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Frontiers and Challenges in Warm Dense Matter

Springer

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Cover illustration: Snapshot of a DFT-MD simulations box with a hydrogen-helium mixture at warm dense matter conditions (4000 K, 1 Mbar). Red: protons, blue: helium nuclei, grey: electron density. (Author: Winfried Lorenzen; for details, see Lorenzen, Becker and Redmer, Chapter 8 of this book)

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Introduction

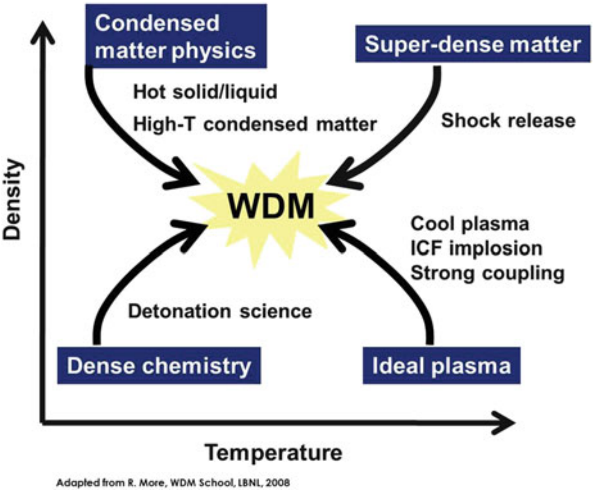
In Spring 2012, the Institute for Pure and Applied Mathematics (IPAM) of the University of California, Los Angeles, sponsored a Long Program devoted to the computational and theoretical challenges in high energy density physics. A major component was a series of workshops, one of which focused on the exciting field of warm dense matter (WDM). WDM was described in the 2009 Fusion Energy Sciences Advisory Committee's report [1] and the Basic Research Needs for High Energy Density Laboratory Physics report [2] as an extreme state of matter characterized as intermediate "…between condensed matter (solids and liquids), gases, and ideal plasmas. It exists in the lower-temperature portion of the high energy density regime, under conditions where the assumptions of both condensed-matter theory and ideal-plasma theory break down, and where quantum mechanics, particle correlations, and electric forces are all important".

Typically WDM conditions span the eV range ($1\,\mathrm{eV} = 1.16 \times 10^4\,\mathrm{K}$) with densities typical of solids up to very high compressions. For both theoretical methods and for their computational implementation, such magnitudes and large ranges pose immense but fascinating challenges. This volume is devoted to expositions of approaches to those WDM challenges from experts who attended the IPAM workshop. Each chapter is meant to review a specific topic. Hence the chapters are extended and provide plenty of references for the interested reader. We, the editors, feel this volume captures the breadth and depth, along with the excitement of WDM physics.

What makes WDM such an exciting topic is its unique position in density-temperature space. WDM is a meeting point of several distinct physical regimes. Figure 1 (adapted from lectures on WDM given by Richard More at Lawrence Berkeley Laboratory) schematically demonstrates the WDM challenge.

As the meeting point of dense chemistry, condensed matter physics, super-dense matter, and ideal plasmas, WDM exposes severe problems for attempts at straightforward extension of well-developed models. For example, the kinetic equations for ideal plasmas rely on the fact that the number density times the Debye length cubed is a large number. This statement is equivalent to stating that all particle correlations are weak. This is the basis of the kinetic theory description of plasmas

Fig. 1 Warm dense matter is at the confluence of several areas of high energy density physics



Adapted from R. More, WDM School, LBNL, 2008

expressed in the Vlasov, Fokker-Planck, and Lenard-Balescu equations. For WDM, this approximation breaks down since particle correlations tend to be large and the number density times the cube of the Debye length is not large. Conversely, the approaches of condensed matter physics, specifically the so-called electronic-structure methods and ab initio molecular dynamics, are well-developed for systems in which the electrons can be treated as being at zero-temperature, but not for WDM temperatures. Those methods also have computational costs which scale unfavorably with both temperature and number of electrons.

