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Ab initio study of stopping power for ions in partially ionized Al and Be plasmas

Bin He, Jian-Guo Wang

何 斌， 王 建 国

Institute of Applied Physics and Computational Mathematics,
Beijing, China

Outline

1. Background

2. Introduction to average atom (AA) model
   and atomic structures in Al and Be plasmas

3. Inelastic stopping of H^+ in Al, Be plasmas

4. Stopping due to free electrons in Al, Be plasmas

5. Comparisons with experiments and other models

6. Summary

1. Background

- Stopping power ($SP = -\frac{1}{n_T}\frac{dE}{dX}$) for ions in plasmas is important to fusion study.

- The plasmas were usually in partially ionized states in relevant experiments, where the bound e^- may be in excited states which is different from solid. In some relevant experiment, such as for D^+ in Al plasmas and H^+ in Be plasmas, enhanced stopping power was observed compared with the cold targets.

- Inelastic, plasma wave and nuclear stopping are three major mechanisms of stopping power in plasmas.

- Bethe equation $SP_{Bethe} = \frac{4\pi Z_{eff}^2 (Z - \bar{Z})}{V_p^2} Log[\frac{2V_p^2}{\bar{I}}]$ is often used to estimate the inelastic stopping at high projectile energy, where $\bar{I}$ is excitation energy and Mehlhorn gave its results for Al and Au in different charge states in his model (J. Appl. Phys. **52,** 652). Zimermann gave an expression to calculate it in LLNL UCRL-JC-105616.

Measurements of Enhanced Stopping of 1-MeV Deuterons in Target-Ablation Plasmas

F. C. Young, D. Mosher, S. J. Stephanakis, and Shyke A. Goldstein[a]
Naval Research Laboratory, Washington, D. C. 20375

and

T. A. Mehlhorn
Sandia National Laboratory, Albuquerque, New Mexico 87115
(Received 28 April 1982)

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aluminum at $\rho = 0.02$ g/cm^3. This is the Al density at peak power based on hydrocode calculations

aluminum (Mylar) at peak power, the electron temperature is 4–5 eV (2.5–3.5 eV) at 50 kA/cm^2 and 13–17 eV (9–11 eV) at 250 kA/cm^2. Code-

In summary, we report measurements of enhanced stopping of ions in dense plasmas. The stopping power of 1-MeV deuterons in aluminum is enhanced by 20% at the 50 kA/cm^2 level and by 40% at the 250 kA/cm^2 level. For Mylar, the

First experiment of stopping power for ions in plasmas

PRL 114, 215002 (2015) PHYSICAL REVIEW LETTERS week ending 29 MAY 2015

Measurement of Charged-Particle Stopping in Warm Dense Plasma

A. B. Zylstra,[1,*] J. A. Frenje,[1] P. E. Grabowski,[2] C. K. Li,[1] G. W. Collins,[3] P. Fitzsimmons,[4] S. Glenzer,[5] F. Graziani,[3] S. B. Hansen,[6] S. X. Hu,[7] M. Gatu Johnson,[1] P. Keiter,[8] H. Reynolds,[4] J. R. Rygg,[3] F. H. Séguin,[1] and R. D. Petrasso[1]

[1]*Plasma Science and Fusion Center, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA*

[2]*University of California Irvine, Irvine, California 92697, USA*

We measured the stopping of energetic protons in an isochorically heated solid-density Be plasma with an electron temperature of ~32 eV, corresponding to moderately coupled $[(e^2/a)/(k_B T_e + E_F) \sim 0.3]$ and moderately degenerate $[k_B T_e/E_F \sim 2]$ "warm-dense matter" (WDM) conditions. We present the first high-accuracy measurements of charged-particle energy loss through dense plasma, which shows an increased loss relative to cold matter, consistent with a reduced mean ionization potential. The data agree with stopping models based on an *ad hoc* treatment of free and bound electrons, as well as the average-atom local-density approximation; this work is the first test of these theories in WDM plasma.

P+Be: 1.77g/cc Be at room temperature and plasmas with T_e=32eV .

Projectile energy E_p=15MeV

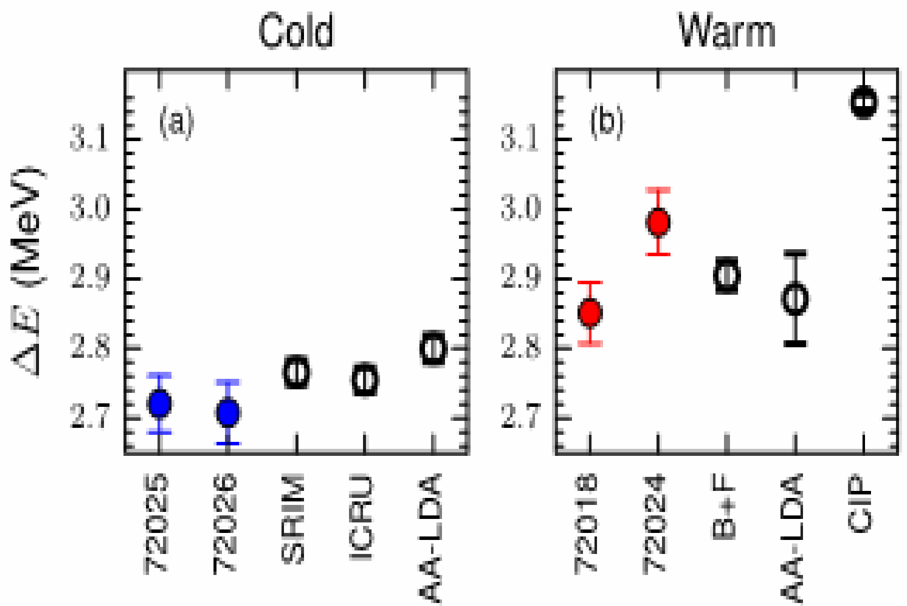

FIG. 4 (color online). Downshift (ΔE) for cold (a) and warm (b) shots compared to theory. The solid points are data (denoted by shot number), and theories are hollow points. The uncertainties in theoretical calculations are due to uncertainties in ρL and plasma conditions.

TABLE I. Data summary: initial (E_i) and final (E_f) energies, and downshift (ΔE) for each shot.

Shot	E_i (MeV)	E_f (MeV)	ΔE (MeV)
72018 (Warm)	15.019 ± 0.020	12.167 ± 0.039	2.851 ± 0.044
72024 (Warm)	15.025 ± 0.029	12.043 ± 0.037	2.981 ± 0.047
72025 (Cold)	15.075 ± 0.018	12.355 ± 0.036	2.720 ± 0.040
72026 (Cold)	15.004 ± 0.017	12.296 ± 0.040	2.708 ± 0.044

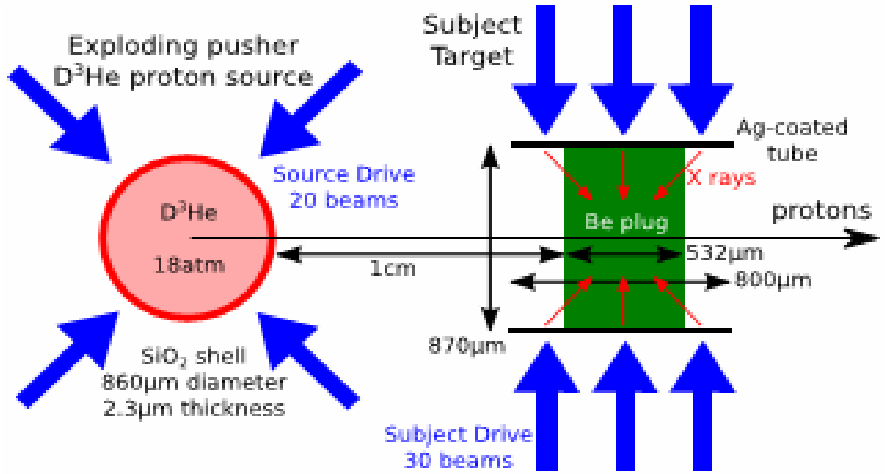

FIG. 1 (color online). Experimental geometry. A thin-glass exploding-pusher proton source (left) imploded by 20 laser beams creates energetic D^3He protons used to probe a subject plasma, which is created by isochorically heating a solid Be plug with x rays (right). These x rays are created by the 30 laser beams irradiating the Ag-coated CH tube.

