Ion Kinetics at the Plasma Material Interface in Oblique Magnetic Fields

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Multiscale, interlinked PSI phenomena

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Feedback Loop of Plasma Sheath & Material Release

**PLASMA SHEATH STRUCTURE**

- Release of particles from the wall (depending on $E, \theta$)
- Plasma particles accelerated by the $\text{ExB}$ fields through the sheath

$J_{\text{wall}}$

$E, \theta$ distributions at the wall
Outline

• Ion distribution functions at the material wall of a magnetized plasma
  • Fluid model
  • PIC model
• Wall response
  • BCA methods for material properties
  • Development of Fractal-TRIDYN
• Coupling methodologies with fluid-kinetic codes
  • SOLPS, EMC3, EIRENE
  • Using only the “relevant” information
A Simple Question

What is the **energy** and the **angle** of plasma ions at the boundary of a magnetized plasma?

\[ f(E, \theta) \]

Material Wall

- \( B_0 \)
- \( v \parallel \)
- \( v_y \)
- \( v_x \)
- \( V_z \)
- \( \psi \)

45°!

0°!

As \( \psi \)!
Release of Material Particles (e.g. Y, $\delta_e$) and wall reflection coefficients depend on $f(E,\theta) @ wall$. E.g.: SY(E,\theta)
Classical picture of the Magnetized Plasma Sheath

Ion Energy-Angle Distribution Function

Marginal distributions derived from $f(E, \theta)$
## Models of the Magnetized Sheath

<table>
<thead>
<tr>
<th>Authors (list of selected works)</th>
<th>Fluid Model</th>
<th>Kinetic Model</th>
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<tbody>
<tr>
<td>Chodura, Phys. Fluids 25, 1628 (1982)</td>
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<td>x (pic)</td>
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<tr>
<td>P. C. Stangeby, PoP 2, 702 (1995)</td>
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<tr>
<td>E. Ahedo, PoP 4, 12 (1997)</td>
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<td>G. Kawamura and A. Fukuyama, PoP, 14, 083502 (2007)</td>
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<td>x (gyrokin)</td>
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<tr>
<td>T.M.G. Zimmermann et al, PoP 15, 072301 (2008)</td>
<td>x</td>
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<td>P. C. Stangeby, NF, 2012</td>
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Riemann Fluid Model including fluid Collisions and Ionization

1. Continuity
2. Momentum
3. Isothermal ideal-gas EoS
4. Quasi-neutrality
5. Boltzmann electrons

Dimensionless variables

\[ X = \frac{x}{\lambda_{mfp}}; \quad V = \frac{v}{c_s} \quad \phi = -\frac{eU}{k_B T_e}, \]

\[ \Delta = \frac{v_i}{v_t}; \quad \lambda_{mfp} = \frac{c_s}{v_t}; \quad \omega \tau = \frac{eB}{m_i v_t}, \]

\[ \alpha = \frac{\pi}{2} - \psi \]
Typical profiles from Fluid Model

\[ \omega_c \tau_i = 100, \quad \psi = 85 \text{ deg}, \quad \Delta = 0.1 \]

\[(V_x, V_y, V_z)_{SE} = (1.47, 1.00, 1.38) V_s\]

Integration is terminated at SE where \(V_y = V_s\)

\(V_{||}\) becomes sonic at MPE

Plasma assumed initially at rest

Chodura Edge (CE)
Collisional and Magnetic Presheath structure in Strongly-Magnetized, Weakly-Collisional case

Strongly magnetized, weakly collisional plasma

\( \omega_c \tau_i = 100, \psi = 0 \text{ deg}, \Delta = 0.1 \)

- CP only
- No magnetic preheat
- Drift velocity different than zero only in parallel direction, \( V_{\parallel} = V_y \)

\( \omega_c \tau_i = 100, \psi = 60 \text{ deg}, \Delta = 0.1 \)

- CP+MP
- Drift velocity has 3D features, with \( V_x, V_y, V_z \) all different than zero
- \( V_{\parallel} \) gains additional momentum by the presence of the MP, becoming supersonic inside MP, before quasi-neutrality is broken (DS)

\( \omega_c \tau_i = 100, \psi = 85 \text{ deg}, \Delta = 0.1 \)

- CP+MP
- At grazing angles the MP size becomes larger
- \( V_{\parallel}, V_x, V_z \) are all supersonic
- Interestingly, \( V_x \) (parallel to the wall) begins to decrease
- Sheath size decreases with
Ion Drift Velocity at Debye Sheath Entrance depends on the inclination of the B-field.
Fluid Ion Kinetic Energy $E_i$ at Sheath Entrance (SE)

Collisions provide a mechanism to dissipate ion kinetic energy across the pre-sheaths (CP and MP).

