Importance of ion stopping power research for IFE

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Executive summary

We advocate for a joint experimental and theoretical research effort designed to improve understanding of ion transport and stopping power in inertial confinement fusion (ICF) relevant plasma conditions. Ion transport is important in many areas of ICF, including central hot spot ignition, fast ignition, and heavy ion fusion. Not only is it directly relevant for the energy transfer process between ions and electrons, it also serves as an energy-resolved probe of the response function of these complicated systems. Hence, it informs us indirectly of other transport properties and the equation of state. Theoretical modeling of ion stopping power in high energy density (HED) plasmas is a difficult task and there are only a few experimental data to validate and benchmark models, resulting in large discrepancies between models. This is particularly salient at the Bragg peak regime in extreme states of matter. The new generation of high repetition rate laser facilities offer the potential for high precision experimental measurements of ion stopping power in a variety of HED plasma states, including warm dense matter (WDM). In addition, the new emerging experimental stations with high power laser systems coupled together with free electron lasers (MEC-U, X-FEL) open new possibilities for a more precise characterization of the plasma parameters. This white paper describes the current status and research needs in this field.

Introduction

Ion transport and stopping power is one of the fundamental physical process relevant to many areas of inertial fusion energy science where HED and WDM states are present. In particular, in the study of alpha particle transport in inertial confinement fusion (ICF)[1], proton and ion-driven fast ignition approach to ICF[2], and heavy ion fusion[3]. While a number of experimental studies have been performed on ion stopping power in classical plasmas, the stopping power in extreme states of matter from WDM to HED plasma states has barely been investigated to date (Figure 1).

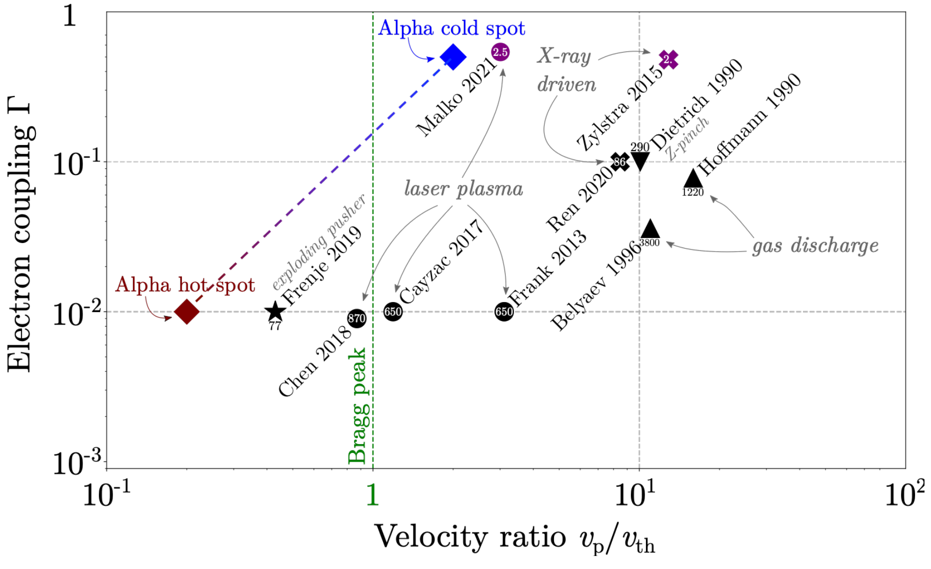

__Figure 1__. Overview of the relevant stopping power experiments[3-12]. Experiments displayed in the parameter space of the velocity ratio v_p/v_{th} of the beam-plasma interaction and the target electron coupling Γ. The electron degeneracy θ is indicated. The dashed line represents the approximate range of v_p/v_{th} and Γ values corresponding to the α-particle trajectory in an igniting ICF experiment, ranging from the cold fuel to the hot spot conditions.

The theoretical description of the ion stopping power in such regimes is difficult due to moderate electron coupling (Γ) and high degeneracy (θ) as well as partial ionization. These conditions typically require first-principles calculations for the most accurate results, but these can be computationally demanding in WDM conditions. And whilst there are computationally cheaper approximate and semi-empirical treatments of stopping powers, the overall scarcity of experimental data for benchmarking the various models in the WDM regime has led to a large theoretical uncertainty in stopping power predictions.[13]

In addition, the Bragg peak region, where the proton velocity v_p is similar to the thermal velocity of the plasma electrons v_{th}, is theoretically even more challenging due to the presence of both moderate electron-ion coupling and dynamic screening. Such strong interaction conditions are typically present in the compressed dense shell in ICF implosion. For example, in typical ICF implosions, the dense DT fuel reaches conditions corresponding to $\Gamma = 0.8$, where alpha particles approach the Bragg peak regime $v_p/v_{th} \approx 1$[14,15]. Disagreement between theoretical models, particularly near the Bragg peak, can lead to large uncertainties in the predicted performance of ICF implosions near the ignition cliff.