Higher energy loss is observed at plasmas than cool Be at solid density

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1. Background

- More than 40 years McGuire did a series of work to study inelastic stopping in plasmas by plane wave Born approximation, where the target electron was assumed in ground state.

- Basing on average atom model, Wang discussed this problem by local density approximation (LDA)(where free electron gas model is used to describe the contribution of both bound and free electron and it is often used in the research of solids) (Phys. Plasmas **5,** 2977 (1998)).

- One motivation for this work is to get more reliable results of stopping power in plasmas in *ab initio* way , where all the inelastic with their reverse processes are included. Our results will be compared with other models and experiment. New experiments are suggested to further test our model and others.

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A unified self-consistent model for calculating ion stopping power in ICF plasma

P. Wang
Fusion Technology Institute, University of Wisconsin—Madison, Wisconsin 53706

T. M. Mehlhorn
Sandia National Laboratory, Albuquerque, New Mexico 87185-5800

J. J. MacFarlane

$$SP_{LDA} = \frac{Z_p^2}{2\pi^2 V_p \rho_{Al}} \int_{(r\le R)} d\vec{r}[n_{bound}(r) + n_{free}(r)]\{\int d\vec{k}\frac{\vec{k}\cdot\vec{V}_p}{k^2}\operatorname{Im}[1+\frac{4\pi}{\hbar k^2}\int d\vec{v}\frac{f(\vec{v},r)-f(\vec{v}-\hbar\vec{k},r)}{\omega-\vec{k}\cdot\vec{v}+\frac{\hbar k^2}{2}+i\delta}]^{-1}\}$$

$$= SP_{LDA-bound} + SP_{LDA-free}$$

Fermi-Dirac statistics:

$$f(\vec{v},r) = \{1+\exp[(0.5v^2 - V(r) - \mu)/T_e]\}^{-1}$$

Inelastic stopping is obtained
by dielectric function and charge density distribution

1. Background

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- One motivation for this work is to get more reliable results of stopping power in plasmas in *ab initio* way , where all the inelastic and their reverse processes are included. Our results will be compared with other models and experiment. New experiments are suggested to further test our model and others.

2. Average atom (AA) model—basic ideas

- The model is often used to describe the atoms in plasmas and it was suggested more than 40 years ago (Rozsnayai Balazs F. 1972 *Phys. Rev. A*. **5** 1137)

- In the model all the ions in the plasmas are represented by the average atom with the average charge state and an average occupation number for each energy level including the bound and free state, where Fermi-Dirac statistics is used.

- The atom is enclosed in an ion sphere with its radius R determined by the matter density and the electrical neutrality must be satisfied within the sphere;

- Electron density $n_e(r) = \sum_{m(\varepsilon_m<0)} \frac{1}{1+\exp[(\varepsilon_m-\mu)/T_e]} |\psi_m(\bar{r})|^2 + \sum_{s(\varepsilon_s\geq 0)} \int \frac{1}{1+\exp[(\varepsilon_s-\mu)/T_e]} |\psi_{\varepsilon s}(\bar{r})|^2 \, d\varepsilon_s$

- Electron wave functions, energy levels, electron potential, chemical potential, and so on are obtained by iteratively solving Dirac equation and Poisson equation.

2. Average atom model results

-- Bound states for Al at 0.02g/cm^3 and T_e=13eV

(N: population number)

States	-Energy (eV)	N(Al ion)	N(Al atom)
1s	1544.8	2.0	2.0
2s	141.9	1.99	2.0
$2p_{1/2}$	104.7	1.85	2.0
$2p_{3/2}$	104.3	3.70	4.0
3s	24.68	0.052	2.0
$3p_{1/2}$	17.42	0.03	1.0
$3p_{3/2}$	17.40	0.06	0.0
$3d_{3/2}$	8.41	0.03	0.0
$3d_{5/2}$	8.409	0.046	
4s	6.36	0.013	
$4p_{1/2}$	4.193	0.011	
$4p_{3/2}$	4.191	0.022	
$4d_{3/2}$	1.6397	0.018	
$4d_{5/2}$	1.6395	0.027	
$4f_{5/2}$	0.79696	0.025	
$4f_{5/2}$	0.79690	0.034	
5s	1.49	0.009	
$5p_{1/2}$	0.783	0.0085	
$5p_{3/2}$	0.782	0.017	

19 total bound states;

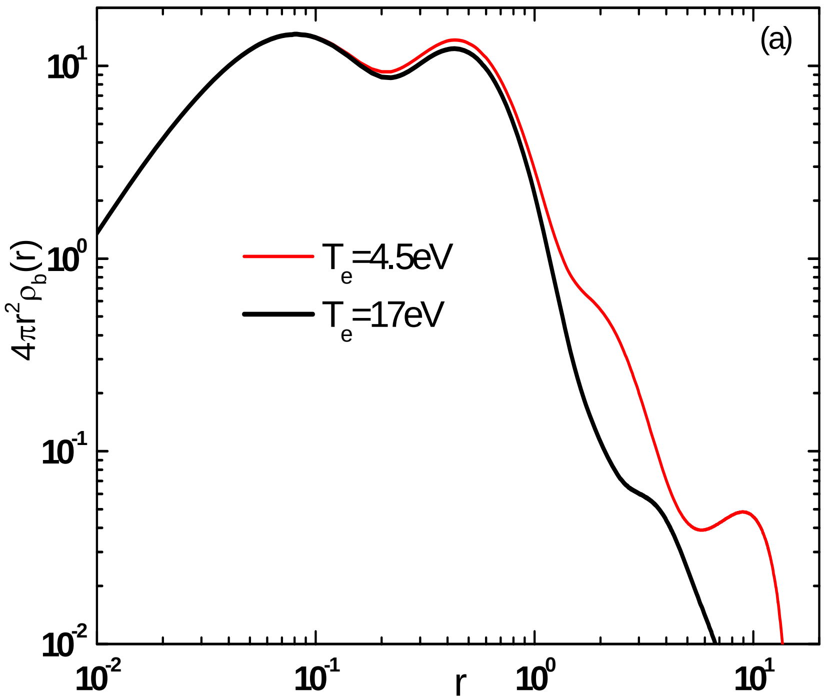
Some electrons populated in excited states; generally speaking, the population number in the excited state decrease with the increasing of its energy level.

Average ionization degree, 3.06, lies in the experimental range (PRL45 549 (1982)).

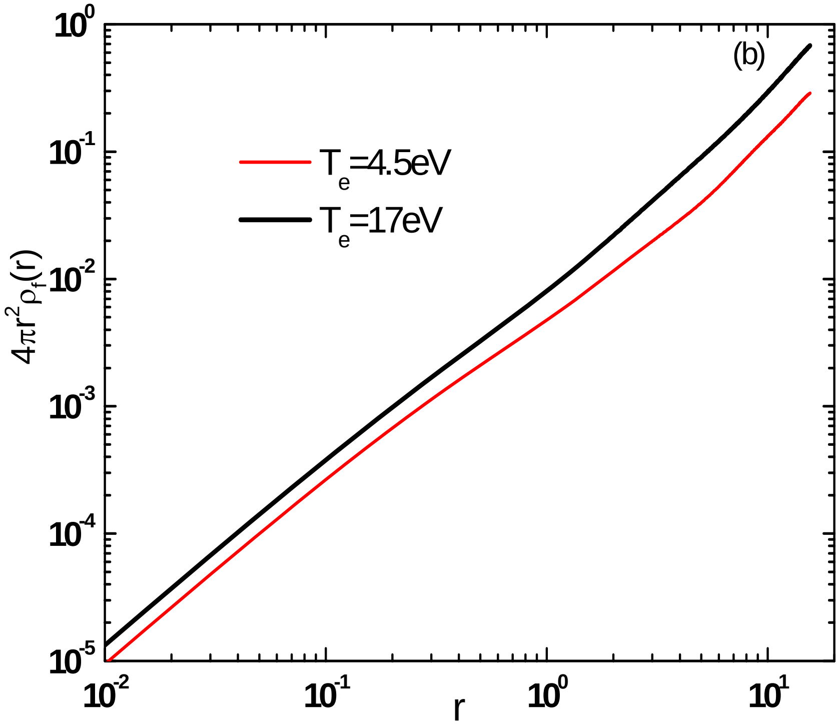
For other T_e our results also agree with the experiment.

