Collisionless Electron Heating by Capacitive rf Sheaths

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High-frequency plasma discharges are often sustained by collisionless heating of electrons; the nature of these mechanisms is a central problem in the theory of such discharges. In capacitive discharges, collisionless heating occurs near boundaries, and is usually attributed to inelastic collisions of electrons with oscillating plasma sheaths, regarded as moving rigid barriers. We show that, when current conservation is required, such heating necessarily vanishes, and we conclude that this model of the heating process is not correct. We develop an alternative view that associates the heating with acoustic disturbances in the electron fluid. An analytic model, based on moments of the Vlasov equation, gives results in good agreement with particle-in-cell simulations. In terms of individual particle dynamics, this acoustic heating may be interpreted as a transit-time effect.

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At low pressure, where the electron mean-free path is comparable to the typical plasma dimension, capacitive rf plasmas are maintained by collisionless heating of electrons in the strongly modulated sheaths adjacent to the electrodes. This is known as "stochastic heating," and is generally viewed as a type of Fermi acceleration [1]. Originally proposed as a model for cosmic ray acceleration [2], this paradigm is now often applied to any mechanism involving a collisionlike interaction with a localized field structure. In the context of rf-driven plasma sheaths, stochastic heating was first discussed in the early 1960's [3]. Later, Godyak [4] used the assumption that an electron with initial velocity v returns from the sheath—modeled as a rigid barrier—with velocity $v_r = 2u_w - v$, where u_w is the instantaneous sheath velocity at the time of interaction. This assumption, now known as the "hard wall model," has been used extensively [1]. In this view, the power transfer from the sheath to electrons with mass m and velocity distribution $f(v)$ is [1]

$$P = \int_{u_w}^{\infty} \frac{1}{2} m(v_r^2 - v^2)(v - u_w) f(v)\, dv\,, \tag{1}$$

$$= -2m\left\{ \int_{u_w - u_s}^{\infty} (u_w - u_s)(v' + u_s - u_w)^2 g(v')\, dv' + \int_{u_w - u_s}^{\infty} u_s (v' + u_s - u_w)^2 g(v')\, dv' \right\}, \tag{2}$$

where $g(v') = f(v - u_s)$ and in Eq. (2) we have used the expansion $v = u_s + v'$, with u_s the drift velocity of the electron fluid at the sheath edge and v' the electron thermal velocity. However, the condition for current conservation at the sheath edge is $u_w = u_s$. Then $v_r = u_s - v'$, i.e., reflection from the sheath does not change the thermal distribution of velocities, g, and the first integral in Eq. (2) vanishes. The second integral merely maintains the drift energy—which is not a heating effect—and its time average is zero for periodic current. These analytic conclusions are supported by a detailed examination of kinetic simulation results [5]. There is, therefore, no heating localized at the sheath edge, and models suggesting otherwise are based on assumptions inconsistent with current conservation [6,7]. It was previously suggested that heating is produced by so-called pressure effects, the cyclic compression and rarefaction of electrons in the sheath region [8–10], but this suggestion has not been fully articulated, nor has it been shown that the proposed mechanism completely accounts for the heating that is found, e.g., in kinetic simulations. In the remainder of this Letter, we present a new heating model, which admits analytic solution, explicitly allows for the details of the oscillating sheath structure (such as the moving boundary), expresses the time-averaged heating as a simple quadrature, and agrees well with simulations designed specifically to test the theory.

We consider a one-dimensional collisionless sheath driven by a sinusoidal current source with amplitude $\tilde{J}$. In common with typical sheath structure models (e.g., [6]), we assume an instantaneous sheath edge at $x = s(t)$, separating the sheath region into a positive space-charge region with no electrons and a quasineutral part where the current is carried by electrons such that $-enu = \tilde{J}\sin(\omega t)$, with e the absolute electron charge, n the electron density, and u the average electron velocity [6]. The electrons are described by Vlasov's equation, and we write $f(v) = g(v - u)$, as above, such that $\int_{-\infty}^{\infty} v' g(v')\, dv' = 0$ and where an effective temperature T (in joules) is defined by $\int_{-\infty}^{\infty} \frac{1}{2} m v'^2 g(v')\, dv' = \frac{1}{2} nT$. With this definition, all terms involving the drift energy and the electric field E can be eliminated between the first three velocity moments of Vlasov's equation, giving

$$\frac{\partial}{\partial t}\left(\frac{1}{2} nT\right) + \frac{\partial}{\partial x}(D + Q) - u\frac{\partial}{\partial x}(nT) = 0\,, \tag{3}$$

