of figure A1. Therefore,

$$P[y \leqslant V(\omega t) \leqslant y + dy] = \frac{\text{support}(y, y + dy)}{2\pi}$$
$$= \frac{1}{2\pi} \sum_{\substack{\text{# of intervals in } 0 < \omega t < 2\pi \\ y \leqslant V(\omega t) \text{ for } y + dy}} \frac{dy}{\left|\frac{dy}{d(\omega t)}\right|} \Rightarrow f(y)$$
$$= \lim_{\substack{dy \to 0}} \frac{P[y \leqslant V(\omega t) \leqslant y + dy]}{dy}$$
$$= \frac{1}{2\pi} \sum_{\substack{\text{# of points in } 0 < \omega t < 2\pi \\ \text{such that } V(\omega t) = y}} \frac{1}{\left|\frac{dV}{d(\omega t)}\right|}$$
(A2)

where f(y) is the IED (density) function. The final expression for f(y) must not contain ωt . To eliminate ωt in favor of y,

$$y = V(\omega t) \Rightarrow \omega t = V^{-1}(y) \Rightarrow 1 = \frac{d(\omega t)}{d(\omega t)} = \frac{dV^{-1}(y)}{d(\omega t)}$$

$$= \frac{dV^{-1}(y)}{dy} \frac{dy}{d(\omega t)} \Rightarrow \frac{dV}{d(\omega t)} = \frac{1}{\frac{dV^{-1}(y)}{dy}}$$
(A3)

Therefore,

$$f(y) = \frac{1}{2\pi} \sum_{\substack{\text{\# of points in } 0 < \omega t < 2\pi \\ \text{such that } V(\omega t) = y}} \left| \frac{\mathrm{d}V^{-1}(y)}{\mathrm{d}y} \right|.$$
(A4)

Note that because of the absolute value in the summation in equation (A2) parts of $V'(\omega t)$ over intervals for which $V'(\omega t) \neq 0$ can be replaced by $-V'(\omega t)$ without any change in f(y). Figure A2 shows how this transformation works for $V(\omega t) = V_0 \sin(\omega t - (\pi/2)) + V_m$. Three profiles of $V(\omega t)$ result in the same IED, f(y).



Figure A2. Three profiles (heavy dotted, dotted and solid lines) of sheath voltage $V(\omega t)$ resulting in the same IED f(y).

Appendix B. Solution of the inverse problem of example 1

Consider the IED in equation (4), i.e.

$$f(y) = \frac{1}{\pi} \frac{1}{V_0 \sqrt{1 - \left(\frac{y - |V_{\rm m}|}{V_0}\right)^2}}.$$

Then equation (A4) yields

$$\frac{1}{\pi} \frac{1}{V_0 \sqrt{1 - \left(\frac{y - |V_m|}{V_0}\right)^2}} = \frac{1}{2\pi} \sum_{\substack{\# \text{ of points in } 0 < \omega t < 2\pi \\ \text{such that } V(\omega t) = y}} \frac{1}{\left|\frac{\mathrm{d}V}{\mathrm{d}(\omega t)}\right|}.$$
(B1)

To ensure continuity from cycle to cycle, $V(\omega t)$ must satisfy the constraint $V(0) = V(2\pi)$. Further, if $V(\omega t)$ is continuous in $0 \le \omega t \le 2\pi$, then $dV/d(\omega t)$ switches signs at least once. To identify voltages that result in f(y) given by equation (4), assume that the summation term contains two entries for the same $y = V(\omega t)$, corresponding to $dV/d(\omega t) > 0$ followed by $dV/d(\omega t) < 0$. To find the voltage $V(\omega t)$ consider a parameter 0 < x < 1 and split the left-hand side of equation (B1) to get

$$x\frac{1}{V_0\sqrt{1-\left(\frac{y-|V_{\rm m}|}{V_0}\right)^2}} = \frac{1}{2}\frac{1}{\frac{\mathrm{d}V}{\mathrm{d}(\omega t)}}, \qquad \frac{\mathrm{d}V}{\mathrm{d}(\omega t)} > 0 \tag{B2}$$

and

$$(1-x)\frac{1}{V_0\sqrt{1-\left(\frac{y-|V_{\rm m}|}{V_0}\right)^2}} = \frac{1}{2}\frac{-1}{\frac{{\rm d}V}{{\rm d}(\omega t)}}, \qquad \frac{{\rm d}V}{{\rm d}(\omega t)} < 0.$$
(B3)

