White Paper for *Frontiers of Plasma Science Panel*

Date of Submission:	***6/19/2015***

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Title:	Structural Dynamics of the Ions: a New Window to Investigate High-Energy-Density Matter
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- ***Describe the research frontier*** **and importance of the scientific challenge.**

- ***Describe the approach to advancing the frontier and indicate if new research tools or capabilities are required.***

- ***Describe the impact of this research on plasma science and related disciplines and any potential for societal benefit***.

Structural Dynamics of the Ions: a New Window to Investigate High-Energy-Density Matter

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1 Background on High-Energy-Density Matter

High-energy-density matter, and particular warm dense matter with temperatures in the range of 0.1-10 eV and densities comparable with solids, are a very challenging research subject as such matter combines strong interactions of the particles with a distinct quantum behaviour including bound states and degeneracy. One crucial point for reduced modelling is the effective ion-ion potential which is often strongly modified from the screened Coulomb potential applicable for ideal plasmas. As this potential is determined by the charge state, electron screening as well as the interaction of bound and free electrons in this parameter region, it can be seen as a summary of the complex interaction in the matter under investigation.

Experimental investigations of dense matter cannot rely on usual plasma physics techniques as well as the high density makes the matter opaque in the visible and beyond. Moreover, the remaining atomic structure can change absorption considerably and only transient states can be created in the laboratory. Most existing techniques thus focus on the macroscopic behaviour like the equation of state or absorption. Over the last decade, x-ray Thomson scattering has been developed as a suitable technique to investigate the micro-physics in warm dense matter. The x-rays can penetrate dense matter and couple to the electron structure in the matter probed. As part of the electron density follows the ion motion, the ionic structure can be observed as well.

2 Limitations of the Current X-ray Scattering Experiments

X-ray Thomson scattering has been successfully applied to determine the basic plasma properties in a large number of experiments [1]. It employs the direct connection between the scattering intensity and the electron structure [2]

$$P(\theta,\omega) \sim S_{ee}^{tot}(k,\omega) = \Big|f(k)+q(k)\Big|^2 S_{ii}(k,\omega) + W_e^{\text{ineleastic}}\,,$$

where the second part contains the inelastic scattering due to free electrons and bound-free transitions driven by the x-rays. The first term is of interest when considering the ion motion as it is related to the ion-ion structure factor. The prefactors are the atomic/ionic form factor of bound electrons and the Fourier components of the screening cloud.

The largest uncertainty in the description above stems from the ion-ion structure factor. If the experiment is sufficiently restricted or combines x-ray scattering with other diagnostics (such as VISAR), the data may also yield information on the form of the ion structure factor S_{ii}. However, x-ray sources from laser-driven plasmas and most detectors cannot resolve the dynamics in the structor factor (order of fractions of eV even for lighter elements). As a result, the dynamic structure factor can be replaced by the static one: $S_{ii}(k,\omega) = S_{ii}(k)\,\delta(\omega)$.

Of course, the static ion-ion structure factor reflects the spatial arrangement in the sample and, thus, contains already much information about the effective ion-ion potential. Theoretical models applying different potentials yield often very significant differences in the ionic structure that can be clearly distinct in experimental data or *ab initio* simulations. For example, a strong repulsion at short distances has first be suggested to when comparing to DFT-MD simulations [3] and then also found to be necessary to describe experimental data [4, 5].

Are static structure factors in principle sufficient to fully determine the effective ion-ion potential? Unfortunately, the answer is 'no'. X-ray diffraction data are not sufficiently complete to define the interaction potential between the ions. Specific features can be identified but the general for of the potential cannot be deconvoluted from data of static structure factors. Indeed, mapping simple models (like OCP) to complicated data by matching the static structure is often used. The problem is even more complicated by the fact the experimental data are mostly only available for the limited range of wave numbers. Accordingly, different effects may result in the same features. For instance, the extra short-range repulsion strongly increase the effective interaction in dense matter and, thus, the ion-ion structure factor has more pronounced peaks. The same effect can be created by reducing the screening from the electrons. Although these model represent very different physics, they might not be distinguished from one another in an experiment giving only static structure factors for finite wavelengths.