where $D = \frac{3}{2}nuT$ is the convective thermal flux and $Q = \int_{-\infty}^{\infty} \frac{1}{2}mv'^3 g(v')\,dv'$ is the random thermal flux. We further assume that the electron temperature T is uniform within the sheath, as expected if the heating is by pressure waves with wavelengths longer than the characteristic sheath length [11]. Integrating Eq. (3) from the ion sheath edge, i.e., the Bohm point at $x = 0$, to the electron sheath edge at $x = s(t)$, we find

$$\frac{1}{2}(1 + \cos\omega t)\frac{\tilde{J}}{e\omega}\frac{dT}{dt} + \frac{\tilde{J}T}{e}\ln\left(\frac{n_s}{n_0}\right)\sin\omega t - Q_0 + Q_s - D_0 + D_s = 0, \tag{4}$$

where the quantities with index 0 and s are respectively defined at the Bohm point and the electron sheath edge, and we have used the relation $\int_0^{s(t)} n\,dx = (\tilde{J}/e\omega) \times (1 + \cos\omega t)$, which is obtained from electron conservation within the sheath region, neglecting electron current to the electrode. Although the thermal flux at the electron sheath edge, Q_s, is zero, the convective flux is not because of the expansion and contraction of the sheath during the rf cycle. Since $T_s = T_0 = T$ by assumption, and $u_s n_s = u_0 n_0$ owing to current conservation, we have $D_0 = D_s$ and there is no net convective flux. Equation (4) is closed by an ansatz for the heat flux Q_0. We suppose that the thermal distribution of electrons at the sheath edge, g_0, can be characterized by separate densities and temperatures for electrons entering and leaving the sheath, $n_{\rm in}$, $n_{\rm out}$, $T_{\rm in}$, $T_{\rm out}$, respectively. For compatibility with previous assumptions, we require the first three moments of g_0 expressed in these terms to be

$$n_0 = n_{\rm in} + n_{\rm out}, \tag{5}$$

$$n_0 T = n_{\rm in}T_{\rm in} + n_{\rm out}T_{\rm out}, \tag{6}$$

and

$$0 = \bar{v}_{\rm in}n_{\rm in} - \bar{v}_{\rm out}n_{\rm out}, \tag{7}$$

where $\bar{v}_{\rm in} = \sqrt{8T_{\rm in}/\pi m}$, etc., and the last equation implies zero random particle flux. We further assume that $T_{\rm in} = T_b$, the constant temperature of the bulk plasma, hence Q_0 is uniquely determined to be

$$Q_0 = \tfrac{1}{2}n_0\bar{v}_b T_b[\tau(1 - \tau)] = Q_b[\tau(1 - \tau)], \tag{8}$$

where $\bar{v}_b$ is the electron thermal speed in the plasma, $\tau = T/T_b$, and Q_b is the electron heat flux arriving at the sheath edge from the bulk plasma. By assuming that T_b is constant (in common with previous models [6,7]) we imply assumptions about thermalization of electrons in the plasma bulk that we do not have space to elaborate (see [12]). We note, however, that the present theory can be generalized to the case where T_b is a given function of time without undue difficulty. Finally, then, we get the evolution equation for T:

$$(1 + \cos\theta)\frac{d\tau}{d\theta} + 2\tau\ln\left(\frac{n_s}{n_0}\right)\sin\theta - \frac{\bar{v}_b}{u_0}\tau(1 - \tau) = 0, \tag{9}$$

where $\theta = \omega t$ and $u_0 = \tilde{J}/en_0$ is the amplitude of the drift velocity at $x = 0$. The solution of (9) can be expressed as a power series in $\delta \equiv u_0/\bar{v}_b \ll 1$,

$$\tau = \tau^{(0)} + \delta\tau^{(1)} + \delta^2\tau^{(2)} + \ldots, \tag{10}$$

where the $\tau^{(0)}$, etc., are functions of θ. By retaining terms up to $O(\delta^2)$ and requiring that coefficients of each order vanish separately, we obtain

$$\tau^{(0)} = 1,$$

$$\tau^{(1)} = -2\ln\left(\frac{n_s}{n_0}\right)\sin\theta, \tag{11}$$

$$\tau^{(2)} = 2(1 + \cos\theta)\left\{\cos\theta\ln\left(\frac{n_s}{n_0}\right) + \sin\theta\,\frac{1}{n_s}\frac{dn_s}{d\theta}\right\}.$$

The average power per unit area can now be calculated given the density profile in the sheath region

$$\langle P\rangle = -\langle Q_0\rangle = Q_b\langle\delta\tau^{(1)} + \delta^2(\tau^{(2)} + \tau^{(1)2})\rangle + O(\delta^3). \tag{12}$$

This result vanishes in the limit $m \to 0$ which corresponds to electrons in Boltzmann equilibrium.