2. Average atom model results

- Electron distribution in ionic sphere of Al plasmas *at 0.02g/cm³*



Bound e⁻ distribution



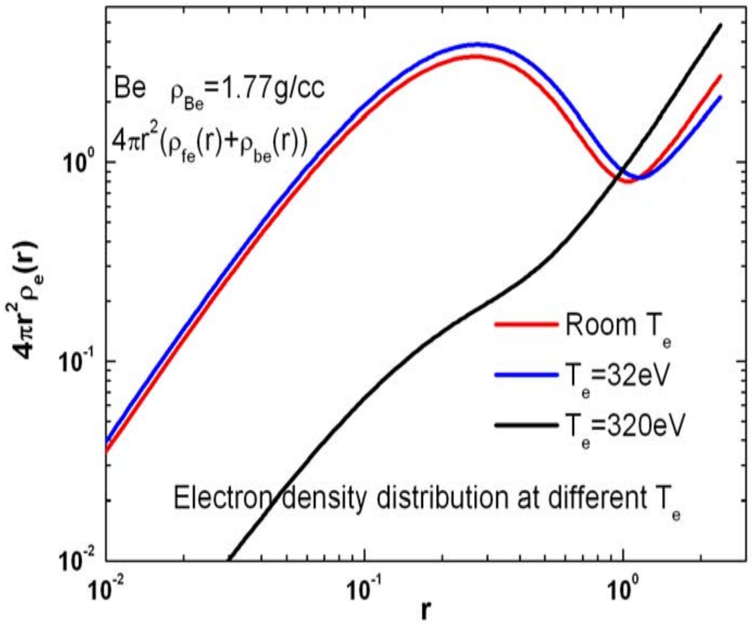
Free e⁻ distribution

Bound electrons distribute around the nucleus and free electrons distribute near the boundary of the ionic sphere.

2. Average atom model results

-Be in solid and plasmas of T_e=32eV *at 1.77g/cm³*

Average ionization degree <Z>=2.33 while the experiment gives 2.46±0.15. All the bound electrons are in 1s state and no higher bound state is permitted. Same result is found for solid Be at room Te with 1s is fully occupied. So in the two case excitation is forbidden.



All electron spatial distribution

Different from Al plasmas there is only one bound state in Be at solid density, which is the ground state.

3. Inelastic stopping --Our calculation method

Relativistic plane wave Born approximation is used to get inelastic stopping with excitation, ionization and their reverse processes included

Excitation contribution (electron occupation number $N_{i,f}$ is considered)

$$SP_{exc} = \sum_{i,f} N_i (1 - \frac{N_f}{2j_f + 1}) \Delta E \int_{q_{\min}}^{q_{\max}} \frac{8\pi q Z_{eff}^2}{V_p^2 (q^2 + \lambda_D^{-2})^2} |< \Psi_i | \exp(i\vec{q} \cdot \vec{r}) | \Psi_f >|^2 \, dq$$

Ionization contribution (electron occupation number is considered)

$$SP_{ion} = \sum_{i,f} N_i \int_0^{E_p - I_i} [1 - \frac{N_f(\varepsilon)}{2j_f + 1}](\varepsilon + I_i) d\varepsilon \int_{q_{\min}}^{q_{\max}} \frac{8\pi q Z_{eff}^2}{V_p^2 (q^2 + \lambda_D^{-2})^2} |< \Psi_i | \exp(i\vec{q} \cdot \vec{r}) | \Psi_f(\varepsilon) >|^2 \, dq$$

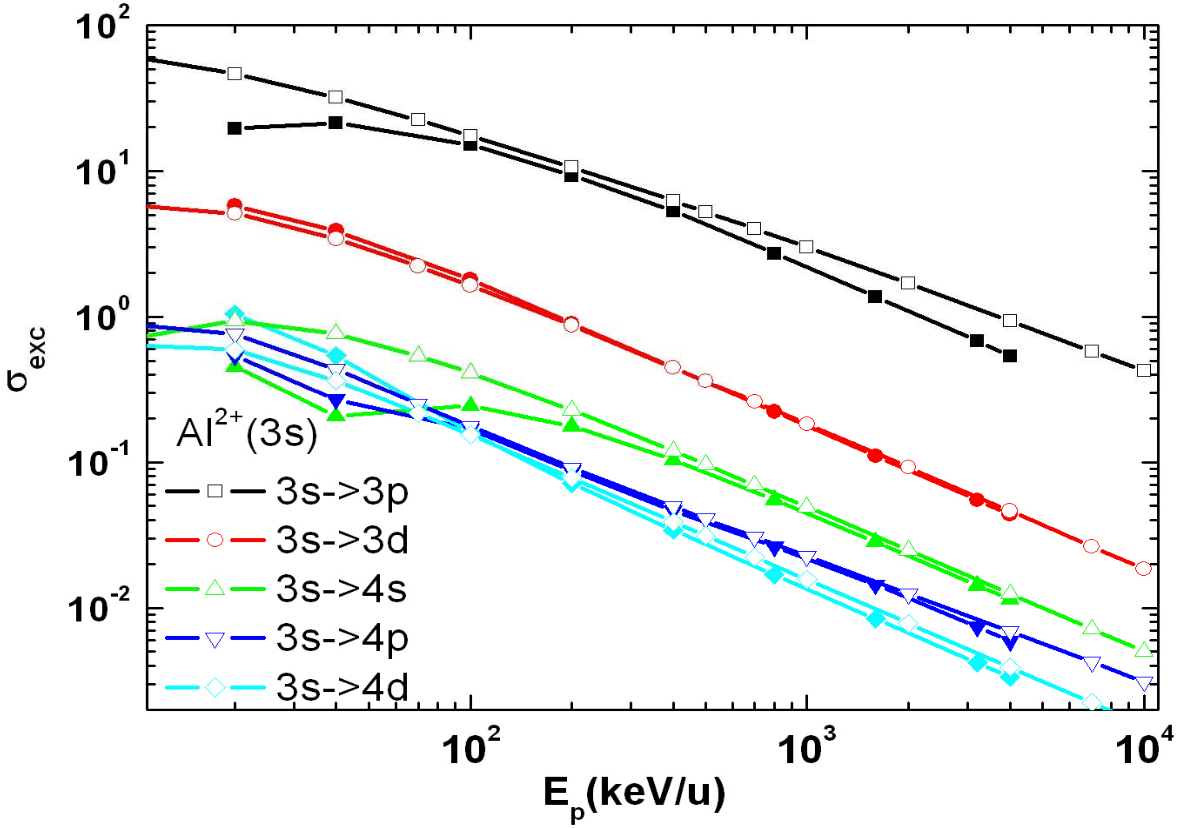
Here $\lambda_D = [\frac{T_e}{4\pi n_e}(1 + \frac{V_p^2}{v_{th}^2})]^{1/2}$ Correction to the projectile charge state:

$$Z_{eff} = Z_p [1 - Exp(-0.92 u Z_p^{-2/3})] \qquad u = \int f(\vec{v_e}) | \vec{V_p} - \vec{v_e} | d\vec{v_e}$$

Contribution from the reverse processes is obtained by exchange of the initial and final states, which are denoted with i and f in the above equations.

