**Workshop Schedule**

*All talks will be in the Österreich-UngarnRoom*

### Monday, September 29th

<table>
<thead>
<tr>
<th>Time</th>
<th>Event</th>
</tr>
</thead>
<tbody>
<tr>
<td>7:45-8:30</td>
<td>Registration</td>
</tr>
<tr>
<td>8:20</td>
<td>Welcome</td>
</tr>
</tbody>
</table>

**Session 1: ICF**

<table>
<thead>
<tr>
<th>Time</th>
<th>Speaker</th>
<th>Title</th>
</tr>
</thead>
<tbody>
<tr>
<td>8:30</td>
<td>T. Ma</td>
<td>Alpha Heating in ICF Implosions on the National Ignition Facility</td>
</tr>
<tr>
<td>9:00</td>
<td>S. Hansen</td>
<td>Analysis of Magnetized Liner Inertial Fusion (MagLIF) experiments on Z</td>
</tr>
<tr>
<td>9:30</td>
<td>H. Nishimura</td>
<td>Quantitative Kα line spectroscopy for energy transport in fast ignition plasma driven with LFEX PW laser</td>
</tr>
<tr>
<td>10:00</td>
<td>S. Le Pape</td>
<td>Optimizing Near-vacuum NIF hohlraum drives for ICF</td>
</tr>
</tbody>
</table>

**Coffee break**

**Session 2: ICF II and Astrophysical Related**

<table>
<thead>
<tr>
<th>Time</th>
<th>Speaker</th>
<th>Title</th>
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<tbody>
<tr>
<td>10:50</td>
<td>P. Patel</td>
<td>Measurements of hot spot conditions and mix in DT implosions on the NIF</td>
</tr>
<tr>
<td>11:20</td>
<td>S. Turck-Chiëze</td>
<td>Different Opacity Activities Dedicated to Astrophysical Objects</td>
</tr>
<tr>
<td>11:50</td>
<td>J. Colgan</td>
<td>Light element opacities from ATOMIC</td>
</tr>
<tr>
<td>12:20</td>
<td>C.J. Fontes</td>
<td>Relativistic Opacities for Astrophysical Applications</td>
</tr>
</tbody>
</table>

**Lunch break**

**Session 3: Opacity I – Theory**

<table>
<thead>
<tr>
<th>Time</th>
<th>Speaker</th>
<th>Title</th>
</tr>
</thead>
<tbody>
<tr>
<td>14:30</td>
<td>D. Gilles</td>
<td>Opacity calculation with the code HULLAC-v9</td>
</tr>
<tr>
<td>15:00</td>
<td>B. Wilson</td>
<td>New Developments for VISTA: the LLNL super-transition array opacity code</td>
</tr>
<tr>
<td>15:30</td>
<td>Y. Frank</td>
<td>Developments of the SEMILLAC NLTE atomic code</td>
</tr>
<tr>
<td>16:00</td>
<td>J.-C. Pain</td>
<td>Accounting for satellite lines due to high-n spectators in detailed opacity calculations</td>
</tr>
</tbody>
</table>

**Coffee break**

**Session 4: Opacity II – Experiment & Population Kinetics I**

<table>
<thead>
<tr>
<th>Time</th>
<th>Speaker</th>
<th>Title</th>
</tr>
</thead>
<tbody>
<tr>
<td>16:50</td>
<td>M. Dozières</td>
<td>X and XUV opacity measurements in dense plasmas</td>
</tr>
<tr>
<td>17:50</td>
<td>T. Nagayama</td>
<td>Investigations for systematic uncertainties in the Fe opacity measurements at solar interior conditions</td>
</tr>
<tr>
<td>18:20</td>
<td>A.V. Demura</td>
<td>Statistical Approach to Radiation-Collisional Processes with Heavy Atoms in Plasmas</td>
</tr>
</tbody>
</table>

**19:00**  *Reception in the Kaiserlounge*

### Tuesday, September 30th

**Session 5: Population Kinetics II**

<table>
<thead>
<tr>
<th>Time</th>
<th>Speaker</th>
<th>Title</th>
</tr>
</thead>
<tbody>
<tr>
<td>8:30</td>
<td>H.-K. Chung</td>
<td>Comparison and analysis of collisional-radiative models at the NLTE-8 workshop</td>
</tr>
<tr>
<td>9:00</td>
<td>A.J.B Cerdan</td>
<td>Collisional Radiative Average Atom Code Based on a Relativistic Screened Hydrogenic Mode</td>
</tr>
<tr>
<td>9:30</td>
<td>C. Gao</td>
<td>Radiation transfer of ultra-intense x-ray laser pulses through solid aluminium</td>
</tr>
<tr>
<td>10:00</td>
<td>A. Sasaki</td>
<td>Study of nLTE kinetic model of high-Z ions for laser plasma produced (LPP) EUV sources to fusion plasma</td>
</tr>
</tbody>
</table>

**Coffee break**

**Session 6: Population Kinetics, Radiation Transport, Line Shapes**

<table>
<thead>
<tr>
<th>Time</th>
<th>Speaker</th>
<th>Title</th>
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</thead>
<tbody>
<tr>
<td>10:50</td>
<td>D.A. Kim</td>
<td>NLTE radiation transport and level kinetics modeling in-line with plasma gasdynamics</td>
</tr>
<tr>
<td>11:20</td>
<td>M. Patel</td>
<td>Radiation hydrodynamics with in-line NLTE atomic kinetics applied to ICF plasmas</td>
</tr>
<tr>
<td>11:50</td>
<td>R. London</td>
<td>Radiation transfer effects in short-pulse heated targets</td>
</tr>
<tr>
<td>12:20</td>
<td>S. Alexiou</td>
<td>Developments in the Frequency Separation Technique for Spectral Line shape Calculations</td>
</tr>
<tr>
<td>12:50</td>
<td>S. Ferri</td>
<td>Review of the 2nd Spectral Line Shapes in Plasmas Code Comparison Workshop</td>
</tr>
</tbody>
</table>

**13:20**  *Lunch break*

**Session 7: Posters in the Kaiserlounge**

**14:30 to 18:00**

**Atomic Physics**

1. Y. Aglitskiy  KrF Nike Laser as a Powerful Platform for Experimental X-Ray Spectroscopy of High-Z Ions
2. T. Blenski    Studies on frequency-dependent linear response of atoms in plasma
3. M. Busquet    Dense Plasma effect and average atom model
4. Y. Kurzweil   The effect of ion-ion correlation on the atomic energy levels and absorption of radiation in dense plasmas
5. M. Polasik    The K X-Ray Line Structures of the 3d-Transition Metals in Warm Dense Plasma
7. L. Syrocki     Modeling of the K and L X-Ray Line Structures for Molybdenum Ions in Warm Dense Plasma
**Session 8: Plasma Spectroscopy and Simulations I**

8:30 A.K. Rossall  
Generation of Warm Dense Matter using an Argon based Capillary Discharge Laser

9:00 M. Smid  
Analysis of Cu K-shell spectra emitted from partially ionized non-equilibrium plasma

9:30 B. Loupias  
Theoretical and experimental studies of electronic heating of tamped targets with UHI lasers

10:00 E. Marley  
T_e measurement of mixed Z buried layer targets using time-resolved and -integrated K-shell spectroscopy