Collisional Dumping of Ion Energy is more effective at higher B-field inclinations.

Strong magnetization

Weak magnetization

$\psi$ [deg]

$E_i/E_i(\psi=0)$
Flow Inclination from Fluid Model

\[ \omega_{ci}, \tau_i = 100, \psi = 85 \text{ deg}, \Delta = 0.1 \]

The plasma flow remains parallel to the magnetic field along most the collisional presheath.

The flow is then bent mostly in the magnetic pre-sheath.

Flow Inclination \( \theta \) [deg]

\( \chi [\lambda_{mfp}] \)

63.6 deg
Flow Inclination $\theta$ at Debye Sheath Entrance vs. Inclination $\psi$ of the B-field

Collisions provide a mechanism to bend the plasma flow toward normal incidence.
Flow Inclination $\theta$ at Debye Sheath Entrance vs. Inclination $\psi$ of the B-field

Collisions provide a mechanism to bend the plasma flow toward normal incidence.

Strong magnetization

Weak magnetization
$f(E)$ and $f(\theta)$ of a Deuterium Plasma in $B_0=1.0$ Tesla field, $\theta_0=30^\circ, 45^\circ, 60^\circ$

$\psi=30^\circ$  
$\psi=45^\circ$  
$\psi=60^\circ$

Field inclination has small effect on energy distributions; Density does not affect the distributions.

Increasing density $n\sim 10^{16}-10^{20}$ m$^{-3}$

Angular distributions are affected by the plasma density.
A Fully-Kinetic Analysis is Necessary: PIC

• Methodology
  – kinetic-kinetic explicit PIC (kinetic ions, kinetic electrons)
  – electrostatic
  – Particle pusher: Leapfrog, parallelized w/ MPI
  – Field solver: PETSc Multigrid on structured mesh; unstructured mesh also available but not used for plasma sheath analysis
  – MPI: OpenMPI
  – Viz: Paraview, Post-proc: Python

• Simulations
  – 2D3V
  – kinetic ions ($10^7$), kinetic electrons($10^7$), ppc~75
  – $dt = (1/20)\min(\omega_{ce}, \omega_{pe})$, O(~500 fs)
  – $dx = (1/20)\min(\lambda_{D}, r_L)$, O(~0.5 µm)
  – B-field inclinations 0,30,60,85 deg
  – Uniform ionization source
  – Lorentz collision operator
    – Collisionless
    – $\omega_{ci} < v < \omega_{ce}$
    – $\omega_{ci} < \omega_{ce} < v$

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<tr>
<td>$&lt; n$</td>
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<tr>
<td>$B$</td>
</tr>
<tr>
<td>$\theta_B$</td>
</tr>
<tr>
<td>domain size,</td>
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<tr>
<td># of iterations</td>
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<tr>
<td>particles per cell</td>
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Fluid Moments obtained from the electron and ion particle state-vector

- The qualitative features of the fluid moments agree with the simpler "classical" fluid models (Riemann, Zimmermann, etc.)
- Sheath size decreases with increasing inclination of the B-field
- However, the kinetic simulations reveal that ions and electrons are not isothermal over the domain and electrons are not Boltzmann
- Ion temperature decreases during the acceleration through the CP +MP sheath
- Local deviations from classical fluid models are observed (not today’s topic)
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At \( \theta_0 = 0 \) deg (normal incidence), the energy-angle peak occurs at \( \sim 5E_{th} \) and \( \sim 15-18 \) degrees; surprisingly, most of the ions do not arrive at normal incidence! All the ion energy is contained within 45-50\( E_{th} \), over three decades of amplitude of the distribution.

Increasing the B-field inclination causes a shift in both energies and angles at the wall; At grazing angles the angular distribution is narrower along the angular coordinate, but it becomes wider along the energy coordinate.
Fluid vs. PIC - Comparison of Energy Peaks

Fluid Ion Kinetic Energy $E_i$ at Sheath Entrance (SE)

$(\Delta=0.1)$

$E_i/E_i(\psi=0)$ vs $\psi$ (deg) at $\omega t=5$ and $\omega t=25$
Scaling is now with respect to the total acoustic energy of the plasma
Ion Energy Distribution Functions @ Wall

![Graph showing ion energy distribution functions at the wall with different angles.]
Influence of a Lorentz Scattering Operator

• The addition of a Lorentz scattering operator does not change the trends of the IEDF, as expected by diffusion on a sphere of $\nu = \text{constant}$

