White Paper for *Frontiers of Plasma Science Panel*

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Title:	Fully exploiting x-ray scattering experiments on warm dense matter
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(Limit text to 3-pages including this form. Font Times Roman size 11.
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Fully exploiting x-ray scattering experiments on warm dense matter

C. Starrett, J. Daligault and D. Saumon

- ***Describe the research frontier* and importance of the scientific challenge.**

Warm dense matter lies at the intersection of solid, gas, liquid and plasma physics, where ions and electrons strongly interact with themselves and each other. As such it is sometimes called the inner frontier of materials research. It is an important aspect of many open problems in inertial confinement fusion as well as stellar and planetary science [1].

In the last decade, many X-ray scattering experiments on warm dense matter (WDM) have been performed and published in high profile journals [2,3]. These challenging experiments have established the value of this technique to diagnose properties of the plasma (electron temperature, electron density, observation of plasmons) [4]. The recent combination of XFEL light sources with platforms to create WDM states is opening a new realm of experimental diagnostics of the microphysics of WDM plasmas with X-ray scattering, such as the time-resolved evolution of the ionic structure of a cooling WDM plasma of Al [2]. X-ray scattering arises from a host of atomic-scale and collective phenomena and, in principle, these new experimental capabilities and those foreseen in the next 5-10 years can probe the number and energies of bound states, continuum resonances, the response of a correlated, partially degenerate electron fluid (beyond the RPA), plasmons, ion acoustic waves, electron screening in strongly non-linear regimes, ion-ion correlations and pressure ionization. Despite steady advances in modeling capability [5-7], current models of WDM can show significant disagreements in their predictions of these quantities. Experiments on these new platforms will be extremely valuable in guiding the development of better theory and models of WDM.

In addition, a theory of X-ray scattering is necessary to link models of WDM with experiments. The current and widely used paradigm for calculating the X-ray scattering cross sections of warm dense matter in thermodynamic equilibrium is known as the "Chihara formula" [8]. This formalism was developed for simple plasmas and is based on a clear separation between bound and valence electrons. In practice, the Chihara formula has so far proven to be adequate to model most of the X-ray scattering data. However, the key assumption of separability is not valid under conditions of pressure ionization. Furthermore, the Chihara formula is unable to handle plasmas where chemical bond may form. This situation is thought to occur in carbon and CH plasmas at solid density and a few eV temperature such as in the initial phases of the implosion of inertial confinement capsules. Thus, progress in understating WDM relies not only on conducting better experiments and developing better models of the dense plasmas, but also on a reliable theory of X-ray scattering by warm dense plasmas. Ideally, the warm dense plasma and the X-ray scattering theory should be developed consistently at the same level of physical approximation.

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

For the analysis of experiments on plasmas in thermodynamic equilibrium, a more direct approach to calculating the X-ray spectra is needed. Some progress has been made by adapting real-space Green's functions methods from solid state physics [10]. However, the underlying model has not been developed

for warm dense matter and lacks some important physics such as a disordered ionic structure. Further development along these lines could prove very fruitful.

Perhaps the most sophisticated and widely used simulation tool for warm dense matter is known as density functional theory molecular dynamics (DFT-MD). While computationally expensive, this method uses few assumptions and approximations. The direct calculation of X-ray scattering cross-sections with this method has not yet been realized, though contact with experiment through the Chihara formula has been made [6].

So-called average atom models of WDM have been used successfully to calculate the X-ray scattering spectra using the Chihara formula [9, 11]. These models are more approximate than DFT-MD methods but due to their computational economy, they are widely used for generating tables of physical data (e.g. equation of state) that are necessary for fluid dynamics simulations. However, even these more approximate models include physics that is not captured by the Chihara formula and a more direct approach is needed to fully explore the limitations of these models.

For experiments probing non-equilibrium warm dense matter the situation is even more uncertain as the underlying models are much less developed. Promising avenues include the development simulation tools in which the classical ions and quantum electrons are both treated dynamically. For example, one such method is time-dependent density functional theory; an approach still in its infancy.

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

Direct comparisons of WDM models and simulation tools to experiments would directly test the validity of the models at the micro-physical level and guide further theoretical developments in the field. These comparisons would also enable the models to better guide experimental design. The synergy of modeling and experiments would lead to improved understanding of numerous physical phenomena including inertial confinement fusion, white dwarf physics and planetary science. Given the level of experimental effort on X-ray scattering in warm dense matter, it is remarkable that such a focused theoretical program has not yet been undertaken. Such an effort is necessary to reap the full benefits of the recent advances in experimental X-ray scattering techniques and those that will be enabled by XFEL platforms.

References (Maximum 1 page)

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Figures (maximum 1 page)