10:30 Coffee break

**Session 9: Plasma Spectroscopy and Simulations II**

10:50 J.F. Seely  
Energetic Electrons Driven in the Polarization Direction of an Intense Laser Beam Incident on a Solid

11:20 D. Hoarty  
Spectroscopic properties of high energy density plasma and Comparisons to Atomic Kinetics Models

11:50 Y. Ralchenko  
Analysis of X-Ray Nike Spectra from Highly-Charged High-Z Ions

12:20 R. Srivastava  
Modeling of plasma through reliable electron-impact cross-sections

10:30 Coffee Break

**Session 10: Density Effects and Ionization Potential Depression I**

08:30 C.A. Iglesias  
A plea for a reexamination of ionization potential depression measurements

09:00 S.-K. Son  
Quantum-mechanical calculation of ionization potential lowering in dense plasmas

09:30 D. Gericke  
Ionisation energies in strongly driven matter

10:00 A. Calisti  
Statistical properties of coupled plasmas employing classical two component plasma MD simulations

10:30 Coffee Break
<table>
<thead>
<tr>
<th>Time</th>
<th>Session</th>
<th>Speaker(s)</th>
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<tbody>
<tr>
<td>10:50</td>
<td>Session 11: Density Effects and Ionization</td>
<td>S. Vinko</td>
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<tr>
<td></td>
<td>Potential Depression II</td>
<td>O. Ciricosta</td>
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<td></td>
<td>N. Argaman</td>
</tr>
<tr>
<td>12:20</td>
<td>Lunch Break</td>
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<tr>
<td>10:50</td>
<td>Session 12: FEL Experiments and Theory I</td>
<td>B. Ziaja-Motyka</td>
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<td>C. Caleman</td>
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<td>M. Bussman</td>
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<td>D.S. Rackstraw</td>
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<tr>
<td>16:00</td>
<td>Coffee break</td>
<td></td>
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<tr>
<td>16:15</td>
<td>Session 13: FEL Experiment and Theory II</td>
<td>B. Deshaud</td>
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<td></td>
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<td>Y. Li</td>
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<td>E. Galtier</td>
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<td></td>
<td>T. Timneanu</td>
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<tr>
<td>18:15</td>
<td>Bus to Banquet Dinner at the Heurigen Wolff</td>
<td></td>
</tr>
<tr>
<td>08:30</td>
<td>Session 14: FEL Experiments and Theory III</td>
<td>M. Nakatsutsumi</td>
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<tr>
<td></td>
<td></td>
<td>G.O. Williams</td>
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<tr>
<td></td>
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<td>U. Zastrau</td>
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<td></td>
<td></td>
<td>F. Wang</td>
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<tr>
<td>10:30</td>
<td>Coffee break</td>
<td></td>
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<tr>
<td>10:50</td>
<td>Session 15: Atomic Physics in Plasmas</td>
<td>M. Poirier</td>
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<td></td>
<td></td>
<td>E.G. Hill</td>
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<tr>
<td></td>
<td></td>
<td>S.J. Rose</td>
</tr>
<tr>
<td>12:30</td>
<td>Workshop adjourns</td>
<td></td>
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</tbody>
</table>
Inertial confinement fusion experiments at the National Ignition Facility have recently demonstrated fuel gains >1 and significant alpha heating. An increase in laser power early in the pulse used in ignition experiments makes the capsule more robust to the hydrodynamic instabilities that typically cause mix of the ablator into the hot spot and can quench the ignition process. To quantify the level of mix, we have developed a model that infers the level of contamination using the ratio of the measured x-ray emission to the calculated DT-only x-ray emission based on the ion density and electron temperature inferred from the measured 14.1 MeV neutron yield, core size, burn duration, and ion temperature. The presence of excess x-ray emission is an indication of carbon from the ablator mixed into the compressed core. The recent "high foot" NIF shots have displayed high hot spot temperatures, indicating low conductive and radiative losses due to mix, consistent with the yield performance and level of alpha heating. We will discuss these experiments and future avenues to spatially and temporally resolve where and when the hot spot mix occurs as we seek to improve implosion performance.

Analysis of Magnetized Liner Inertial Fusion (MagLIF) experiments on Z


Sandia National Laboratories, P.O. Box 5800, Albuquerque, New Mexico 87185, USA

The first integrated experimental tests of the Magnetized Liner Inertial Fusion (MagLIF) concept have been performed at Sandia’s Z facility, demonstrating significant fusion neutron yields (~10^{12} DD neutrons) and effective confinement of charged fusion products by the flux-compressed magnetic field (signaled by few x 10^{20} secondary DT neutrons). The neutron diagnostics are complemented by an extensive suite of visible, VUV, and x-ray diagnostics providing power, imaging, and spectroscopic data. This talk will present analysis of x-ray signatures from the imploding and stagnating plasma that provide a consistent picture of the temperatures, densities, mix, and gradients in the fuel and liner at stagnation.

Quantitative Kα line spectroscopy for energy transport in fast ignition plasma driven with LFEX PW laser


1) Institute of Laser Engineering, Osaka University, 2-6 Yamada-oka, Suita, Osaka 565-0871, Japan
2) Lawrence Livermore National Laboratory, Livermore, California 94550, USA
3) National Institute for Fusion Science, LHD, High Temperature Plasma G. 322-6 Oroshi Toki, Gifu 509-5292, Japan

Kα emission, caused by hot electrons propagation in a hot dense matter, can provide abundant information about the laser plasma interaction. Quantitative Kα line spectroscopy is a potential method to derive energy transfer efficiency from laser to hot electrons. A Laue spectrometer, composed of a cylindrically curved crystal and a detector, has been developed and calibrated absolutely for high energy x-rays ranging from 17 to 77 keV. Either a visible CCD detector coupled to a CsI phosphor screen or a sheet of imaging plate can be chosen as detector. The absolute sensitivity of the spectrometer system was calibrated using pre-generated x-ray sources [Z. Zhang, et al., Opt. Exp. 19, 4560 (2011)] and radioisotopes, for the detectors and crystal respectively. The integrated reflectivity for the crystal is in good agreement with predictions by an open code for x-ray diffraction.

The energy transfer efficiency from incident laser beams to hot electrons, as the energy transfer agency is derived as a consequence of this work. The absolute yield of Au and Ta Kα lines were measured in the fast ignition experimental campaign performed at ILE Osaka U. By applying the electron energy distribution from ESM data and scaling laws, energy transfer efficiency of incident LFEX, a kJ-class PW laser, to hot electrons was derived.
Near Vacuum Hohlraum (NVH) is a high coupling platform1 that might provide a path to ignition using High Density Carbon (HDC)2 with 10 ns long pulses. We have investigated in a series of experiments on the National Ignition Facility (NIF), our ability to control the symmetry of the implosion in this high efficiency platform. Keeping control of the symmetry as the hohlraum fills in with ablated gold is the main challenge of NVH hohlraum. To help inner beam propagation by increasing the distance from the hohlraum wall to the capsule, the hohlraum diameter was increased from 5.75 mm to 6.72 mm, results from of these experiments will be presented. To reach an ignition relevant design, the adiabat has to be lowered. To lower the adiabat, the 2 shock pulse shape length was increased from 4.5 ns up to 8 ns, results will be presented.

