# A surface physics inspired model for particle charging in plasmas

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## Introduction

qualitative discussion of the build-up of surface charges

#### Physisorption-inspired charging model

- surface states for electrons and ions
- "effective" electron and ion surface densities

#### Results

- criteria to determine  $Z_p = Q_p/(-e)$
- power, pressure, and radius dependence of Z<sub>p</sub>

## **Conclusions**

sum-up and to do's

## Introduction (1)



## Macroscopic objects in an ionized gas acquire a charge

- plasma boundaries in general
- artificial satellites in the ionosphere of planets
- dust particles in the interstellar medium
- contaminants in processing discharges
- aerosols in the upper atmosphere
- grains in laboratory plasmas

## Problem of plasma-boundary interaction

- solid state physics meets plasma physics
- quantum meets classical mechanics in a plasma context



A. Piel et al. 2008



L. Stollenwerk et al. 2007

## Introduction(2)





## Introduction (3)



Lets consider a spherical grain with radius  $R \ll \lambda_D$ .



Quasi-stationary surface charge density (in units of -e)

$$\begin{array}{l} 0 = d\sigma_e/dt = s_e j_e^{\mathrm{plasma}} - \tau_e^{-1} \sigma_e - \alpha_R \sigma_e \sigma_i \\ 0 = d\sigma_i/dt = s_i j_i^{\mathrm{plasma}} - \tau_i^{-1} \sigma_i - \alpha_R \sigma_e \sigma_i \\ \Longrightarrow \sigma_\rho = \sigma_e - \sigma_i \end{array}$$

phenomenological!

## Introduction (4)



#### Standard approach

• ions reach surface 
$$\implies \tau_i^{-1} = 0$$

•  $\tau_e^{-1} = 0$  or at least  $\tau_e^{-1}\sigma_e \ll s_i j_i^{\text{plasma}} = \alpha_R \sigma_e \sigma_i.$ 

• 
$$s_e = s_i = 1$$
 or at least  $s_e = s_i$ 

 $\implies \text{grain} \triangleq \underline{\text{perfect absorber}} \text{ for } e^- \text{ and } A^+$  $\implies j_e^{\text{plasma}}(\sigma_p) = j_i^{\text{plasma}}(\sigma_p) \text{ at } r = R$ 

#### We challenge all 3 assumptions

- ► surface states ⇒ A<sup>+</sup> & e<sup>-</sup> spatially separated
- if  $A^+$  &  $e^-$  spatially separated then  $\alpha_R \sigma_i \sigma_e \ll \tau_{e,i}^{-1} \sigma_{e,i}$

• physisorption 
$$\implies s_e \ll s_i$$

$$\implies \sigma_p = (s\tau)_e \cdot j_e^{\text{plasma}}(\sigma_p) \text{ at } r_e = R$$
  
$$\sigma_i = (s\tau)_i \cdot j_i^{\text{plasma}}(\sigma_p) \text{ at } r_i \gtrsim r_e$$

Within our approach  $(s\tau)_{e,i}$  important surface parameter!

phenomenology  $\implies (s\tau)_{e,i} \simeq (s\tau)_{e,i}^{\text{LJD}} \equiv \frac{h}{kT_{p,g}} \exp\left[\frac{E_{e,i}^d}{kT_{p,g}}\right]$  with  $T_g \sim 300K$ and  $T_p$  adjustable parameter  $\rightarrow T_p$  measurement  $\rightarrow$  H. Maurer *et al.* P4.7

## Charging model (1)



#### Electron and ion surface states

$$\frac{\text{grain}}{U_f} (R, Z_p, \epsilon) \Longrightarrow V_{e,i}(x) = [U_C(r) + U_p(r)]/U_f = \frac{1}{1+x} [\pm 1 - \frac{\xi}{x(1+x)(2+x)}],$$
$$U_f = e^2 Z_p/R, \ x = r/R - 1, \text{ and } \xi = (\epsilon - 1)/2(\epsilon + 1)Z_p$$

$$\frac{\text{electrons:}}{\lambda_e^{dB}/R} \propto |V_e(x) \simeq 1 - \xi/2x \text{ (image potential)} \\ \lambda_e^{dB}/R \simeq |V_e/V_e'| \simeq 10^{-4} \text{ @ } x \simeq 10^{-4} \Longrightarrow e^- \text{ quantum mechanical}$$

$$\frac{\text{ions:}}{\lambda_i^{size}} \propto 10^{-4}, V_i(x) \simeq -1/(1+x) \text{ (Coulomb tail)} \\ \lambda_i^{dB}/R \ll |V_i/V_i'| \text{ @ } x \ge x_i^{size} \Longrightarrow A^+ \text{ classical}$$