In our results the occupation number is considered both for cross section and stopping.

3. Our calculation method --- *Validity test*



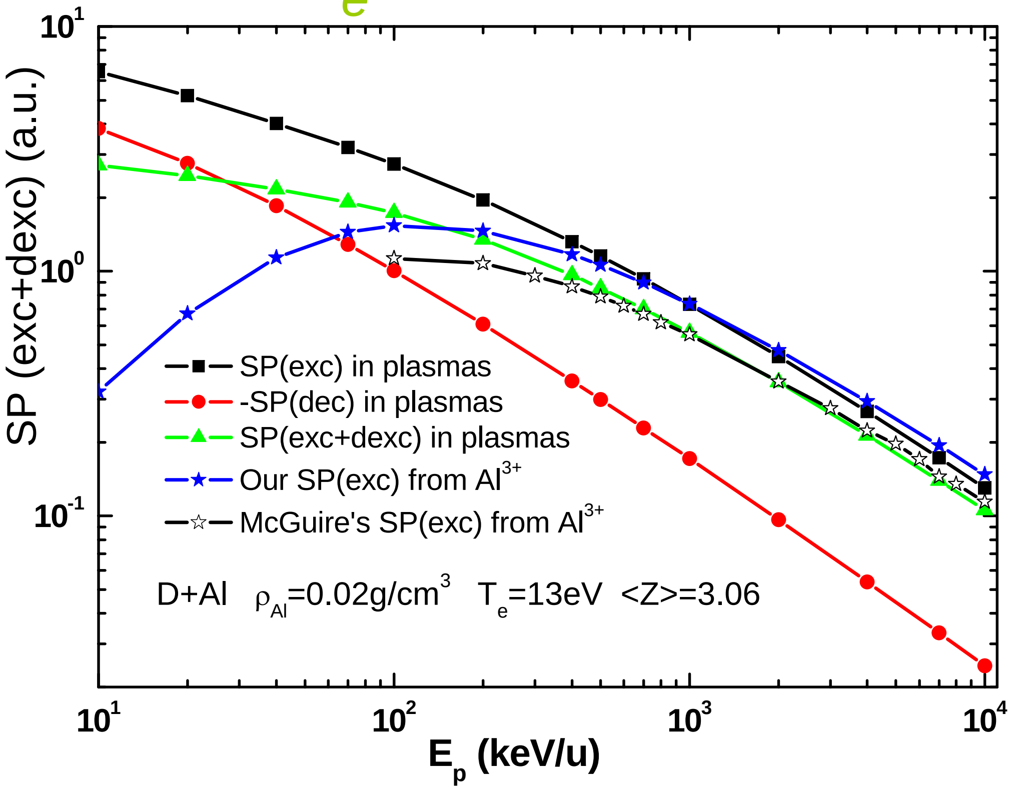
$P + Al^{2+}$

TDSE: solving the time-dependent Schrödinger equation

For other charged Al ion similar results are obtained.

Comparison indicates that our method RPWBA is valid at least for E_P>100keV/u.

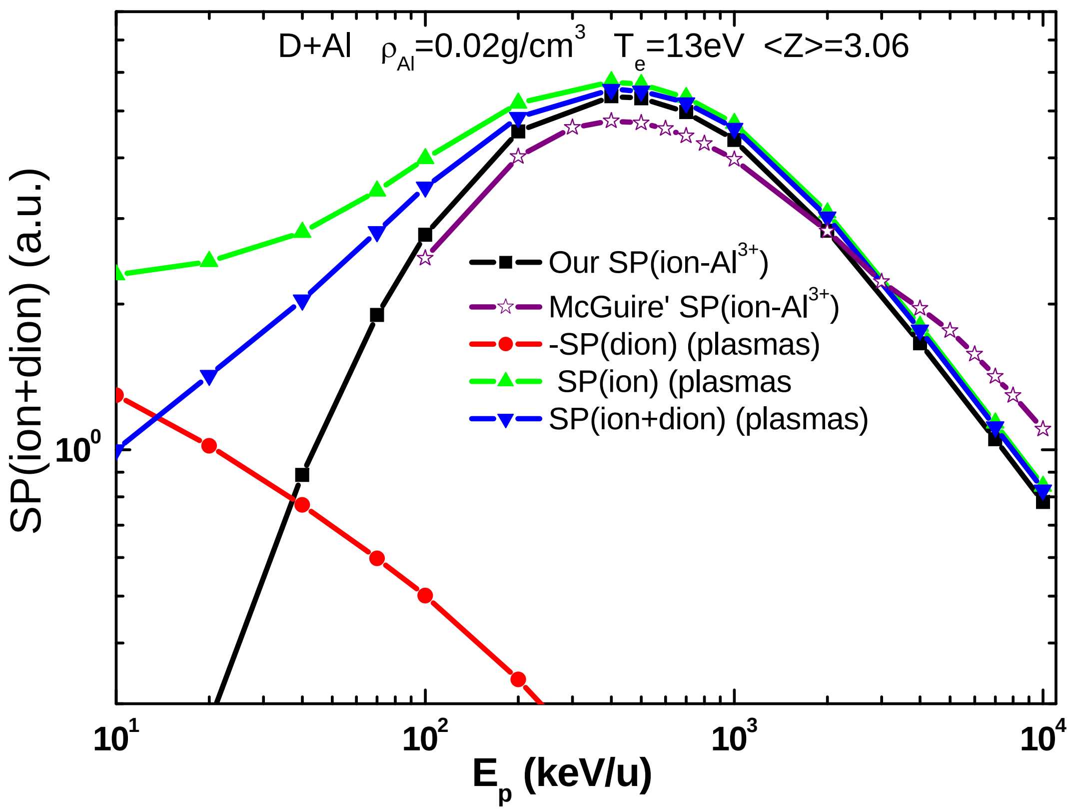
3a. Inelastic stopping for deuterons in Al plasmas *at 0.02g/cm³ and T_e=13eV----excitation + de-excitation*



Contribution from excitation (black line), de-excitation (red line) and their total results (green line) in plasmas. We can see the de-excitation must be included to get the final results. Blue line is for the isolated Al^{3+} ion. Our result for Al^{3+} (blue line) is higher than McGuire's due to fewer final states included in McGuire's calculation. Difference between green and blue line may arise from the different occupation number and energy level between the two model.