References:

This work was performed under the auspices of the U.S. Department of Energy by the Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344.

Session 2. ICF II and Astrophysical Related

Measurements of hot spot conditions and mix in DT implosions on the NIF


Lawrence Livermore National Laboratory, L-637, PO Box 808, Livermore, CA 94550, USA

We describe a 1D model that uses experimentally measured data to derive the thermodynamic conditions at stagnation of the hot spot, dense fuel, and ablator, in deuterium-tritium (DT) layered implosions on the National Ignition Facility (NIF). Neutron measurements—spectrally, spatially and temporally resolved—are used to infer the hot spot burn-averaged pressure, density, areal density, ion temperature, volume, and internal energy. X-ray spectral measurements are used to infer electron temperature, radiative energy loss, and the presence of ablator mix in the hot spot. The signature of ablator mix is the increase in radiation loss due to CH(Si) contamination of the hot spot. In addition, we can calculate the fraction of alpha-particle energy trapped in the hot spot and, hence, estimate the degree of self-heating. Recent DT layered implosions using the high-foot design [Hurricane et al., Nature 506, 343 (2014)] have achieved areal densities and temperatures in the hot spot whereby a significant fraction of the internal energy at stagnation can be attributed to alpha-particle self-heating.

Different Opacity Activities Dedicated to Astrophysical Objects

S. Turck-Chièze

SAp/IRFU/DSM CEA France

In this talk, on behalf of the OPAC consortium, I shall quickly recall the two astrophysical problems that we investigate in questioning the reliability of the opacity calculations generally used in Astrophysics. The talk will have two parts. I shall present the conclusions that we get for the envelopes of massive stars thanks to some detailed comparison realized this year between the experimental campaign at LULI2000 on iron, nickel and some SCO-RCG, ATOMIC, HULLAC, OP and OPAL calculations. In the second part of my talk, I shall recall the OPAS effort to produce new tables for the solar interior conditions and a new technique we develop to probe experimentally a large part of the solar radiative zone conditions with the hope to check some plasma effects for some dominant contributors.

Light element opacities from ATOMIC

1James Colgan, 1D. P. Kilcrease, 1N. H. Magee, Jr, 1J. Abdallah, Jr., 1M.E. Sherrill,2C.J. Fontes, 2H.L. Zhang, and 2P. Hakel

1Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM, USA

2Computational Physics Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA

The effort to compute new local-thermodynamic-equilibrium (LTE) light element opacity tables using the Los Alamos ATOMIC code is well underway. New OPLIB tables are anticipated for hydrogen through zinc and are expected to be completed in the near future. These tables will eventually supplant the previous OPLIB tables that were generated using the legacy LEDCOP code.

In this talk we present a brief overview of the new physics and more complete modeling in the current ATOMIC calculations as compared to the previous LEDCOP calculations. The atomic structure calculations required for all the elements hydrogen through zinc are complete and encompass several tens of terabytes of data.
We show how an improved treatment of the electron-ion contribution to the equation-of-state can have a significant effect on the monochromatic opacity of Fe. We briefly describe comparisons of our new opacities with ongoing experimental efforts to measure opacities of astrophysical interest. Finally, we present comparisons of our new ATOMIC calculations with external opacity databases (such as the Opacity Project) for Rosseland mean opacities as well as monochromatic opacities for selected elements, including Ni and Cr.


Relativistic Opacities for Astrophysical Applications

Christopher J. Fontes, C.L. Fryer, A.L. Hungerford, P. Hakel, J. Colgan, D.P. Kilcrease and M.E. Sherrill
Los Alamos National Laboratory, Los Alamos, NM 87545, USA

Ongoing efforts to improve and expand the relativistic capabilities in the Los Alamos suite of atomic physics codes have produced a more robust approach that can accommodate larger fine-structure models with configuration interaction. We report on the use of this capability to generate opacities that are relevant for astrophysical modeling. In the first application, we consider the generation of cold lanthanide opacities for the study of light curves produced in neutron star mergers (NSMs). The astrophysical site of the nucleosynthesis r-process (rapid neutron capture) remains unknown. While the r-process is widely accepted to occur in core-collapse supernovae, it cannot account for the relative abundances of all of the heavy elements in the universe. Therefore, it is of interest to study compact objects with large concentrations of neutrons, such as NSMs, which may provide alternative sites for r-process production. In order to know if/how it is possible to distinguish NSMs from other events, one needs to simulate the light generated by them, which requires the use of heavy-element opacities calculated at cold, low-density conditions. Thus, we present opacities for lanthanide elements in fine-structure detail and discuss the consequences of these data for the possible detection of NSMs. In the second application, we discuss the generation of opacities for iron-peak elements in support of ongoing experimental efforts related to the solar convection zone and stellar envelopes.

This work was performed under the auspices of the U.S. Department of Energy by Los Alamos National Laboratory under Contract No. DE-AC52-06NA25396.

Session 3. Opacity I - Theory

Opacity calculation with the code HULLAC-v9

1D. Gilles, 2M. Busquet and 3M. Klapisch

1CEA/IRFU/Service d'Astrophysique, CE Saclay, 91191, Gif sur Yvette, France
2Research Support Instruments, Lanham, MD 20706, USA
3Berkeley Research Associates, Beltsville, MD 21042, USA

In its latest development (release > 9.50), the HULLAC code has been dramatically improved [1] and is now able to compute spectrum with several billions of lines, addressing opacity spectra. User can play with the Configuration Interaction scheme to investigate effect of CI in various frequency, temperature and density domains, and obviously can play with the "completeness" of the set of configurations (i.e. large extended set including scarcely populated but numerous levels). Even if “full relativistic CI” mode between all levels of a given charge states is the proper scheme, the computing time which behaves as the third power of the size of the matrices to be inverted can be a limitation as much as the number of configurations considered in the calculations, due to hardware resources limit. Fortunately the “CI in one Non-Relativistic Configuration” scheme, i.e. CI only between levels of a same non-relativistic configuration used in most recent codes, is often a good alternative scheme, which make possible opacity calculations over the whole energy range. These two modes are implemented in HULLAC-v9 and are powerful to quantify importance of CI effect, particularly for the Δn=0, n=3 transition contributions, where it is well known that CI effect play a large role. User can also take a first ride, computing computation averages (i.e. not going to Detailed Levels) to obtain a low resolution spectrum, which might be sufficient for high n - configurations. "Sampling-interpolation" of the spectra for given temperatures and/or for a given spectral range is also possible and accelerates the calculation of opacity spectra.

Some examples of iron and nickel LTE M-shell opacity spectra will be presented and compared to other sources [2], like STA [3] code or OPCD [4] opacity database, for temperatures between 15 and 30 eV and for a wide range of electronic densities. Importance of "full CI" and of "completeness" will be discussed.

References:
New Developments for VISTA: the LLNL super-transition array opacity code

Brian Wilson, Carlos Iglesias, and Mau Chen

Lawrence Livermore National Laboratory L-473, 7000 East Ave Livermore CA 94550-9234 USA

Results will be presented from a new modification of the LLNL super-transition array opacity code VISTA which extends and incorporates the partially resolved transition array algorithm previously developed for detailed configuration accounting. This new approach incorporates the effects of intermediate coupling without ad-hoc closure approximations previously resorted to in STA approaches. Applications to mid-Z opacities where pure j-j coupling treatments are inadequate will be illustrated.