In proton-driven fast ignition, where protons must heat compressed matter from very low temperature states to high temperature, the proton stopping power and material state are tightly coupled. The stopping power depends on the material state (density and temperature), which conversely is directly affected by the stopping power through energy deposition. Thus, uncertainties in the stopping power lead directly to uncertainties in the total proton energy and laser energy needed in the ignitor pulse.

We therefore advocate for a joint experimental and theoretical research effort to improve the understanding of ion transport and stopping power in ICF relevant plasma conditions.

Current state of the art

I. Experiments

Figure 1 is a selection of ion stopping experiments in HED plasmas as a function of the plasma coupling parameter, Γ, and the ratio between the ion velocity and the plasma thermal velocity, v_p/v_{th}. Most experimental studies are limited to large projectile velocities, significantly above the thermal velocity of plasma electrons ($v_p >> v_{th}$)[3-9] and ideal ($\Gamma \ll 1$) and nondegenerate ($\Theta \gg 1$) plasmas, validating the perturbative stopping-power models in that range.

Only a few focused (i.e. non-integral) ion stopping experiments have been performed in the HED regime[11], including Warm Dense Matter ($\Gamma \approx 1$)[9,12], relevant to the central hot spot and proton fast ignition schemes. We note that integrated data from ICF implosions has been used to constrain stopping power[16], but not at a single material condition. The focused experiments have used three different platforms for producing the particle source and the plasma to be probed, which reached different regimes:

(i) Monoenergetic ions (1, 3, 3.7, 14.6 MeV) produced through fusion reactions in a D^3He exploding pusher that self-probe the plasma of the exploding pusher itself. The experiment based on this platform provided validation of ion-stopping formalisms in the regime ranging from low-velocity ion stopping (below the Bragg peak) to high-velocity ratio ion stopping ($v_p/v_{th} \approx 0.3$ to 10) in hot dense plasmas ($T_e \sim 1.5$ - 2 keV)[11].

(ii) Monoenergetic protons (14.6 MeV) produced through fusion reactions in an exploding pusher, that probe a WDM sample isochorically heated by X-rays with electron temperature of $T_e \sim$ 30 eV. The experiment based on this platform validated proton stopping power models in WDM at high velocity ratio ($v_p/v_{th} \approx 13$)[9]. In the regime accessed the temperature and degeneracy effects on the stopping power were negligible, but adequately isolated to test differences between WDM and cold stopping models.

(iii) Quasi-monoenergetic proton beams (500 keV) extracted (via magnetic selector) from a Target Normal Sheath acceleration (TNSA) distribution, that probe laser heated WDM achieving $T_e \sim 10$ eV. This experimental approach allowed one to study proton stopping power at significantly lower velocity projectile ratios of ($v_p/v_{th} \approx$ 3-10) in WDM conditions[12]. The results of the experiment showed closest agreement with Density Functional Theory (DFT), such as time-dependent orbital free (TD-OF-DFT)[17,18] and Kohn-Sham DFT (TD-KS-DFT)[19], which showed reduced stopping power compared to time-independent DFT approaches.

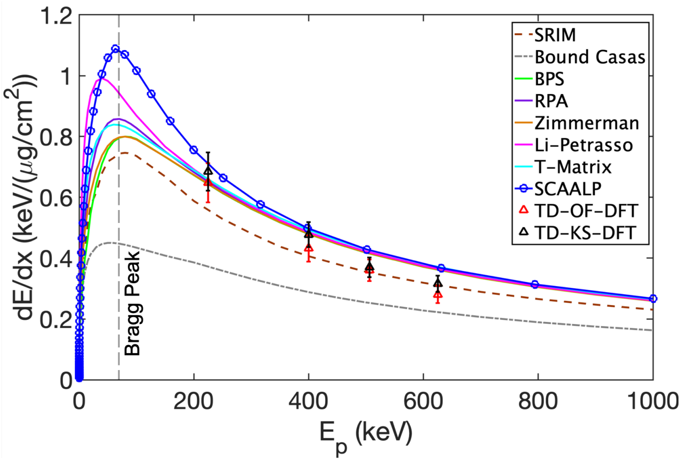

Figure 2. Comparisons of proton stopping power in warm dense carbon of ρ = 0.5 g/cm³ and T_e = 10 eV predicted by different proton stopping power formalisms[17-26]. Figure from[12]

These results are still short of reaching the regime of $v_p/v_{th} = 1$ (Bragg peak), where the largest discrepancies of up to 30-40% between theoretical models are reported (Figure 2) and which ultimately remains an important unexplored parameter domain for understanding partially ionized systems. In order to bridge this gap, one needs to achieve the necessary conditions of v_p and v_{th}, which requires lower proton energies and higher WDM temperatures than have yet been achieved, along with a proton beam duration that is shorter than or comparable to the sample lifetime.