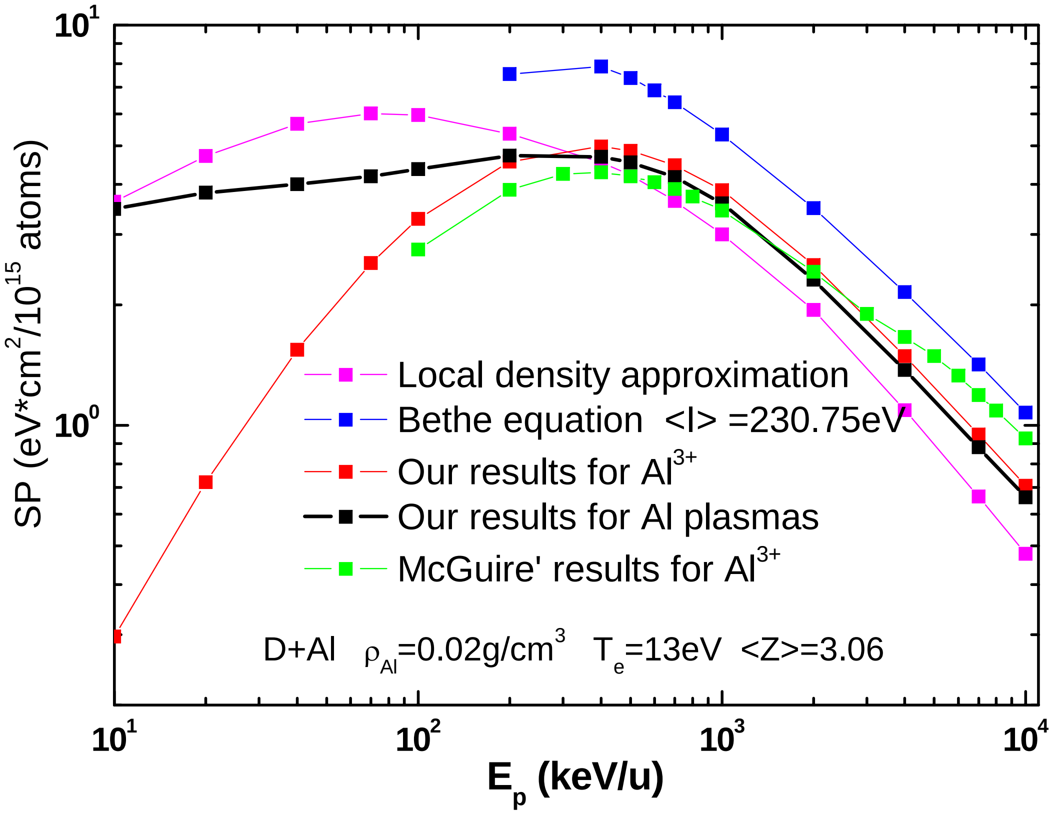
3b. Inelastic stopping for deuterons in Al plasmas

at 0.02g/cm^3 and T_e=13eV----ionization and its reverse process



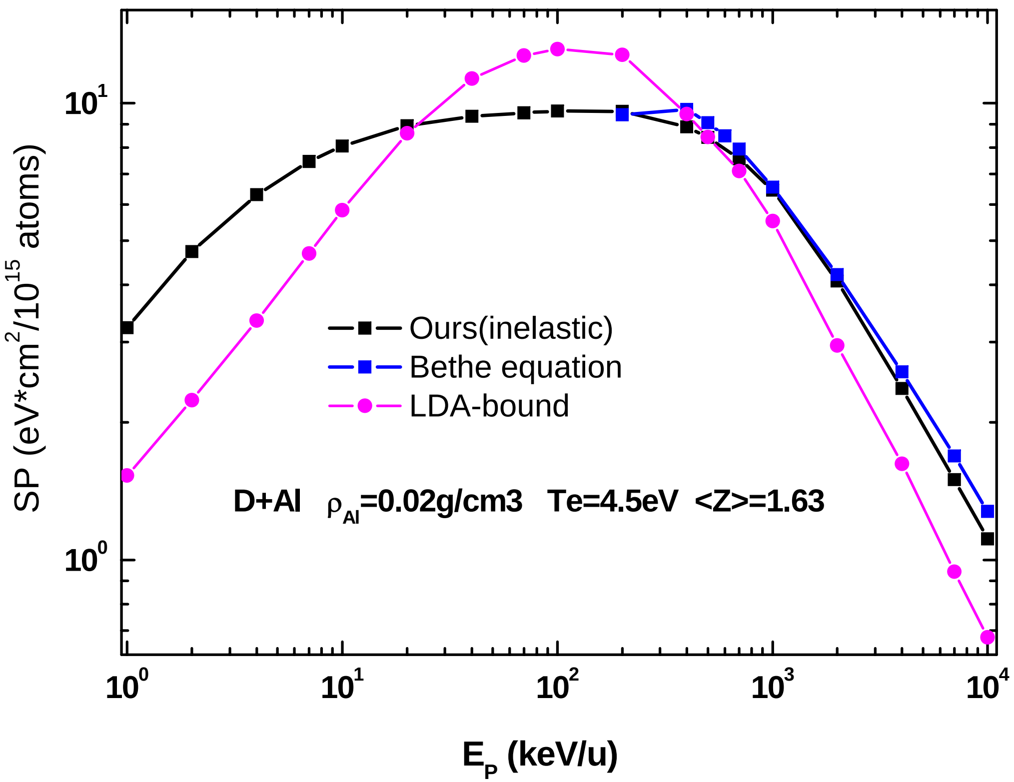
Total results from ionization and its reverse process in plasmas and comparison with the isolated Al^{3+} ion. The total result in plasmas is close to that for isolated Al^{3+} ion when E_p>200keV/u.

3c. Inelastic stopping for deuterons in Al plasmas *at 0.02g/cm^3 and T_e=13eV----total inelastic stopping*



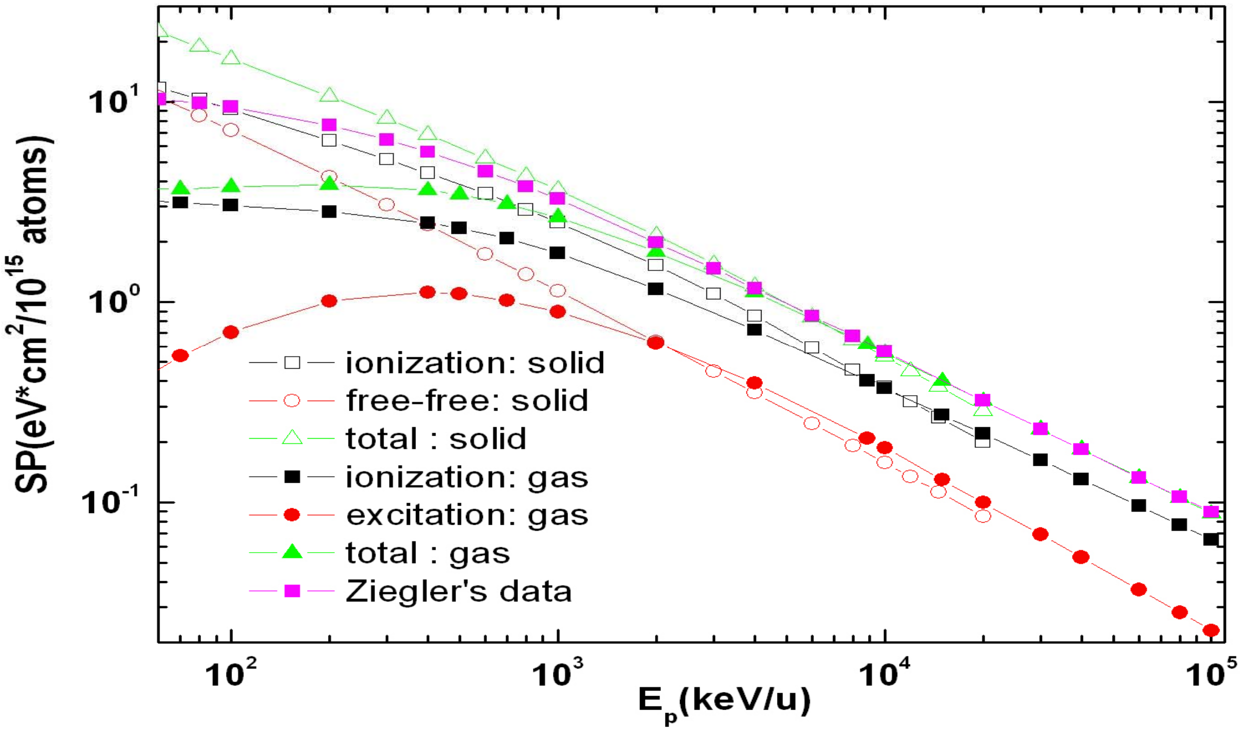
Comparison of total inelastic stopping for different models. We think that Bethe equation overestimates the result. Local density approximation gives different result from our model due to different physical picture.

3c. Inelastic stopping for deuterons in Al plasmas *at 0.02g/cm^3 and T_e=4.5eV----* *total inelastic stopping*



Comparison of total inelastic stopping for different models. With T_e decreasing, the result from Bethe equation is close to ours.