Developments of the SEMILLAC NLTE atomic code.

1Yechiel Frank, 2Pinchas Mandelbaum, 3Zohar Henis

1Racah Institute of Physics, Hebrew University, Jerusalem 91904, Israel & Soreq Research Center, Yavne 81800, Israel
2Jerusalem College of Engineering, Ramat Beth Hakarem, 91035
3Soreq Research Center, Yavne 81800, Israel

Recent modifications now allow us to calculate radiative properties of various laser-produced plasmas. We present the novel extension method developed to calculate the absorption and emission spectra.

This model is based on a limited set of detailed MCDF calculations, extended to a wider set of atomic configurations using simple algebraic relations. The model uses similar principles to those used in the SEMILLAC population dynamics code. The model can be used in local thermal equilibrium and non-local thermal equilibrium conditions.

Results are presented for emission and absorption spectra as well as for average radiative properties.

Accounting for satellite lines due to high-\(n\) spectators in detailed opacity calculations

Jean-Christophe Pain* and Franck Gilleron

CEA, DAM, DIF, F-91297 Arpajon, France
*jean-christophe.pain@cea.fr

In multiply-charged ion plasmas, a significant number of electrons may occupy high-lying loosely-bound orbitals. These “Rydberg” electrons, when they act as spectators, are responsible for a number of satellites of X-ray absorption or emission lines, yielding an effective broadening of these resonance lines (red wing) [M. Busquet, et al., Phys. Scr. 31, 137-148 (1985)]. The contribution of such satellite lines may be important, because of the high degeneracy of the relevant excited configurations, which give a large Boltzmann weight. However, it is in general difficult to take those satellites into account since they give rise to a large number of lines. Usually, they are partially discarded, or described by semi-empirical models. For instance, in Ref. [K. Honda, K. Mima and F. Koike, Phys. Rev. E 55, 4594-4601 (1997)], the authors proposed a model that extrapolates the satellite emission spectra of ions with a single spectator electron to those of ions with an arbitrary number of electrons. Such an approach is interesting, but inadequate when two or more spectator electrons are in the same shell.

In the hybrid statistical / detailed opacity code SCO-RCG [Q. Porcherot, J.-C. Pain, F. Gilleron and T. Blenski, HEDP, 7, 234-239 (2011), J.-C. Pain, F. Gilleron, Q. Porcherot and T. Blenski, Proceedings of the 40th EPS Conference on Plasma Physics, P4.403 (2013): http://ocs.ciemat.es/EPS2013PAP/pdf/P4.403.pdf], the high-\(n\) orbitals-representing the Rydberg electrons, are gathered in a single super-shell. The grouped orbitals are chosen so that they weakly interact with inner orbitals. In one option of the code, the transitions starting from this super-shell are modeled by a limited number of relativistic super transition arrays. However, such a statistical modeling of Rydberg spectators may be irrelevant for some well-resolved transition arrays. Indeed, a Rydberg electron is weakly bound to the ion, so that it does not interact much with the core electrons and perturbs weakly the transition. The detailed calculation of satellites differs then from resonance lines only by a small shift and broadening. On the contrary, the statistical treatment of spectators tends to fill the gaps between the lines more efficiently than the detailed one.

We propose to model the perturbation induced by the spectators in a detailed way in a manner similar to the Partially Resolved Transition Array [C. A. Iglesias and V. Sonnad, High Energy Density Phys. 8, 154-160 (2012)] method. It consists in a partial detailed-line-accounting calculation in which the effect of the Rydberg spectators is included through a shift and width, expressed in terms of canonical partition functions.

Session 4. Opacity II - Experiment & Population Kinetics I

X and XUV opacity measurements in dense plasma

1M. Dozières, 1F. Thais, 2S. Bastiani-Ceccotti, 1T. Blenski, 3W. Fölsner, 4F. Gilleron, 5D. Khaghani, 4J.-C. Pain, 1M. Poirier, 4C. Reverdin, 2F. Rosmej, 4G. Soullié, 4B. Villette.

1CEA, DSM, IRAMIS, Saclay, Gif-sur-Yvette (France)
2LULI, École polytechnique, CNRS, UPMC, Palaiseau (France)
3Max-Planck-Institut für Quantenoptik, Garching (Germany)
4CEA, DAM, Dif, Arpajon (France)
5EMMI, GSI Helmholtzzentrum, Darmstadt (Germany)
We present the recent experimental work at the LULI-2000 facility about X and XUV opacity measurements in medium-Z laser produced plasma. We were interested in plasma conditions characterized by temperatures from 20eV to 25eV and densities of the order of magnitude of $10^{-2} \text{g/cm}^3$ to $10^{-3} \text{g/cm}^3$. The aim of this work was to simultaneously measure absorption structures in X and XUV range using different approaches to estimate the plasma temperature and validate the atomic physics codes. We sought to investigate the 2p-3d x-ray absorption structures of Ni, Fe and Cu targets as well as the 1s-2p transition of an additional aluminum layer to confirm the in-situ temperature. Moreover in medium-Z plasma the Planck and Rosseland average opacities under these conditions are often dominated by XUV $\Delta n=0$ ($n=3$) transitions whose strength is highly sensitive to plasma temperature.

Furthermore, the experimental scheme was based on two different target designs. The first one was a thin foil of main material, inserted between two gold cavities that were heated by two nanosecond beams in the 300J range. The plasma was probed by x-ray backlighter created by a third nanosecond beam with an energy $E\approx20J$. This x-ray source was in the same axis as the two cavities and the foil. In the second set-up the two cavities were perpendicular to the axis defined by the x-ray source and the foil. For these two schemes, the temperature gradient inside the sample was reduced during the spectroscopic measurement because of both-side irradiation of the foil by the cavities.

In addition to the main spectrometer, several other diagnostics were used. An independent measurement of the radiative temperature of each cavity was performed with a broadband spectrometer. A spherical crystal spectrometer with a high spectral resolution was dedicated to the study of the x-ray source, which was also controlled by a third spectrometer. Finally a pinhole camera was placed to observe the x-ray emission of the cavities.

The association of every diagnostic allowed us to complete and well characterize the opacity data.


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The Z Astrophysical Plasma Properties collaboration is staging Z experiments that simultaneously investigate multiple topics in radiative properties of hot dense matter. The four astrophysics questions presently guiding this research are: 1) Why can’t we predict the location of the convection zone base in the Sun?; 2) How does radiation transport affect spectrum formation in accretion-powered objects?; 3) Why doesn’t spectral fitting provide the correct properties for White Dwarfs?; and 4) Why can’t we predict the heating and charge state distribution in photoionized plasmas? The benefits and challenges associated with designing, executing, and interpreting four simultaneous experiments will be discussed. Recent progress in the first two of these four projects will also be described. Stellar opacities are an essential ingredient of stellar models and opacity models have become highly sophisticated, but laboratory tests have not been done at the conditions existing inside stars. Our opacity research is presently focused on measuring Fe at conditions relevant to the base of the solar convection zone, where the electron temperature and density are believed to be 190 eV and $9\times10^{22} \text{e/cc}$, respectively. The second project is motivated by the fact that emission lines from L-shell ions are not observed from iron in black hole accretion disks, but are observed from silicon in x-ray binaries. We investigate photoionized silicon plasmas using absorption spectroscopy to infer the plasma conditions and emission spectroscopy to determine the dependence of spectrum formation on plasma column density.