Equation (B2) yields

$$\int x \frac{\mathrm{d}V}{V_0 \sqrt{1 - \left(\frac{y - |V_{\mathrm{m}}|}{V_0}\right)^2}} = \int \frac{1}{2} \mathrm{d}(\omega t) \Rightarrow \sin^{-1}\left(\frac{V - |V_{\mathrm{m}}|}{V_0}\right)$$
$$= \frac{1}{2x} \omega t + c_1 \Rightarrow V = V_0 \sin\left(\frac{1}{2x} \omega t + c_1\right) + V_{\mathrm{m}} \quad (B4)$$

and equation (B3) yields

$$\int (1-x) \frac{dV}{V_0 \sqrt{1 - \left(\frac{y - |V_{\rm m}|}{V_0}\right)^2}}$$

= $-\int \frac{1}{2} d(\omega t) \Rightarrow \sin^{-1} \left(\frac{V - |V_{\rm m}|}{V_0}\right)$
= $\frac{-1}{2(1-x)} \omega t + c_2 \Rightarrow V = V_0 \sin\left(\frac{-1}{2(1-x)} \omega t + c_2\right) + V_{\rm m}.$
(B5)

Now select $c_1 = -(\pi/2)$, for which $dV/d(\omega t) > 0$ in equation (B2) for $0 < \omega t < 2x\pi$. Similarly, pick $c_2 = \pi(1+x)/2(1-x)$, for which $dV/d(\omega t) < 0$ for $2x\pi < \omega t < 2\pi$. These choices result in equations (5) and (6), respectively. Clearly, there is an infinite number of voltage waveforms all yielding the same IED.

Appendix C. Solution of the inverse problem of example 2

Consider the bell-shaped IED of equation (7). Then, as in appendix B, consider a parameter 0 < x < 1 and split the left-hand side of the equation

$$c \exp\left[-\frac{(y-|V_{\rm m}|)^2}{2\sigma^2}\right] = \frac{1}{2\pi} \sum_{\substack{\text{\# of points in } 0 < \omega t < 2\pi \\ \text{such that } V(\omega t) = y}} \frac{1}{\left|\frac{\mathrm{d}V}{\mathrm{d}(\omega t)}\right|}$$
(C1)

into two terms,

$$xc \exp\left[-\frac{(y-|V_{\rm m}|)^2}{2\sigma^2}\right] = \frac{1}{2\pi} \frac{1}{\frac{\mathrm{d}V}{\mathrm{d}(\omega t)}}, \qquad \frac{\mathrm{d}V}{\mathrm{d}(\omega t)} > 0$$
 (C2)

and

$$(1-x)c\exp\left[-\frac{(y-|V_{\rm m}|)^2}{2\sigma^2}\right] = \frac{1}{2\pi}\frac{-1}{\frac{\mathrm{d}V}{\mathrm{d}(\omega t)}}, \qquad \frac{\mathrm{d}V}{\mathrm{d}(\omega t)} < 0.$$
(C3)

Equation (C2) yields

$$\frac{\operatorname{erf}\left[-\frac{V_{0}}{\sigma\sqrt{2}}, \frac{V-V_{m}}{\sigma\sqrt{2}}\right]}{\operatorname{erf}\left[-\frac{V_{0}}{\sigma\sqrt{2}}, \frac{V_{0}}{\sigma\sqrt{2}}\right]} = \frac{\omega t}{2\pi x}$$

$$\Rightarrow V(\omega t) = V_{m} + \sigma\sqrt{2}\operatorname{erf}^{-1}\left[\frac{\omega t}{2\pi x}\operatorname{erf}\left[-\frac{V_{0}}{\sigma\sqrt{2}}, \frac{V_{0}}{\sigma\sqrt{2}}\right]\right]$$

$$+ \operatorname{erf}\left[-\frac{V_{0}}{\sigma\sqrt{2}}\right]\right]$$
(C4)

for $0 < \omega t < 2x\pi$, (corresponding to $dV/d(\omega t) > 0$), and equation (C3) yields

$$\frac{\operatorname{erf}\left[-\frac{V_{0}}{\sigma\sqrt{2}}, \frac{V-V_{m}}{\sigma\sqrt{2}}\right]}{\operatorname{erf}\left[-\frac{V_{0}}{\sigma\sqrt{2}}, \frac{V_{0}}{\sigma\sqrt{2}}\right]} = \frac{2\pi - \omega t}{2\pi(1-x)} \Rightarrow V(\omega t)$$
$$= V_{m} + \sigma\sqrt{2}\operatorname{erf}^{-1}\left[\frac{2\pi - \omega t}{2\pi(1-x)}\operatorname{erf}\left[-\frac{V_{0}}{\sigma\sqrt{2}}, \frac{V_{0}}{\sigma\sqrt{2}}\right]\right]$$
$$+ \operatorname{erf}\left[-\frac{V_{0}}{\sigma\sqrt{2}}\right]\right]$$
(C5)
for $2x\pi < \omega t < 2\pi$, (corresponding to $dV/d(\omega t) < 0$).

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These are equations (8) and (9), respectively. Again, there is an infinite number of voltage waveforms all yielding the same IED.

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