3. Inelastic stopping for proton in Be materials *at gas and solid state--- inelastic stopping*



All the possible transitions for the bound states are considered. For free electrons their maximum energy is 500 a.u. maximum angular momentum is 50, and the energy interval is below 0.2a.u. or even smaller. So far no such calculation of inelastic process for solid Be has been made.

Reliable results in *ab initio* way are obtained for high enough E_p at both gas and solid state.

3d. Summary for inelastic stopping

Based on average atom model and PWB approximation, the inelastic stopping for D^+ in Al plasmas at density 0.02g/cm^3 and T_e around 10eV is studied in detail with both excitation, ionization and their reverse processes included. Comparison with other models is made and their difference is explained. In addition, we find that

1. Bethe equation usually overestimates the result at least 10% and its result is close to our model with T_e decreasing;

2. With E_p decreasing, the neutralization from the inelastic and its reverse process strongly weakens the inelastic stopping;

3. With E_p decreasing the inelastic stopping from the electrons at n=2 in plasmas becomes dominant, which is close to that from Al^{3+}. This can explain that in this case why the model where all bound electrons in ground state gave the results consistent with the experiment.

4. Plasma wave stopping ---some different models

Electron plasma wave is excited as the projectile moves in the plasmas, which leads to the energy loss of the projectile.

$$SP_{Lindhard} = \frac{Z_p^2}{2\pi^2 V_p \rho_{Al}} \int d\vec{k} \frac{\vec{k}\cdot\vec{V}_p}{k^2} \mathrm{Im}[1+\frac{4\pi}{\hbar k^2}\int d\vec{v} \frac{f(\vec{v})-f(\vec{v}-\hbar\vec{k})}{\omega - \vec{k}\cdot\vec{v} + \frac{\hbar k^2}{2} + i\delta}]^{-1}$$

PRA16, 727 (Skupsky), J. Physique V46, 1113 (Marnard & Deutsch)

$$SP_{CD} = \frac{Z_p^2}{2\pi^2 V_p \rho_{Al}} \int d\vec{k} \frac{\vec{k}\cdot\vec{V}_p}{k^2} \mathrm{Im}[1+\frac{4\pi}{\hbar k^2}\int d\vec{v} \frac{\vec{k}\cdot\partial f(\vec{v})/\partial\vec{v}}{\omega - \vec{k}\cdot\vec{v} + i\delta}]^{-1}$$

PRA43, 1998 (Peter & Meyer-ter-Vehn)

$$SP_{JK} = \frac{4\pi <Z> Z_p^2}{V_p^2}[Erf(\sqrt{\eta}) - 2\sqrt{\eta/\pi}e^{-\eta}]Log\{\frac{0.216V_p}{\sqrt{<Z>}Max[Z_p u^{-2},(2u)^{-1}]}\}$$

J.Appl.Phys.52, 6522 (Mehlhorn)

$$\eta = V_p^2(2V_{th}^2)^{-1} \qquad u = \int |\vec{V}_p - \vec{v}| f(\vec{v}) d\vec{v}$$

Fermi-Dirac velocity distribution f(v)
Is used in all the models

Phys. Plasmas 5, 2977 (Wang *et al*)
AA model → charge density distribution

$$-\frac{dE}{dx}\Big|_e = \frac{4\pi \bar{Z}_0^2 e^4}{mV_0^2} N_i \int d\mathbf{r}\rho_e(\mathbf{r}) L_0[\rho_e(\mathbf{r}), T_e, V_0], \quad L_0 = \frac{i}{\pi\omega_p^2}\int_0^\infty \frac{dk}{k}\int_{-kV_0}^{kV_0} \omega d\omega \left[\frac{1}{\varepsilon(k,\omega)} - 1\right]$$

4. Plasma wave stopping --- our model

$$SP_{Lindhard} = \frac{Z_p^2}{2\pi^2 V_p \rho_{Al}} \int d\vec{k} \frac{\vec{k}\cdot\vec{V}_p}{k^2} \mathrm{Im}[1 + \frac{4\pi}{\hbar k^2} \int d\vec{v} \frac{f(\vec{v}) - f(\vec{v} - \hbar\vec{k})}{\omega - \vec{k}\cdot\vec{v} + \frac{\hbar k^2}{2} + i\delta}]^{-1}$$

The free electron velocity distribution f(v) should be different from Fermi-Dirac's due to the electric field in the plasmas.

$$f(v_x) = c\int_{-\infty}^{\infty} dv_y \int_{-\infty}^{\infty} dv_z \int_{r_0}^{R_0} \frac{4\pi r^2 dr}{1 + e^{(-\mu + \varepsilon_e)/T_e}}$$

$$\varepsilon_e = \frac{1}{2} m_e v_e^2 - V(r)$$

R_0 : radius of ionic sphere

V(r): potential in the sphere

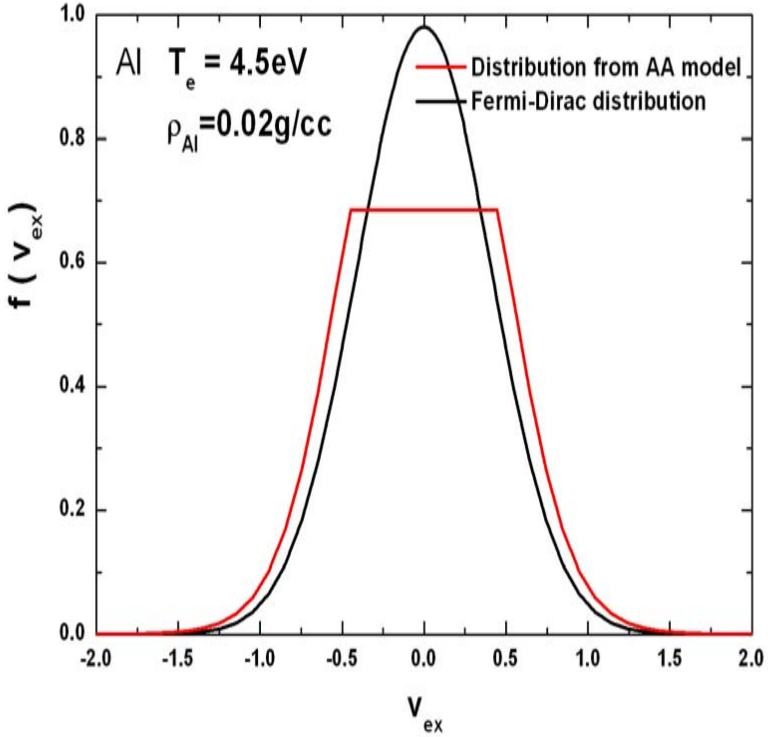
μ : chemical potential

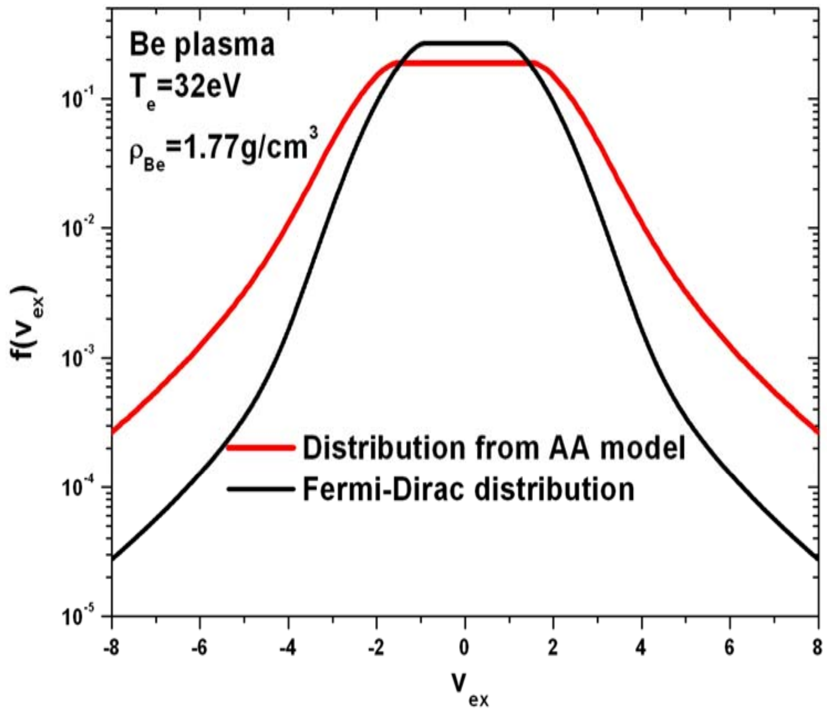
$$r_0 : \frac{1}{2} m_e v_e^2 - V(r_0) = 0$$