The first two of the above experimental approaches[9,11] are limited to ion energies above 1 MeV as a product of the exploding pusher fusion reaction, and the complexity of reaching needed T_e of WDM to study Bragg peak regime, however it allows much higher temperatures to study hot dense plasmas. The third method[12] is very promising for studying various extreme states of matter from warm dense matter to hot dense plasmas. It can provide a large span of proton energies (100 keV – 2 MeV), allow low WDM temperatures up to 30 eV, and can access the Bragg peak at lower velocity ratio. It also has a potential to achieving higher temperatures of plasma to study other regimes. Simultaneously, this method provides a multi-shot statistical measurement which can provide more precise benchmarking of the models.

II. Theory

Concurrently, further work is needed to improve theoretical models and better understand the sources of differences between them. There are three state-of-the-art methods, for calculating stopping power:

(i) Ad-hoc calculations – A combination of a free-electron and a bound-electron contribution to stopping power. The free-electron term calculated using several models that have the same Bethe-like high-velocity limit determined from dielectric stopping theory [20-24], meanwhile the bound-electron stopping term, calculated using a model by Casas et al,[25] that is valid for all projectile velocities.
(ii) Time-independent DFT – A DFT calculation is performed to obtain the electron density around an ion (or field of ions). This density is used within a stopping power functional, usually the local density approximation. This method is the basis of SCAALP.[26]
(iii) Ab-initio time-dependent DFT[17-19] (KS-DFT, OF-DFT) – A projectile ion explicitly interacts with an electron density. The ion produces a time-dependent potential, which causes the electrons to dynamically screen it and exert a retarding non-adiabatic force on it. Dynamical bound states, including at the onset of non-linear screening are considered. The model is self-contained (independent of other models phenomenological or not), although with a steep computational cost.

While the several models from the first approach provide a good agreement with experimental data in high to low velocity ratio and in classical and HED plasmas with the right fit parameters, the two other approaches are in active development and are a promising way of understanding dynamic WDM systems. However, even among *ab initio* KS-DFT[19] approaches, there are potentially many sources of systematic discrepancies between methods and codes (e.g., pseudization and countless other implementation details). More broadly, OF-DFT[17,18] methods cut down on computational costs by avoiding a formulation that explicitly represents each of the many thermally-populated orbitals, relying instead on approximate expressions for the kinetic energy functional. The success of these models depends heavily on the accuracy of these density-dependent kinetic energy functionals, although much progress has been made in the WDM regime[10,11,12]. From another side, the developments in DFT will prepare the way for the exascale computing age, when large DFT calculations will become the norm for calculating HED properties as we attempt to bridge the gap between the atomic scale and mesoscale.

Additionally, theoretical models that make various approximations to generate tractable expressions for the stopping power, like the dielectric formulation[20-24], are important because they are computationally cheap. These approximate models must be benchmarked against the *ab initio* methods to determine the validity of the approximations used. As illustrated in Figure 2, more work is required to improve the agreement between these simpler models and the *ab initio* approaches. We note that developers and practitioners of four distinct first-principles approaches are co-authors on this white paper, indicative of the breadth and maturity of this field.

Research needs

The principal scientific questions can be summarised as:

- How well do we understand ion stopping in extreme states of matter relevant to ICF, such as hot dense plasma and WDM?
- Are current models, adequate to describe such physical processes to the fidelity required for predictive modeling of ICF targets?
- If not, how can the models be improved and experimentally validated?

Key elements of an integrated experimental and theoretical program to address these questions should include:

(i) To develop a platform for precise measurements at near-Bragg-peak conditions over a range of HED plasma conditions using the new generation of high repetition rate multi-beam high repetition rate (HRR) laser facilities coming online available through LaserNetUS (e.g.., MEC-U, Texas PW upgrade, CSU, etc.). The main experimental challenge is to generate a well-defined proton beam with short pulse duration and homogenous HED plasma conditions with simultaneous characterization of these conditions and measure proton beam energy loss in plasma with high precision to distinguish difference between theoretical models. In particular this includes:

- Proton source: development of monoenenergetic (dE/E~ 1%) short time (< 100 ps) spread proton bunches from laser-driven TNSA by improving existing proton energy selection platforms[27] and/or designing proton beam time-compressor systems.
- Plasma generation: Isochoric and homogenous heating of target samples by proton heating[28], x-ray heating, laser heating.
- Full plasma characterization: measuring plasma temperature and density (X-ray Thomson Scattering, XUV spectroscopy, Streak Optical Pyrometry) as well as ionization state (x-ray absorption spectroscopy via betatron probing).
- Diagnostic development: developing high resolution proton energy spectrometers (< 2 keV), methods to measure proton pulse duration, methods to mitigate proton beam scattering after passing through probed plasma by proton focusing systems.
- HRR operation: developing tools for performing experiments at HRR (up to 1 Hz), including HRR targetry, HRR data acquisition and data processing toolbox.

(ii) To test and progress on development of theoretical models:

- Test models against experimental data in a wide range of HED and WDM plasma conditions and velocity ratios.
- Conduct a detailed comparison among the first-principles stopping power codes for an exemplary range of conditions in order to identify and potentially eliminate sources of discrepancies.
- Study the sensitivity to ion stopping power models in integrated ICF simulations of the various schemes (Central Hot Spot, Fast Ignition, Heavy Ion Beam, etc.).
- Development of a global alpha-particle stopping power model, validated against TD-DFT calculations and benchmarked with precision experiments, for accurate IFE target designs.
- Improve the accuracy of approximate stopping power models in order to increase agreement with TD-DFT calculations. These models can be used in place of the more accurate calculations when the latter become computationally intractable, for instance for target systems with high temperatures ($T_e > 20$ eV) or projectiles with large velocities ($v_p > 10$ atomic units).
- Develop and validate stopping power functionals.
- Connect results to other transport properties.

References:

1. Nuckolls, J. *et al., Nature* **239,** 139–142 (1972).
2. Roth, M. *et al.*, *Phys. Rev. Lett.* **86**, 436–439 (2001).
3. Hoffmann, H.H. *et al.*, *Phys. Rev. A* **42** (1990).
4. Belyaev, G. *et al.*, *Phys. Rev. E* **53**, 2701 (1996).
5. Dietrich, K.-G. *et al.*, *Z. Phys. D Atoms Molec. Clust.* **16,** 229–230 (1990).
6. Frank, A. *et al.*, *Phys. Rev. Lett.* **110**, 115001 (2013).
7. Chen, S. N. *et al.*, *Sci. Rep.* **8**, 14586 (2018).
8. Ren, J. *et al.*, *Nat. Commun.***11**, 5157 (2020).
9. Zylstra, A. *et al.*, *Phys. Rev. Lett.* **114** (2015).
10. Cayzac, W. *et al.*, *Nat. Commun.* **8**, 15693 (2017).
11. Frenje, J. A. *et al.*, *Phys. Rev. Lett*. **122**, 015002 (2019).
12. Malko, S. PREPRINT (Version 1) *available at Research Square [https://doi.org/10.21203/rs.3.rs-880993/v1].*
13. Grabowski, P. E. *et al.*, *High Energy Density Phys.* **37**, 100905 (2020).
14. Hurricane, O. *et al.*, *Phys. Plasmas* **26**, 052704 (2019).
15. Zylstra, A. *et al.*, *Phys. Plasmas* **26**, 800–806 (2019).
16. Hayes, A.C., *et al., Nat. Phys.* **16,** 432–437 (2020).
17. White, A. J. *et al.*, *Phys. Rev. B* **98**, 144302 (2018).
18. Ding, Y. H. *et al.*, *Phys. Rev. Lett.* **121**, 145001 (2018).
19. White, A. J. & Collins, L. A, *Phys. Rev. Lett.* **125,** 055002 (2020).
20. Zylstra, A. *et al.*, *Phys. Plasmas* **16**, 122703 (2019).
21. Brown, L. S., Preston, D. L. & Singleton, R. L., Jr., *Phys. Rep.* **410**, 237–333 (2005).
22. Zimmerman, G. LLNL, *Report No. UCRL-JC-105616.* (1990).
23. Gericke, D. O. & Schlanges, *Phys. Rev. E* **60**, 904–910 (1999).
24. Gericke, D. O. *et al.*, *Phys. Rev. E* **65**, 036406 (2002).
25. Casas, D. *et al.*, *Phys. Rev. E* **88**, 033102 (2013).
26. Faussurier, G. *et al.*, *Phys. Plasmas* **17**, 052707 (2010).
27. Apinaniz, J. *et al.*, *Sci. Rep.* **11**,6881 (2021).
28. Patel, P. *et al.*, *Phys. Rev. Lett.* **91**, 125004 (2003).