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under contract DE-AC04-94AL85000.

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**Synthetic investigations for systematic uncertainties in the iron opacity measurements at solar interior conditions**


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Iron opacity experiments near solar interior conditions are performed at Sandia National Laboratories Z machine [J.E. Bailey et al., Phys. Plasmas 16, 058101 (2009)]. Z-pinch dynamic hohlraum radiation heats the sample as it implodes and backlights the sample at its stagnation [G.A. Rochau et al., Phys. of Plasmas 21, 056308 (2014)]. Space-resolved iron-transmitted backlighter images are recorded on x-ray film to maximize the image resolution, spectral resolution, and signal-to-noise ratio. While the time resolution of the absorption spectra is provided by the backlighter duration, both the backlighter radiation and the sample conditions slowly change over the duration. Potential systematic uncertainties in the time-integrated measurements and in the resultant opacity measurements are
synthetically studied with a detailed modeling of the drive radiation, the sample hydrodynamics, and the backlighter radiation taking into account the time- and space-integrations. We report on the systematic uncertainties due to the plasma self-emission, tamper transmission, time- and space-integration, and non-local-thermodynamic equilibrium effects.

## Statistical Approach to Radiation-Collisional Processes with Heavy Atoms in Plasmas

A.V. Demura, M.B. Kadomtsev, V.S. Lisitsa, V.A. Shurygin

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The statistical approach for calculation of radiation and collisional processes with heavy multielectron ions in plasma is developed. The method consists in consideration of atomic structure as a condensed medium, characterized by the spectrum of elementary excitations with plasma frequency, determined by local atomic electron density. For instance, the radiation losses in this model are due to excitation of plasma type oscillations in atom under its collisions with plasma electrons and have a universal statistical representation for all sorts of multielectron ions. The calculations of radiation losses on tungsten ions are performed in the wide range of plasma temperature variation, typical for physics of high temperature plasma. It is shown that the universal statistical approach results are within the scattering of current numerical codes data. The proposed statistical method for description of complex atoms collective excitations for calculations of plasma radiation losses is of general physical interest and allows to obtain the necessary data with the lesser computational resources.

### Tuesday, September 30th

#### Session 5. Population Kinetics II

**Comparison and analysis of collisional-radiative models at the NLTE-8 workshop**


1. *International Atomic Energy Agency, Atomic & Molecular Data Unit, Nuclear Data Section, P.O. Box 100, A-1400 Vienna, Austria*
2. *Los Alamos National Laboratory, Los Alamos, NM 87545, USA*
3. *Sandia National Laboratories, PO Box 1964 Tijeras, NM 87059 USA*
4. *National Institute of Standards and Technology, 100 Bureau Drive, Gaithersburg, MD 20899, USA*

Advanced collisional-radiative (CR) models are extensively used in plasma spectroscopy to analyze plasma kinetics and spectra produced far from local thermodynamic equilibrium (LTE). Non-LTE atomic models also play a critical role in radiation-hydrodynamic simulations used to help design plasma experiments. Therefore, the verification and validation of these complex CR models are of great interest. Since experimental benchmarks for validation are extremely challenging, computational experiments and comparisons are one of the primary tools for V&V of CR codes.

Since 1995, the NLTE Workshops have played a significant role in developing such tools and techniques. We present results of the 8th NLTE Code Comparison Workshop held in November 2013 Santa Fe, NM, USA. Results of 19 codes from 8 countries have been compared and analyzed for three cases: 1) Ne case for photoionized plasmas, 2) Kr case for an analysis of experimental spectra from Z at SNL, and discussion of CR modeling strategies and 3) W case as a plasma facing components in ITER.

**Collisional Radiative Average Atom Code Based on a Relativistic Screened Hydrogenic Model**

Ana Josefa Benita Cerdan

*Istituto de Fusión Nuclear, ETS de Ingenieros Industriales UPM Universidad Politécnica Madrid*

A steady state and time dependent collisional-radiative “average-atom” AA model (ATMED) is presented for the calculation of atomic and radiative properties of plasmas for a wide range of laboratory and theoretical conditions: coronal, local thermodynamic equilibrium or nonlocal thermodynamic equilibrium, optically thin or thick plasmas and photoionized plasmas. The radiative and collisional rates are a set of analytical approximations, which compare well with more sophisticated quantum treatment of atomic rates yielding to fast calculations and savings in computer running time. The atomic model is based on a new Relativistic Screened Hydrogenic Model (NRSHM) with a set of universal screening constants including nlj-splitting that has been obtained by fitting to a large database of ionization potentials and excitation energies compiled from the National Institute of Standards and Technology (NIST) database and the Flexible Atomic Code (FAC). The model NRSHM has been validated by comparing the results with ionization energies, transition energies, and wave functions computed using sophisticated self-consistent codes and experimental data. All the calculations presented in this work were performed using ATMED code.

**Radiation transfer of ultra-intense x-ray laser pulses through solid aluminium**

Cheng Gao, Jiaolong Zeng and Jianmin Yuan

*Department of Physics, College of Science, National University of Defense Technology, Changsha Hunan, P.R. China, 410073*

A theoretical formalism is developed to deal with the radiation transfer of ultra-intense x-ray laser pulses through solid density of aluminium simultaneously solving the radiation transfer equation and the rate equation. The rate equation determines the evolution dynamics of charge state distribution (CSD) and level populations in the interaction of ultra-intense x-ray pulses with matter, while the radiation transfer equation determines the absorption of x-ray radiation. These two equations are coupled together. With the increase of intensity, the matter becomes transparent due to the empty K-shell states irradiated by the strong radiation field. The physical effects of
Radiation hydrodynamics with in-line NLTE atomic kinetics applied to Inertial Confinement Fusion plasmas*

Mehul V. Patel, Howard A. Scott, and Michael M. Marinak
Lawrence Livermore National Laboratory, USA

In radiation hydrodynamics modeling of inertial confinement fusion (ICF) targets, NLTE atomic kinetics is important for modeling high-Z hohlraum wall materials, high-Z dopants mixed in the central gas hotspot, and is potentially also required for accurate modeling of outer layers of the capsule ablator. Over the past several years, the in-line NLTE atomic physics capabilities [1,2] in the 3D ICF radiation hydrodynamics code HYDRA [3] have been significantly enhanced. The underlying atomic models have been improved, additional kinetics options including the ability to run inline atomic kinetics in cells with dynamic mixing of species has been added, and the computational costs have been significantly reduced using OpenMP threading. To illustrate the improved capabilities, we will show higher fidelity results from simulations of ICF hohlraum energetics, laser irradiated sphere experiments, and ICF capsule implosions.

References:

* This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

Radiation transfer effects in short-pulse heated targets

R. A. London, H. A. Scott, J. J. Castor, and J. Nilsen*
Lawrence Livermore National Laboratory

Emission line spectra are often used to infer the temperature and density of high temperature plasmas. Although optically thin lines are preferred for such diagnostics, this is not always possible. Line diagnostics can still be used in optically thick situations if a proper accounting of radiation transfer effects are taken into account. We discuss how optical depth affects the strengths and emission profiles of X-ray lines from short pulse laser heated targets by using detailed radiation transfer calculations with the Cretin code [H. A. Scott, JQSRT. 71 (2001) 689]. The use of moderately optically thick lines for plasma diagnostics of several recent experiments is described.