• Here “Intermediate collisions” and “High Collisions” are intended w.r.t the ion cyclotron and electron cyclotron frequencies
Ion Angular Distribution Functions at the Wall

\[ f_\theta(\theta, \psi) \]

- \( \psi = 0 \) deg
- \( \psi = 30 \) deg
- \( \psi = 60 \) deg
- \( \psi = 85 \) deg

\[ 0 \leq \theta, \psi \leq 90 \]
Influence of a Lorentz Scattering Operator

- The peak of $f(\theta_w)$ is independent than the collision rate of the Lorentz operator
- In order to quantify the peak trend, we have conducted a larger set of simulations at slightly-reduced resolution
Peak angles of the IADF’s vs. $\psi$

Above ~25 deg of inclination, the distribution peaks at an angle smaller than the B-field angle.

(B-field inclinations) (0°-10°) (60°) (82°) (88°)

Normal incidence  Grazing incidence
Ions 3D features at the time of impact
Kinetic IEADs affect how EIRENE evaluates the impurity release at the surface.
The wall properties are considerably affected not only by $E$, but also by $\theta$! Examples for $Y(E,\theta)$.
Release of Material Particles (e.g. $Y, \delta_e$) and wall reflection coefficients depend on $f(E_w)$ and $f(\theta_w)$ @ wall

$$Y = Y(E, \theta)$$

$$Y(E, 0) = 0.042 \frac{Q(Z_2)\alpha^*(M_2/M_1)}{U_s} \frac{S_n(E)}{1 + \Gamma \kappa_e e^{0.3}} \left[ 1 - \sqrt{\frac{E_{th}}{E}} \right]^s$$

Surface binding energy

Nuclear stopping cross-section

Reduced Energy

Lindhard electronic stopping coefficient

Ratio of Lindhard screening length and average lattice constant
Release of Material Particles (e.g. $Y$, $\delta_e$) and wall reflection coefficients depend on $f(E_w)$ and $f(\theta_w)$ @ wall

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\]

Surface binding energy

Nuclear stopping cross-section

Reduced Energy

Lindhard electronic stopping coefficient

in SOLPS:

\[
Y(E, 0) = Q \cdot s(E) \cdot \left( 1 - \left( \frac{E_{th}}{E} \right)^{2/3} \right) \cdot \left( 1 - \frac{E_{th}}{E} \right)^2
\]
Y(E,0) of He->Be from BCA, low energy range

Sputtering of Be by normal incident He ions

\[ Q = 0.33 \text{ [atoms/ion]}, \]
\[ ETF = 1153 \text{ [eV]} \] Thomas-Fermi energy
\[ Eth = 13.90 \text{ [eV]} \] threshold energy

\[ Q = 0.28 \text{ [atoms/ion]}, \]
\[ ETF = 720 \text{ [eV]} \] Thomas-Fermi energy
\[ Eth = 16.40 \text{ [eV]} \] threshold energy

ecktein_IPP_9_82
$Y(E,0)$ of He->Be from BCA, low energy comparison with PISCES-B data

Sputtering of Be by normal incident He ions

- $Q = 0.33$ [atoms/ion], $ETF = 1153$ [eV] Thomas-Fermi energy $Eth = 13.90$ [eV] threshold energy
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R. Doerner - PISCES-B DATA, +TRIM.CALC/13
Y(E,0) of He->Be, effect of surface roughness using fractal description of surface orientation

\[ Y(E,0) = Q \cdot s(E) \cdot \left( 1 - \left( \frac{E_{th}}{E} \right)^{2/3} \right) \cdot \left( 1 - \frac{E_{th}}{E} \right)^2 \]

All the curves can be fitted using a “Bodhansky-like” formula with 2 free parameters \( Q, E_{th} \):
Y(E,0) of He->Be, effect of surface roughness using fractal description of surface orientation

Results from fitting using a Bodhansky-like formula; non-linear least-squares fitting trend of the 2 free parameters Q [atoms/ions], E\text{th} [eV] vs. Fractal dimension

The decrease in Y(E,0) for corrugated surfaces can be seen as an equivalent increase in the Energy Threshold E\text{th}

Equivalent Energy Threshold [eV]

Equivalent Yield Amplitude [atoms/ions]
The fractal description of the surface roughness can be included in plasma edge codes.
Conclusions

• Ion Energy-Angle Distribution Function at the boundary of a magnetized plasma is strongly dependent on both the magnitude and inclination of the magnetic field

• The peak angle of the ions at wall is always different than the B-field angle

• Proper treatment of the wall response requires the IEADF for the calculation of the material properties

• Progress on BCA codes done with the development of fractal-TRIDYN and

Thanks!