c: normalization coefficient

4. Plasma wave stopping

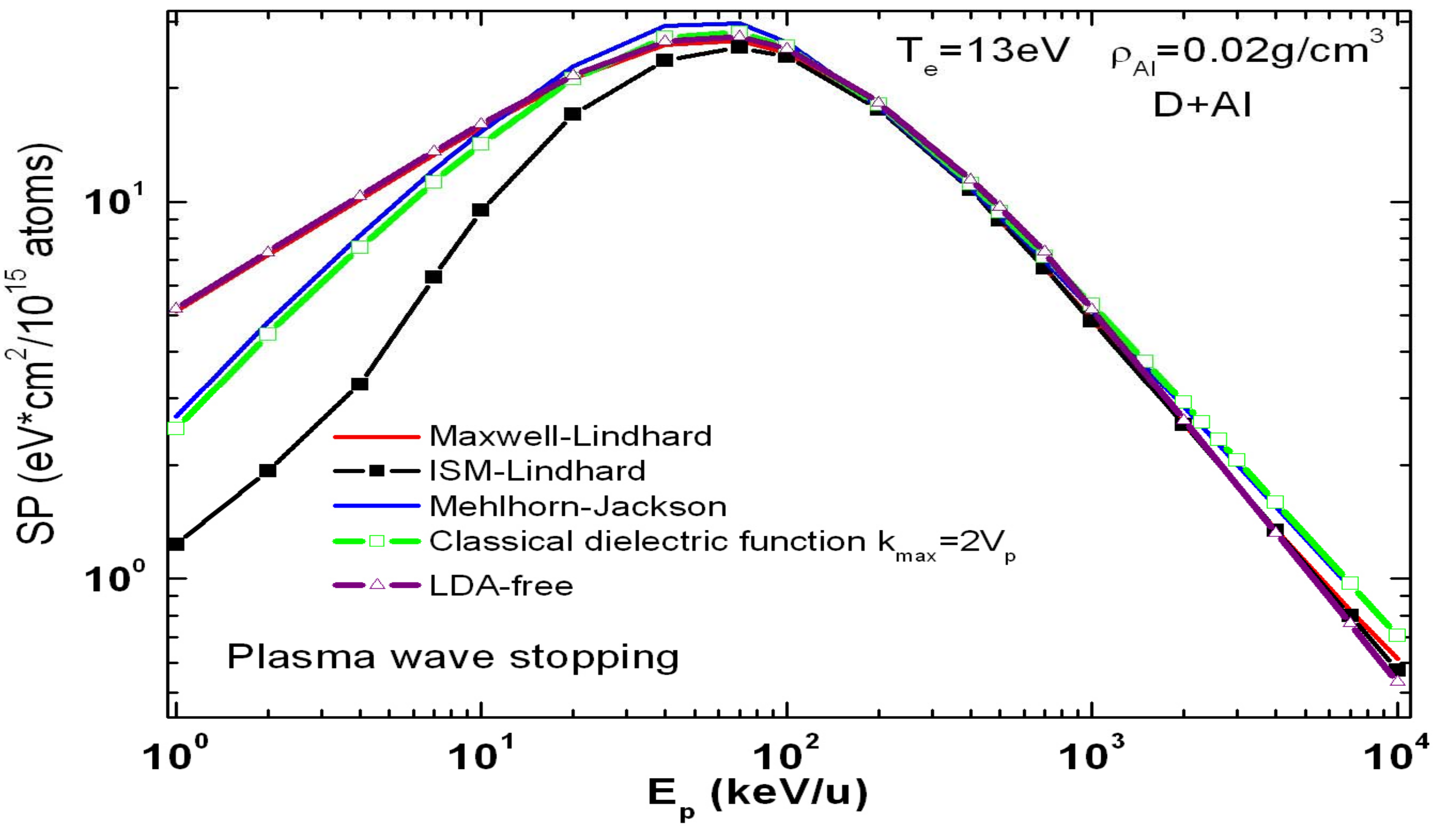
--- free electron velocity distribution





Free electron number with low velocity is decreased and the number with high velocity is increased due to the acceleration of electric field in the ionic sphere.

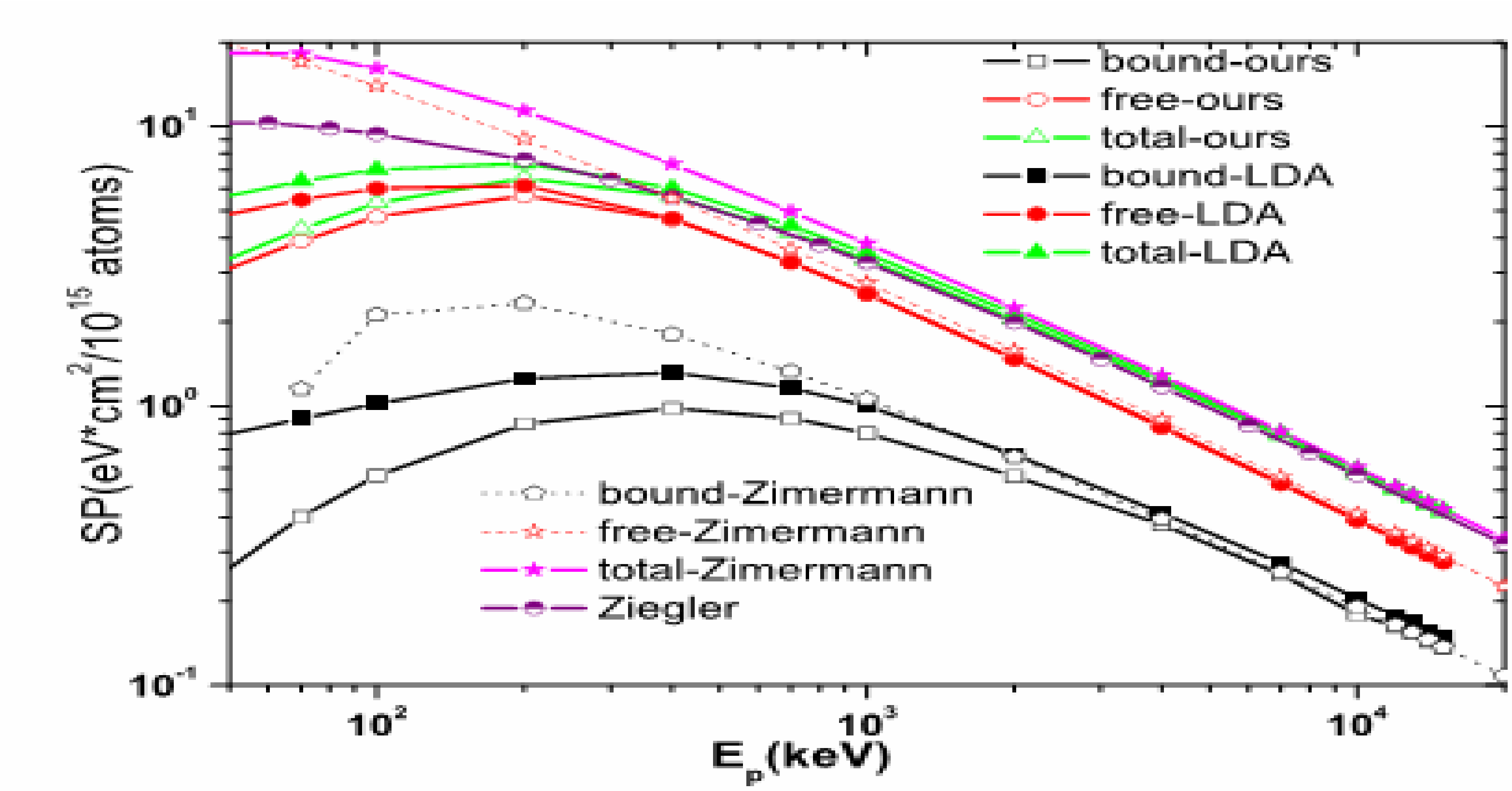
4. Plasma wave stopping --- comparison of different models