* This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.
Developments in the Frequency Separation Technique for Spectral Line shape Calculations

Spuridon Alexiou
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The Frequency Separation Technique is a method capable of improving practically any method for ion dynamics in line shape calculations by separately calculating and including exactly the ion impact part. The basic ideas and practical implementation are discussed and results are given.

Review of the 2nd Spectral Line Shapes in Plasmas Code Comparison Workshop

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Modeling the Stark broadening of spectral lines in plasmas plays a crucial role in the interpretation of spectroscopic observations of lines emitted from laboratory or astrophysical plasmas. It is a complex problem requiring precise calculations for accurate diagnostics. For a long time, different computational and analytic methods of various complexity and applicability have been developed but with a certain lack of useful confrontations. The Spectral Line Shape in Plasmas (SLSP) code comparison workshop series was proposed to correct it, [1, 2].

For the first two SLSP workshops, participants submitted in total over 1,500 line-shape calculations. Different computational cases were selected not only to serve the purpose of code comparison but also for their interest in research of magnetic fusion, astrophysical, laser-produced plasmas, and so on. We will present here a review of the second workshop.

References:

Session 7. Posters (Alphabetical by first author)

Atomic Physics:

1. KrF Nike Laser as a Powerful Platform for Experimental X-Ray Spectroscopy of High-Z Ions*

1Y. Aglitskiy, 2J.L. Weaver, 3M. Karasik, 4V. Serlin, 5S.P. Obenschain, and 6Yu. Ralchenko

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The NRL Nike laser is capable of delivering several kilojoules of ultraviolet light (λ = 248 nm) on a target within several nanoseconds, which is sufficient to produce high-Z ions with multi-keV ionization potentials. As such this system is a unique platform to benchmark high-energy-density plasma diagnostics and relevant atomic physics simulations.

The goal of this study of the Au x-ray spectra is to provide more insight into the M-band contribution to the total energy balance inside hohlraums. For this purpose two high-resolution x-ray spectrometers have been added to the Nike diagnostic suite. One is a survey instrument covering the spectral range from 0.5 to 19.5 angstroms, and the other is an imaging spectrometer using a spherically curved crystal. The survey instrument allows simultaneous high-spectral-resolution observations of both M- and N-spectra of highly charged ions with nuclear charge Z=70-85. The imaging spectrometer provides even more detailed spectra within a narrower variable spectral band with a substantially higher efficiency. Measurements and analyses of isoelectronic spectra from several elements greatly assist in identification of specific spectral lines that are of major interest.

The Nike shots taken with a power density of 2×10^{14} W/cm^2 on the foils of Hf, Ta, W, Pt and Au confirmed presence of strong spectral lines from Ni-like ions along with multiple satellite lines originating from the lower stages of ionization. High-quality n=2-n=3 spectra from L-shell ions of elements from Y to Sn were also measured for calibration and testing. Collisional-radiative simulations with the NOMAD code were used to model the recorded spectra and to identify spectral lines in the x-ray region. This study represents an important milestone for the program of development and testing of similar spectrometers that are to be built by NRL for NIF.

*Supported by DOE NNSS.

2. Studies on Frequency-Dependent Linear Response of Atoms in Plasmas

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A self-consistent model of atoms in plasmas in which all electrons are treated on the same footing [1-4] allows one to calculate from the linear response (LR) theory the dynamic polarizability of plasma electrons [5-6]. Correctly calculated such polarizability should provide photon absorption coefficients taking into account both electron-hole transitions and collective modes with channel mixing (configuration interaction). We give an overview of the present state of our research in this field. The physics and mathematics of the
problem has been well-understood [5] in the case of the dynamic response of the quasi-classical Thomas-Fermi (TF) atom in plasma at finite temperature, which is a special case of the variational average atom in plasmas (VAAQP) approach. We present essential results obtained in this case especially those concerning the contribution of the collective effects to the absorption cross-section, the role of the ion-ion correlation and the verification of the Ehrenfest-Type Atom-In-Plasmas Sum Rule [6-8]. The LR theory in the full quantum VAAQP model will also be discussed. The quantum VAAQP case is from the practical point of view much more challenging than the TF case due to the non-local relation between the frequency-dependent induced density and potential having slowly vanishing tails far from the atom.

*thomas.blenski@cea.fr

References:

3. Dense Plasma effect and average atom model
Michel Busquet, Marcel Klapisch
ARTEP, Inc., Research Support Instruments 4325-B Forbes Blvd. Lanham, MD 20706 USA

We present application of the PIES (Pressure Ionized Effective Statistical Weights), a powerful alternative of the methods of "resonance tracking" to take into account the hybridization of bound and free orbitals in the framework of the (average) ion cell, used for atomic physics of dense plasmas

4. The effect of ion-ion correlation on the atomic energy levels and absorption of radiation in dense plasmas
Y. Kurzweil S. Kahane and G. Hazak
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A realistic model of hot dense plasma requires a combined treatment of two aspects which traditionally were treated as separated disciplines. The first one is the description of the plasma as an ensemble of point ions and electrons interacting via the coulombic interaction. The second aspect concerns the details of the quantum states of the bound and free electrons, and the radiative transitions between them. In the past, and also recently, combined treatments were suggested by several works [e.g., Ref. 1 Rozsnyai, High Energy Density Physics 10 16 (2014) (and the references therein); D. Ofer, E. Nardi and Y. Rosenfeld, Phys. Rev. A 38 5801 (1988) (and the references therein)] mainly for the evaluation of thermodynamic properties of hot dense plasmas. These works treated the ion-ion correlations mostly by the HNC approximation. In the present work we combine both ion-ion correlation and quantum atomic structure, a la Refs. [1], self-consistently. The ion-ion correlation, however, is calculated by Monte-Carlo simulation rather than the HNC approximation. In its turn, the atomic structure is the self-consistent solution of the Dirac equation that contains both electronic and ionic densities. The ion-ion potential, used in the Monte-Carlo simulation, is determined from the resultant atomic structure. Finally, while full self-consistency between the atomic and the Monte-Carlo calculations is obtained, the absorption spectrum is evaluated using the recently developed CR-STA (configurationally resolved super transition arrays) method [2,3].