Schrödinger equation ( $E < 0 \implies e^-$  and  $A^+$  bound states)

$$\frac{d^2}{dx^2}u^{e,i} + \left[-\frac{\alpha_{e,i}^2}{k^2} + \tilde{V}_{e,i}(x) - \frac{l(l+1)}{(1+x)^2}\right]u^{e,i} = 0$$
  
with  $\tilde{V}_e(x) = 2\alpha_e/x$ ,  $\tilde{V}_i(x) = 2\alpha_i/(1+x)$ , and BC @  $x \to \infty$  and  $x = \begin{cases} x_b \simeq 0\\ x_i^{size} \end{cases}$ 

## Charging model (2)





 $\begin{array}{l} \underline{e^-}: \mbox{ high energy, come close to the surface, inelastic scattering with grain} \\ \Longrightarrow E_e^d = |U_C(R) - E_1| = \frac{1}{16} (\frac{\epsilon - 1}{\epsilon + 1})^2 R_y \simeq 0.5 \ eV \Longrightarrow (s\tau)_e^{\rm LJD} \end{array}$ 

 $\begin{array}{l} \underline{A^+:} & \text{low energy } \& \ x_i^{size} > 0, \text{ already trapped in Coulomb tail, inelastic scattering with} \\ & \text{neutrals (CX)} \\ & \Longrightarrow 2\pi r_i = l_{cx} = (\sigma_{cx} n_g)^{-1} \ \text{(largest "stable" orbit)} \\ & \Longrightarrow E_i^d = |U_C(r_i)| = 4\pi \sigma_{cx} a_B n_g Z_p R_y \simeq 0.37 \ eV \Longrightarrow (s\tau)_i^{\text{LJD}} \end{array}$ 

## Charging model (3)



#### Energy relaxation at the grain boundary



## Charging model (4)



#### <u>"Effective"</u> e<sup>-</sup> and A<sup>+</sup> surface densities

quasi-stationary charge in the vicinity of the grain ( $x_D = \lambda_D/R \gg 1$ ):

$$Z(x < x_D) = Q(x < x_D)/(-e) \simeq 4\pi R^3 \int_{x_b}^{x} dx' (1 + x')^2 \left[ n_e^b(x') - n_i^b(x') + \dots \right]$$

- effective surface density:  $n_{e,i}^b(x) \simeq \sigma_{e,i}\delta(x x_{e,i})/R$ , with  $x_e \simeq 0$  and  $x_i \simeq 1 - 10$
- $\stackrel{\text{individual (!) quasi-stationarity of "surface densities"}}{\Longrightarrow \sigma_{e,i} = (s\tau)_{e,i} j_{e,i}^{\text{plasma}} }$

final equations for particle charge and its partial screening due to trapped  $A^+$ :

$$Z_p \equiv Z(x_e < x < x_i) = 4\pi R^2 \cdot (s\tau)_e \cdot j_e^{\text{OML}}(Z_p, n_e, T_e)$$

$$Z_i \equiv Z_p - Z(x_i < x < x_D) = 4\pi R^2 (1+x_i)^2 \cdot (s\tau)_i \cdot j_i^B$$

- ► *Z<sub>p</sub>* resides on grain surface
- $\triangleright$  Z<sub>i</sub> resides on effective surface where we subsume all trapped A<sup>+</sup>

## Results (1)



## Criteria to determine $Z_p$

- 1. orbital motion limited charges:  $j_e^{\text{OML}} = j_i^{\text{OML}} \Longrightarrow Z_p$
- 2. charge-exchange enhanced charges:  $j_e^{\text{OML}} = j_i^{\text{OML}} + j_i^{\text{CX}} \Longrightarrow Z_p$ (M. Lampe *et al.* (01 & 03), S. A. Khrapak *et al.* (05))