3 Experimental Needs to Determining the Dynamic Ion-Ion Structure

Experiments would employ a pump-probe scheme. Ultimately, both should be done by the intense beam of an x-ray laser to yield homogeneously heated targets and well-characterised probe. First experiments will use optical lasers to create the required target conditions. Heating by fast electrons created from ultra-intense, short-pulse lasers or shock-compression by a long-pulse (ns) laser with more energy are viable options.

When measuring the structural ion dynamics, all main features must be resolved. The most prominent are the ion acoustic peaks (equivalent to phonons in solids or plasmons for the electrons). These peaks are roughly 0.1–1 eV separated from the central diffusive peak [6] (of course, separation depends on the wavenumber and conditions). This small separation puts stringent requirements on the band widths of the probe radiation and such measurements were elusive with laser-driven sources. However, the availability of fourth generation light sources with their unprecedented ultra-high brilliance and coherence has now completely changed the situation and made measurements of the ionic response in WDM nowadays feasible. Indeed, the seeded version of the LCLS x-ray beam and a monochromator yields the required resolution and is available for users.

Coupled to the x-ray probe beam, an optical laser with sufficient energy and time structure is required to create the target. Hydrodynamics simulations show that two laser beams with 5 J of energy per beam focused to a 50 μm spot can be compressed an aluminium sample up to 10 gcm^{-3} with a temperature of roughly 10 eV. Of course, such tight focus results in inhomogenities that needs to be addressed. More energy available would allow larger foci and, thus, less gradients in the system. Larger drivers would also allow for greater compression and stronger heating to be investigated.

The combination of two well-timed energetic beams is crucial for these experiments. While the first beam needs to create a very homogeneous region of high-energy-density matter, the second needs to be sufficient to resolve the low-frequency oscillations of the ions. Thus, high energy content and a large penetration depth are requirements for the drive laser and high photon numbers in the x-ray regime together with very low bandwidth is needed for the probe. Of course, the standard diagnostics like VISAR or x-ray diffractions would be beneficial to determine the plasma conditions probed.

4 Theoretical Approaches for the Dynamic Ion-Ion Structure Factor

As the dynamic ion structure is extremely rich in information about the system, a large body of modelling work has be performed. Most older theories and simulations focus on model systems with a given ion-ion potential: typically, the one component system (pure Coulomb interactions) or Yukawa systems (linearly screened Coulomb potential) were studied with classical MD simulations [7]. Alongside hydrodynamics was employed to link the structure factor to macroscopic variables like the sound speed, diffusion coefficient etc. Naturally, these approaches have a limited predictive power as they either fixed already the form of an unknown potential or contain free parameters.

Recently, *ab initio* simulations have been applied to make more realistic predictions without free parameters. Firstly, DFT-MD simulations were used to obtain effective ion-ion potentials and these were then applied in classical MD simulations [8]. In this way, the quantum effects could be fully included and the simulations could be run for a large system. Increase rigour was implemented when orbital-free DFT calculations were directly coupled with MD [9]. This scheme removed the need to extract potentials from the quantum simulations but is restricted to systems with relatively easy electron structure. Most recently full DFT-MD simulations using the Kohn-Sham scheme were performed to extract also dynamic structure factors [10]. These data can be considered as the best standard of modern simulations but are numerically very expensive.

Comparing results of the models and simulations above with experimental data for the dynamic structure factor would bring a large step forward in our understanding of dense strongly coupled matter and the way we describe it. While some common features have been seen in many approaches, there are distinct differences, especially for the strength of the central peak describing diffusive modes in the system. Indeed, the relative hight of the ion acoustic modes and the diffusive mode can be used to discriminate between models.

5 Summary

Measurement of the low-frequency ion dynamics in dense, strongly heated matter will be a new tool that can open many new perspectives on the physics of this interesting state. Indeed, the information contained in the dynamic ion structure factor is so rich that it will open a new window for observations of the complex interplay of bound state structure, strong interactions and quantum degeneracy in dense matter. The resulting deeper understanding of dense matter will then allow for more precise modelling for diverse scientific and technical application such as planetary evolutions, inertial confinement fusion and laser-based material processing.

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