References:

5. The K X-Ray Line Structures of the 3d-Transition Metals in Warm Dense Plasma
E. Szymańska1, K. Słabkowska1, Ł. Syrocki2, N. R. Pereira3, J. Rzadkiewicz4, M. Polasik1

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Outer-shell ionization can affect the energy and shape of characteristic x-ray lines sufficiently for a single line to be of value in plasma diagnostics. Recently, the outer-shell ionization of a hot, dense tungsten plasma was determined from a detailed analysis of a single, highly-resolved L x-ray line shape, and in an iridium plasma the change in energy of a single K x-ray line confirmed a theoretical estimate of the ionization [1-4]. Diagnosing plasmas by these ionization energy shifts depends essentially on computations that can now be performed with sufficient accuracy, e.g. using the multiconfiguration Dirac-Fock (MCDF) method.
References [3-4] emphasize that outer-shell ionization not only affects the energies of the x-ray lines, as was already used in a diagnostics application for heavy elements, but also their shapes. This is important for K x-ray lines emitted by 3d-transition metals, which can be registered with high enough spectrometer resolution to see the different line shapes in x-rays from plasmas produced on the plasma focus (PF-1000) [5]. Figure 1 presents results of our analysis performed for Ka1,2 x-ray lines using the MCDF method [6], where the ‘sticks’ seen inside each spectrum are located at the center energy of the x-ray line. The dotted line is the sum of the Lorentzian natural line shapes with the appropriate natural line width; the solid line convolves this ideal spectrum with the Gaussian instrumental response for easier comparison with experiment. As can been seen from Figure 1, removing an electron from the 2p subshell causes very strong changes for shapes and positions. We believe that the results of this analysis can explain the experimental results registered on the PF-1000 in Institute of Plasma Physics and Laser Microfusion in Warsaw [5].

References:

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A few recent papers on radiating Z-pinches at Sandia National Laboratories [1-3] discuss K-shell x-rays emitted by ions ionized to within the L-shell but below helium-like. In molybdenum [3] the energy needed to create a vacancy in the K-shell is about 20 keV, the energy of neutral Mo’s K-edge; but, a purely Maxwellian energy distribution with the few-keV temperature inferred from other diagnostics has too few electrons with sufficient energy to produce the K-shell radiation observed. Therefore, the plasma must contain non-thermal electrons with energies not described by the thermal electron energy distribution; these are variously referred to as hot or beam electrons. The detailed collisional-radiative plasma model in Ref. [3], which includes many interactions between the plasma’s thermal electrons, Mo’s L-shell and higher-lying shells, and the photons, accounts for the radiation by assuming a stationary, higher-density central rod of plasma surrounded by a cylindrical shell, provided that a pinch of 60 keV electrons is added to excite the K-shell photons.

Other Z-pinch implosions at Sandia similarly produce intense pulses of multi-keV x-rays, from plasmas with local electron temperatures that range from 100 eV up to 12 keV [1,2]. Also in these pinches a hot, dense core of the Z-pinch plasma emits Kα radiation from a thermal plasma, with a contribution from excitation by high-energy electrons that are not in thermal equilibrium with the plasma. These energetic electrons can also generate Kα and Kβ radiation in the cooler plasma in the region outside the compressed Z-pinch plasma [3]. As is well known, the energy of the K-line photons depends on the ionization level, which often reflects the temperature of the plasma: we have recently published an extensive series of relevant computations and measurements on this effect [4-8]. Here we explore the energy shifts to the K-lines of elements such as Mo and Ag as diagnostics of Z-pinch plasmas produced by Sandia’s Z-machine, where the Z-pinch plasma tends to have partially ionized L-shells for elements with Z ~ 40-50. The computations are performed with the multi-configuration Dirac-Fock (MCDF) method. In this work we discuss the increase in K-line energy as a higher-Z atom with Z > 40 or so like Mo or Ag, and higher) ionizes a particular shell.

References:
A recent publication [1] presented high-resolution measurements of the x-ray line structures for partially ionized molybdenum obtained from wire implosions on the Z machine at Sandia. The accompanying modeling of the radiation gives the best results when the plasma is assumed to consist of a hot, dense core of thermal plasma in ionization equilibrium with Mo ions, with bound electrons primarily in the K and L shells [2]. Any non-thermal, energetic electrons that excite these ions generate Kα and Kβ radiation, whose photon energy depends on the ionization level and thus on the plasma temperature. In this work the modeling of the K and L x-ray line structures has been performed using the Flexible Atomic Code (FAC) [3, 4] package within the framework of Collisional-Radiative Model (CRM) approach. Figure 1 shows the individual contributions of the 4 relevant ionization states, and their sum, for a Mo plasma with electron temperature of 4 keV and electron density of 1.7x10²¹ cm⁻³ as might exist in the core of the 70 mm Mo pinch.

The reasonable agreement of our results with the experimental data [1] shows that modeling the K and L x-ray spectra from plasmas with the CRM approach, as implemented in packaged programs such as FAC, can reproduce significant parts of the x-ray spectra from Z-pinches quite well. The parameters of the fast electrons could then be derived from computations of the K-shell spectrum. These should include not only the ionization energy shift, but also fluorescence from absorption of higher-energy photons at the energy-shifted K-edge, and possibly the energy loss by fast electrons as they generate vacancies in the K-shell [5].

References:

* Supported in part by the Polish National Science Center under Grant No. 2011/01/D/ST2/01286. This work has also received funding from the European Union’s Horizon 2020 research and innovation programme under grant agreement number 633053. The views and opinions expressed herein do not necessarily reflect those of the European Commission.

8. Opacity and EOSs

Opacity calculations: Ge and Si dopants in ICF

D. Benredjem

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The opacity is an important issue in the knowledge of radiative properties of ICF and astrophysical plasmas. In this work we present the opacity of dopants embedded in the ablator of some ICF capsules. We focus on germanium and silicon dopants. In recent works, Hill and Rose [1] have calculated the opacity of silicon in LTE and non-LTE plasmas.
We have used two methods to calculate the opacity spectra of mixtures. The first one involves a detailed line calculation where almost all spectral broadening effects, including Zeeman splitting and Stark effect, are taken into account [2]. This method is able to provide accurate opacity spectra but rapidly becomes prohibitive when the number of lines is large. To account for many ionic stages and thousands of lines, a second method – hybrid method – [3] is preferred. This method combines detailed line calculations and statistical calculations. In spectral regions where the lines are sufficiently separated and the number of radiative transitions is moderate, detailed calculations are feasible. When the number of transitions is very large and most of them merge in broad structures, due to line broadening, statistical calculations are inevitable. The hybrid method involves much smaller calculation times than the first one. It is then more appropriate for extensive calculations.

References:

9. Enigmatic photon absorption in plasmas
Carlos A. Iglesias
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Large systematic discrepancies between calculations and experimental transmission of hot dense Fe plasmas were recently reported. The disagreement is examined in context with the Thomas-Reiche-Kuhn f-sum rule. The analysis suggests that the data, in the absence of unidentified systematic experimental errors, reveal extraordinary, previously unobserved photon absorption phenomena in plasmas.

10. An Equation of State for Partially Ionized Plasmas: Coulomb Contribution to the Free Energy
D.P. Kilcrease, J.P. Colgan, P. Hakel, C.J. Fontes, M.E. Sherrill
Los Alamos National Laboratory
We have developed an equation of state (EOS) called ChemEOS for a plasma of interacting ions, atoms and electrons [P. Hakel, D.P. Kilcrease, in Atomic Processes in Plasmas, Eds., J. Cohen, S. Mazevet, D. Kilcrease, AIP Conference Proceedings 730, p. 190, 2004]. It is based on a chemical picture of the plasma and is derived from an expression for the Helmholtz free energy of the interacting species. All other thermodynamic quantities are then derived by minimizing this free energy subject to constraints thus leading to a thermodynamically consistent EOS. The contribution to this free energy from the Coulomb interactions among the particles is treated using the method of Chabrier and Potekhin [G. Chabrier, A. Potekhin, Phys. Rev. E 58, 4941 (1998)]. This treatment is examined and is found to give rise to unphysical behavior for certain values of the density and temperature where the Coulomb coupling begins to become significant and the atoms are partially ionized. We examine the source of this unphysical behavior and suggest corrections that produce acceptable results. The sensitivity of the thermodynamic properties and frequency dependent opacity of iron is studied with and without these corrections. The corrected EOS is used to determine the fractional ion populations and level populations for a new generation of low-Z opacity tables currently being prepared at Los Alamos National Laboratory [J. Colgan, et al., see accompanying presentation at this conference] with the ATOMIC code [P. Hakel, et al., J.Q.S.R.T 99, 265 (2006)]. The new tables also contain the thermodynamic information derived from the newly corrected EOS, namely the Helmholtz free energy, total pressure, and internal energy.