<u>3. surface model:</u> approximate  $(s\tau)_e \simeq (s\tau)_e^{\text{LJD}} = \frac{h}{kT_p} \exp\left[\frac{E_e^d}{kT_p}\right]$  and adjust  $T_p$  such that  $Z_p = 4\pi R^2 \cdot (s\tau)_e^{\text{LJD}} \cdot j_e^{\text{OML}} = Z_p^{\text{exp}}$ 

where the fluxes are defined by  $j_e^{\text{OML}} = n_e \sqrt{\frac{k_B T_e}{2\pi m_e}} \exp\left[-\frac{Z_p e^2}{Rk_B T_e}\right], \ j_i^{\text{OML}} = n_i \sqrt{\frac{k_B T_i}{2\pi m_i}} \left[1 + \frac{Z_p e^2}{Rk_B T_i}\right],$   $j_i^{\text{CX}} = 0.1 n_i \frac{\lambda_i^D}{l_{\text{cx}}} \sqrt{\frac{k_B T_i}{2\pi m_i}} \left(\frac{Z_p e^2}{Rk_B T_i}\right)^2, \text{ and } j_i^{\text{B}} = 0.6 n_i \sqrt{\frac{k_T_e}{m_i}}$  Results (2)



#### MF particle in He discharge (A. Melzer (97))

- ► *R* = 4.7 µ*m*
- $T_{e,i}$  and  $n_{e,i}$  known,  $\sigma_{cx} = 0.32 \times 10^{-14} cm^2$



our approach works, predicted T<sub>p</sub> reasonable

▶  $Z_i \simeq 150$  (at p = 102Pa) in accordance with MD simulations (S. J. Choi *et al.* (94))

Results (3)



### MF particle in Ne discharge (S. A. Khrapak et al. (05))



our approach reproduces non-linear R-dependence of Z<sub>p</sub>

Results (4)



## MF particle in Ar discharge (E. B. Tomme *et al.* (2000))

▶ particles confined in sheath  $\implies n_e(R) = n_e \exp[e\Phi(z_{eq}(R))/kT_e]$ 



- our approach works particularly well for  $R < 5 \ \mu m$
- ad-hoc description of j<sub>e</sub><sup>plasma</sup> perhaps too crude for R > 5 μm (secondary electron emission from electrode?)

## Conclusions



### Sum-up and to do's

- ▶ We questioned the treatment of grains as perfect absorber for e<sup>-</sup> and A<sup>+</sup>
- ► and presented a surface physics inspired charging model (F. X. Bronold *et al*, PRL 101, 175002 (08)). charge of a dust particle ←→ microphysics at its surface



effective surface for ions

- Model based on two main hypotheses:
  - 1. ions get stuck in disturbed region of the grain
  - 2. electrons are bound in external surface states
- Using  $T_p$  as an adjustable parameter model works very well.
  - $\implies$  hypotheses have to be justified theoretically. <u>Thats what we do now!</u>
  - $\implies$  microscopic calculation of  $s_{e,i}$  and  $\tau_{e,i}$ . Thats what we do now!
  - $\implies$   $Z_p$  and  $T_p$  should be measured simultaneously.
- Diagnostics of electronic structure of grain surface would be very helpful (IPES etc.).

## Sticking, desorption



#### e<sup>-</sup> : metal surface



# $\begin{array}{c} 0.0001 \\ \hline \\ 0.0001 \\ \hline \hline \\ 0.0001 \\ \hline \\ 0.0001 \\$

## $\mathcal{W}(...) \Rightarrow s_e \& \tau_e$

- internal electron-hole pairs
- ▶ golden rule & PT  $\Rightarrow$   $s_e$ ,  $\tau_e$ (Bronold *et al.* submitted to EPJD 2009)

 $\Rightarrow s_e \sim 10^{-4} \text{ very small; approximation?}$  $\Rightarrow \tau_e \sim 10^{-2} s \text{ very large; assumption of thermodynamical equilibrium?}$