Equation (12) can be used to evaluate the power deposition for an arbitrary underlying sheath structure model. A convenient example is Lieberman's sheath model [6], which provides a closed analytic expression for n_s/n_0 as a function of a single parameter $H = \tilde{J}^2/(\pi\epsilon_0 T_b\omega^2 n_0)$. The first order deposition term in Eq. (12) averages to zero, because the sheath motion is symmetrical around $\theta = \pi$ (which is not the case for more general sheath models). A good parametric fit of Eq. (12) for $H < 50$ was found to be

$$\langle P\rangle \approx Q_b\delta^2\frac{35H}{60 + H}. \tag{13}$$

We now compare this model with a semi-infinite, planar, collisionless particle-in-cell (PIC) simulation [13,14]. The simulation is driven by a sinusoidal current source and is bounded on one side by a perfectly absorbing electrode. The other boundary emits a constant ion flux $\Gamma_i = n_0 u_B$ with a Maxwellian distribution drifting at the Bohm speed u_B. The electron flux required to maintain the rf current is obtained from a Maxwellian with the appropriately modulated drift velocity. These boundary conditions correspond precisely to those of our model, and previous models. This type of simulation has obvious advantages, in principle [13], and our formulation removes the spurious potential at the plasma boundary often present in previous works [15]. In order to get the closest possible comparison with theory, the PIC simulation was adapted to model a time symmetric sheath. This was achieved by running a simulation to steady state and then stopping the movement of

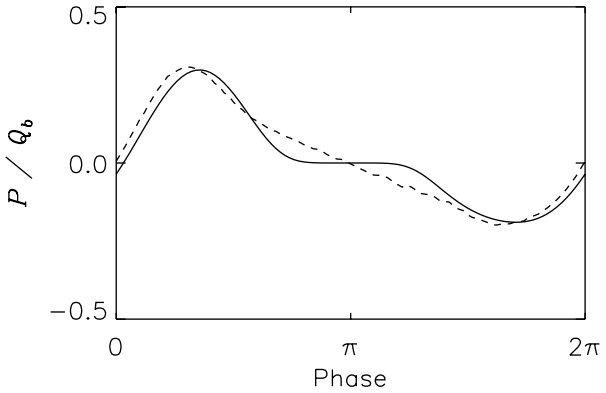

FIG. 1. A comparison of the heating power per unit area, P, normalized by the heat flux from the bulk plasma, Q_b, showing the model prediction and the result of the symmetric PIC simulation discussed in the text. The solid line is the model prediction and the dashed line is the PIC result. Parameters: $\tilde{J} = 130$ A/m^2, $\omega_{\rm rf}/2\pi = 13.56$ MHz, $n_0 = 1.5 \times 10^{16}$ m^{-3}, $T_b = 2.57$ eV, $H = 13.47$.

the ion superparticles. Since this eliminates ion loss, electron loss also stops and the sheath becomes symmetric, in the sense discussed above. For all the results presented hereafter, ion mass was chosen to correspond to helium, the bulk temperature was set to $T = 2.57$ eV, and the density at the Bohm point was set to $n_0 = 1.5 \times 10^{16}$ m^{-3}.

The power deposition calculated from our model using Lieberman's analytic expression for the density profile is compared to the PIC simulation result in Fig. 1 and good agreement is obtained. However, as can be seen in Fig. 2, the discrepancy between the temperature variation predicted by our model, when Lieberman's analytic sheath model is used for the density profile, and that calculated from the PIC simulation can be appreciable, even if this does not seriously affect the calculation of power deposition. Finally, the time-averaged areal power density given

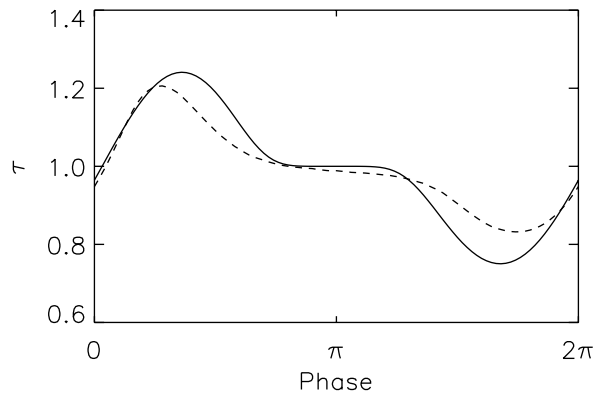

FIG. 2. A comparison of the variation of the normalized temperature τ given by the model, Eqs. (10) and (11), and the symmetric PIC simulation. The solid line is the model prediction and the dashed line is the PIC result. The parameters are the same as in Fig. 1.