The FESAC report identified four WDM issues, relevant for this workshop, for which theoretical, computational, and experimental opportunities would exist in the next 10 years. The methodological and computational implications are numerous. The list, with our commentary, is

1. Phase transitions in WDM: Developing advanced theoretical methods and precision experimental techniques that produce validation quality data is sorely needed. Specifically, the challenges include melting, liquid-liquid phase transitions, plasma phase transitions, the location of the liquid-vapor critical point, and the metal-insulator transition.
2. A comprehensive theory connecting WDM regimes: Developing advanced theoretical and computational tools for WDM is key. In addition, the theoretical methods should provide for connectivity between models. Theoretical and computational methods such as density functional theory (DFT) require further developments in the area of orbital-free DFT, advanced exchange-correlation functionals that include temperature effects consistently. In addition, DFT research in going beyond the Born-Oppenheimer approximation and also the inclusion of magnetic fields is needed. Particle simulations methods based on molecular dynamics coupled to quantum hydrodynamics are offering interesting inroads to a comprehensive theory of WDM.

3. Equations of state (EOS) and their dependence on formation history: Validation data for equations of state requires reliance on experimental techniques for accurate measurements in the WDM regime. In addition, a deep question is whether or not WDM is satisfactorily described by a set of state variables, independent of its formation history. The computation of EOS without decomposition of ionic and electronic contributions is a high priority. Another is reliable computation of the EOS of mixtures. In addition, the validity of equilibrium phase diagrams for WDM needs to be explored more satisfactorily, along with the issue of whether two-temperature equations of state are needed (and, if so, what is their physical basis). Finally, our knowledge of EOS in the WDM regime is impacted directly by experiments and theoretical/computational tools that can provide insights into chemistry at high density. Clear understanding of chemical bonds at high density is particularly needed.
4. Transport properties of WDM: Application of current computational and theoretical tools to the calculation of transport coefficients in WDM is key. Improvement also is needed. The coefficients include viscosity, diffusivity, and electric, ionic, and thermal conductivities. Key data to guide theoretical approaches continues to come from experiments conducted at small and large facilities worldwide.

This volume focuses on the theoretical and computational research progress in the four areas described above. Each of the chapters presents an in-depth review of various theoretical and computational approaches currently being developed and applied to problems in WDM physics. Numerous application areas in the WDM regime also are treated.

This volume does not deal with the wide variety of experimental capabilities that exist worldwide for studying WDM. The spectrum of techniques and instruments ranges from small scale, “table-top” to very large multi-billion dollar facilities. Data from them appear throughout this volume. For context therefore, we close with a cursory summary. There are small-scale facilities world-wide that include well-controlled, intense, short-pulse laser sources. Small scale pulsed-power facilities allow the WDM regime to be reached readily. Large pulsed-power facilities, such as the Z machine at Sandia National Laboratory, can provide ramp loading of materials up to 5 Mbar and shock loading up to 40 Mbar, in experimental configurations that permit long time scales and large sample sizes. The Z machine can address EOS and optical properties of elements and mixtures in WDM, strength, shock and release to WDM states, phase boundaries and X-ray scattering studies of WDM. The Linac Coherent Light source (LCLS) at Stanford University probes WDM states in a controllable manner. It employs a rapid heating source that creates WDM conditions and measures it prior to disassembler. LCLS can address dynamic structure factors with spatially resolved elastic Bragg and spectrally resolved Thomson scattering. Inertial confinement fusion facilities, such as Omega at the University of Rochester and the National Ignition Facility (NIF) at Lawrence Livermore National Laboratory, open new areas of high energy density science. NIF in particular can probe matter in the hundreds of Mbar to Gbar pressure regime. These facilities can address high pressure strength and EOS and the transition from

WDM to hot dense matter. Important large scale facilities also exist outside of the United States. The European X-ray free electron laser being built in Germany and the GSI Helmholtz Centre for Heavy Ion Research are examples. An expansion of GSI is now underway, namely, the Facility for Antiproton and Ion Research (FAIR), which is an international accelerator facility under construction which will use antiprotons and ions to perform research in high density plasma physics. Besides Germany, France has invested heavily in WDM experimental facilities. This includes the Laser Mégajoule(LMJ)/PETAL program and LULI (Laboratoire d'Utilisation des Lasers Intenses). Like NIF, LMJ intends to use the "indirect drive" approach. Rutherford Laboratory in the United Kingdom and various laboratories in Russia and China also have significant experimental facilities devoted to obtaining data in the WDM regime.

The editors thank the authors of the chapters for making this volume possible. We are grateful to the staff and leadership of IPAM for supporting dialogue about research which engages mathematics and physical science. The Long Program on Computational Challenges in High Energy Density Plasmas was of immense benefit to all of us, as well as being extremely well-organized and under-girded operationally.

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