Our result (black line) is lower than others at low E_p due to the flatter velocity distribution. Local density approximation (LDA) model is very close to the result with average e^- density considered because most free electrons are close to the boundary of ionic sphere.

4. Plasma wave stopping --- comparison of different models

Proton moving in Be plasmas



1) Three models (Ours, LDA and Zimermann) are very close at E_p>4MeV.

2) Difference between ours and LDA at low E_p mainly comes from plasma wave stopping at different velocity distribution.

Our result (red line with empty circles)

4. Summary for plasma wave stopping

- Velocity distribution for free e^- in plasmas, which is flatter than Fermi-Dirac's, is found with electron number at low velocity decreased and that with high velocity increased due to the acceleration of electric field in the ionic sphere.

- The plasma wave stopping from our model is lower than others for low E_p under the flatter velocity distribution.

- At high enough E_p the results from different models are close to each other.

5. Stopping for deuterons in Al plasmas *at different* T_e

----comparison of different models with experiment data

Table. The respective stopping power at different T_e in unit of eV from different models together with the comparisons of the total stopping powers with the experiments at E_p=500keV/u. All the stopping powers are in units of eV*$cm^2/10^{15}$atoms.

<table>
<tr><th rowspan="2">T_e</th><th colspan="3">Inelastic</th><th colspan="4">Plasmas</th><th colspan="9">Enhanced rate of SP (%)</th></tr>
<tr><th>Ours</th><th>LDA</th><th>Bethe</th><th>Ours</th><th>LDA</th><th>MJ</th><th>CD</th><th colspan="2">Ours</th><th colspan="2">LDA</th><th colspan="2">MJ+Bethe</th><th colspan="2">CD+Bethe</th><th>Expt</th></tr>
<tr><td>4.5</td><td>8.68</td><td>8.71</td><td>9.35</td><td>4.81</td><td>5.52</td><td>4.81</td><td>5.42</td><td colspan="2">17</td><td colspan="2">23.6</td><td colspan="2">26.7</td><td colspan="2">28</td><td>20</td></tr>
<tr><td>13</td><td>5.72</td><td>4.22</td><td>7.47</td><td>9.2</td><td>9.97</td><td>9.42</td><td>9.68</td><td>30</td><td rowspan="2">37</td><td>23.3</td><td rowspan="2">29.2</td><td>45.8</td><td rowspan="2">51.9</td><td>48.1</td><td rowspan="2">40.6</td><td rowspan="2">40</td></tr>
<tr><td>17</td><td>5.22</td><td>3.71</td><td>6.66</td><td>11.4</td><td>11.9</td><td>11.4</td><td>8.71</td><td>44</td><td>35.1</td><td>58.0</td><td>33.5</td></tr>
</table>

Contribution to stopping power from other mechanism is included

Our model is totally in best agreement with the experimental data in PRL45 549 (1982), which reason is that our results for the inelastic processes should be the most reliable. (Phys. Plasmas 21, 063711 (2014))

5. Stopping power for proton in Be *plasmas with Te=32eV and 1.77g/cc*

----energy loss and comparison with experiment

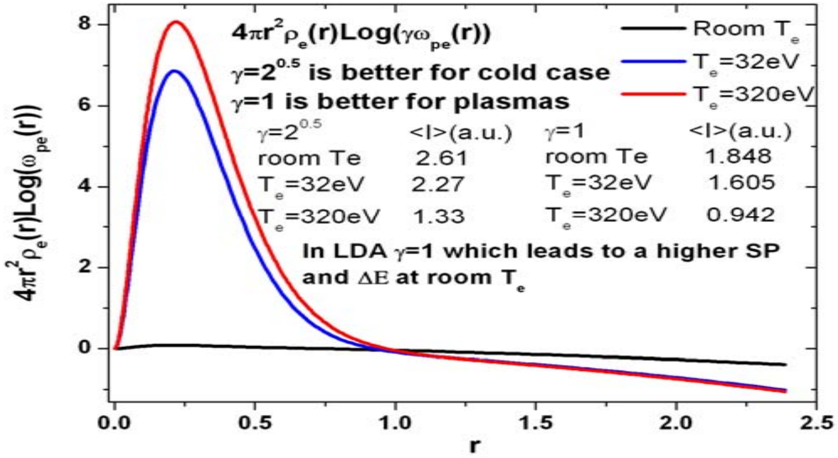
Table I Energy loss ΔE (MeV) for E_p=15MeV, 1.77g/cc and L=532 μm

T_e	Expt	Simulation				
		Our model	LDA		Zimermann	
			Ref.[1]	Ours	Ref.[1]	Ours
Cold	2.71 ~ 2.72	2.71	2.80	2.81		
32eV	2.85 ~ 2.98	2.87	2.85	2.89	2.90	2.94

Three models agree well with the experiment (PRL114, 215002 (2015)).

$$SP_{Bethe} = \frac{4\pi Z_p^2 (Z - \langle Z \rangle)}{V_p^2} Log[\frac{2V_p^2}{\langle I \rangle}]$$

$$Z_{Be} * Log \langle I \rangle = \int 4\pi r^2 \rho_e(r) * Log[\gamma\omega_{pe}(r)]dr$$



Phys. Plasmas 24, 033110 (2017)

5. Stopping power for proton moving in Be *plasmas with Te=32eV and 1.77g/cc*

---Prediction of energy loss from our model and LDA

TABLE II. Initial (E_i) and final (E_f) energies of proton predicted from our model and LDA for $T_e = 32$ eV and $L = 532$ μm.

	E_f (MeV)	
E_i (MeV)	LDA	Ours
8.03	<0	0.176
8.04	0.060	0.268
8.05	0.158	0.354
8.06	0.261	0.434
8.10	0.600	0.700

TABLE III. Similar with Table II for $T_e = 320$ eV and $L = 266$ μm.

	E_f (MeV)	
E_i (MeV)	LDA	Ours
5.15	0.040	0.077
5.20	0.093	0.130
5.25	0.162	0.199

This prediction of energy loss at lower E_p is quite different for our model and LDA model. We hope it will be tested by future experiment since it is related with the view that whether the velocity distribution in dense plasmas is far from the Fermi-Dirac's, which determines the basic property of plasmas.

6. Summary

1. **Based on average atom model and PWB approximation, the inelastic stopping for D^+ in Al plasmas at density $0.02g/cm^3$ and T_e around 10eV is studied in detail with both excitation, ionization and their reverse processes included in *ab initio* way. Comparison with other models is made and their difference is explained. Our model is found in better agreement with the experiment than Bethe equation and Mehlhorn's model.**

2. **Similar calculation for proton in solid Be is made and our result is found in good agreement with the experiment at both cool matter and plasmas .**

3. **Prediction is given to test by future experiment whether the velocity distribution in dense plasmas is far from the Fermi-Dirac's, which is relevant to the basic property of plasmas.**

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Thank you for all your attention !