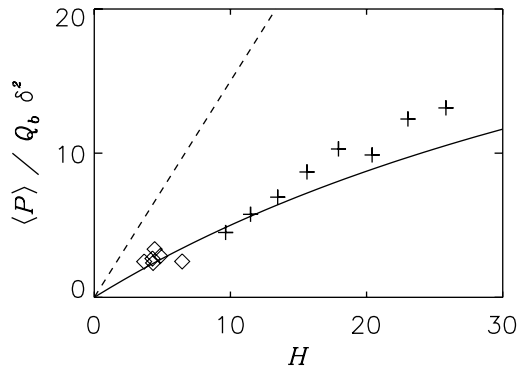

FIG. 3. The time-averaged normalized power deposition as a function of the parameter H. The solid line is the model prediction calculated from Eq. (13), the dashed line is the stochastic heating result from [6], and the symbols correspond to the PIC simulation results for the parameter ranges indicated in the text.

by Eq. (13) is in good agreement with the model, as shown in Fig. 3. The symbols in Fig. 3 correspond to the power calculated by the simulation for a current range between $\tilde{J} = 110$ A/m^2 and $\tilde{J} = 180$ A/m^2 at a fixed frequency equal to $f_{\rm rf} = 13.56$ MHz (+ symbols), and a frequency range from $f_{\rm rf} = 10$ MHz to $f_{\rm rf} = 80$ MHz at a fixed maximum rf voltage at the electrode equal to 400 V ($\diamond$ symbols). Over this range of conditions, δ has a maximum of approximately 0.15, which is large relative to the values typically found in experiments, where usually $\delta \lesssim 0.1$. Power deposition calculated from the hard wall model [6] is also shown in Fig. 3, and it is clearly overestimated.

In Fig. 4 we show the power per unit area as a function of phase, along with the pressure contribution defined as

$$P_{\rm pr} = -T \int_0^{s(t)} u \frac{dn}{dx}\, dx\,, \tag{14}$$

for the same conditions as in Fig. 1 but for a simulation where no time symmetry was imposed. The space-averaged temperature T as well as all other quantities

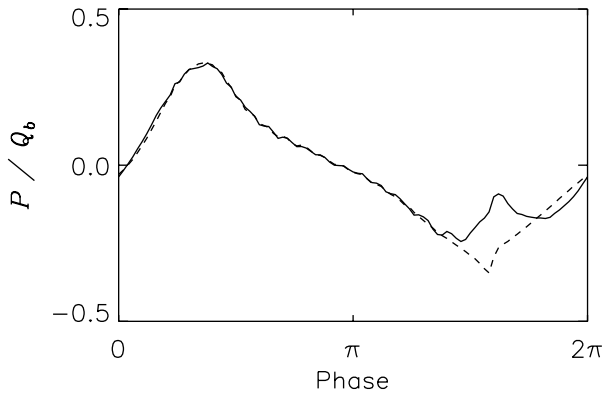

FIG. 4. A comparison of the normalized P (solid line) from the nonsymmetric PIC simulation with $P_{\rm pr}$ (dashed line), where $P_{\rm pr}$ is defined by Eq. (14). The parameters are the same as in Fig. 1.

involved in (14) are obtained from the PIC simulation. We notice that there is close agreement, except for the end of the rf cycle where electron loss at the electrode becomes important. There is, therefore, no reason to believe that any electron heating mechanism other than pressure heating is important. As far as we can determine, the plasma oscillations that are excited at the plasma sheath boundary [5,16] under some conditions do not constitute a significant heating mechanism for the range of parameters considered in this Letter.

We conclude that the pressure heating mechanism gives a complete account of the power dissipation observed in the simulation under the present conditions, and that previously proposed models are formally invalid. Although this mechanism appears quite different to the one previously accepted, this is because our approach is in terms of moments of the velocity distribution. Incidentally, the pressure mechanism would presumably be automatically included in fluid models if an appropriate closure of the moment equations was used [17], which is not typically the case. In terms of single particle trajectories, the pressure mechanism can be understood as a transit time heating effect produced by the change of the electric field during the interval when an electron passes through the sheath: The condition $\delta \ll 1$ is essentially equivalent to the requirement that the electron transit time is small compared to the oscillation period of the discharge current, so that the change in particle speed integrated over the trajectory of a transit will typically be fractionally small. Presumably then, pressure heating can be expressed in a Fermi acceleration formalism by using some effective barrier velocity, but there is no reason to identify this effective barrier velocity with the sheath edge velocity. Moreover, the effective barrier velocity is unlikely to be simple, because a "single electron" picture of the interaction is difficult to reconcile with the various conservation and continuity conditions that must be satisfied. It is essential that the electrons act collectively and that their motion is largely constrained by the nonuniform ion density.

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