11. Transport & optical properties of aluminum in the two-temperature WDM regime
D. V. Knyazev
Institute for Theoretical and Experimental Physics Bolshaya Cheremushkinskaya 25, 117218, Moscow, Russia
At first transport and optical properties were obtained in an ab initio calculation. The ab initio calculation is based on the quantum molecular dynamics, density functional theory and the Kubo-Greenwood formula. Next a semi-empirical model of transport and optical properties was constructed based on the results of ab initio calculations. Ab initio results may also be well described by the Drude theory with the expression for the relaxation time determined in this work.

The results are compared with the other models of transport and optical properties. Most of the models are reduced in the low temperature limit to the Drude expression with different expressions for the relaxation time. The Bloch-Grüneisen expression is commonly used for solid phase and for liquid phase as well. In this work we show that the Bloch-Grüneisen expression is incorrect for liquid phase.

12. Optical and transport properties of hot and warm dense matter with the RESEOS model
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1Russian Federal Nuclear Center – All-Russian Scientific Research Institute of Technical Physics, Snezhinsk, Russia
2Keldysh Institute of Applied Mathematics, Moscow, Russia
Optical properties (opacity, complex functions of ac conductivity, permittivity, and the refraction index) of hot and warm dense plasmas are calculated using both the generalized superconfiguration approach and effective accounting [1] of occupation-number fluctuations of all atomic subshells. The generalized superconfiguration approach enables one to effectively allow for the occupation-number fluctuations of some atomic subshells when the detailed accounting of those is not significant [2–4]. The standard superconfiguration approach [5] is realized as a particular case. RESEOS calculations demonstrate smooth dependence of optical
properties on material’s density under pressure ionization.

The DC conductivity is calculated using the generalized Ziman formula [6,7], the relaxation-time approximation for the Boltzmann equation [8,9], the Kubo-Greenwood formula for an average-atom [10], and the Zubarev method [11–13] previously implemented in the COMPTRA model [13]. The relaxation-time approximation is also used for the thermal-conductivity calculations.

Conductivities based on the Ziman formula and the relaxation-time approximation appear to coincide in the case of strong electron degeneracy. In the nondegenerate case the Ziman formula, however, appreciably underestimates the conductivity [12]. On the other hand, at intermediate degeneracies the relaxation-time approximation may lead to the unphysical behavior of electron and thermal conductivities because of peculiarities of the average-atom electron-ion scattering cross section at low electron energies. The Zubarev method enables one to avoid these disadvantages.

References:

13. The Ionization Equilibrium of Dense Multielectron-Ion Plasmas Based on the Chemical-Picture Representation Using the Modified Superconfiguration Approach

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Simulation of thermodynamic, optical and transport properties of dense multielectron- ion plasmas requires the accurate modeling of the ionization equilibrium in a wide range of temperatures and densities. We present the description of the improved theoretical model CP-SC [1] for consistent calculation of ionization equilibrium and equations of state (EOS) of dense multielectron-ion plasmas based on the chemical-picture representation of plasmas using the modified superconfiguration approach (SC) [2–4]. Using the improved version of the CP-SC model utilizing the modified full-scale superconfiguration approach [4] we illustrate the effect of multiply excited configurations of multielectron ions on the ionization equilibrium of dense plasmas. In addition, we demonstrate the comparison of ion-charge distributions calculated with the accounting of the first-order corrections to the electron configuration energies and also improved by refining the definition of the supershells. Calculations of ion-charge distributions for low-, mid- and higher atomic number (Z = 13, 29, 64, 79) multielectron-ion plasmas are compared to the results calculated using the Liberman model for average-atom implemented in RESEOS code [5].

References:

14. Ab initio calculations of the elastic and thermodynamic properties of aluminum crystal under non-equilibrium heating and different compressions

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Within the scope of density functional theory, we used the all-electron full-potential linear muffin-tin-orbital (FP-LMTO) method to investigate the elastic properties of aluminum in the case where the electron gas is heated to a temperature of ~10 eV and the nuclei are at rest in the lattice nodes. Our calculations were done for three isochors V/V0=1, 0.7, 0.6 (V0 – is specific volume under ambient conditions). The elastic constants of aluminum are shown to change in non-monotonic manner as the electron temperature Te grows due to a significant redistribution of electron density in the crystal. We demonstrate that with the growth of Te aluminum crystal gets strongly anisotropic for all values of V/V0 under consideration. Calculated results were used to determine Debye temperature and melting temperature (by the Lindemann criterion) as function of Te for different compressions. These functions also demonstrate the nonmonotonic variation as the electron temperature grows. Using obtained results, we calculated the electron-phonon coupling factor [Z. Lin, L. V. Zhigilei, V. Celli, Phys. Rev. B 77, 075133 (2008.)] as a function of Te with account for changes in the electron and phonon spectra of the crystal for the three isochors. A detailed analysis of results we obtained is provided.
15. **Comparisons of radiative opacities using the DAVROS DTA opacity code**
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The radiative opacity of a plasma is a key parameter in understanding a diverse range of high energy density systems including inertial confinement fusion and astrophysics. The accurate calculation of opacity is hampered by the potentially enormous number of ionic configurations, the detailed internal structure of each giving rise to the term structure, and the line broadening models which must typically be applicable across densities from $10^6$ g/cc to several times solid.

The DAVROS opacity code (Detailed Accounting of Various configurations for Radiative Opacity Spectra) has been developed at AWE over recent years, and by making use of the large scale High Performance Computing (HPC) systems, implements a number of models and algorithms aimed at a more direct calculation of opacities than has traditionally been feasible. The results are both more physically based and spectrally accurate than codes based upon statistical accounting approximations. In particular, the bound-bound line spectrum can be explicitly calculated using the Detailed Term Accounting (DTA) method, which, although computationally expensive, is necessary to understand the true frequency dependent structure of the opacity spectrum.

We present a selection of results, including systematic comparisons as functions of temperature and density with the average atom code CASSANDRA. Such systematic comparisons are particularly useful for understanding code differences and for validating physics models.

16. **Quantum molecular dynamics simulations of the equation of state and optical properties of expanded beryllium**
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We investigate, by performing quantum molecular dynamics simulations, the equation of states, electrical and optical properties of the expanded beryllium at densities from 0.5 to two $10^2$ lower than the normal solid density and temperatures ranging from 5000 to 30000 K. With decreasing density of Be, the optical response evolves from the one characteristic of a simple metal to the one of an atomic fluid. By fitting the optical conductivity spectra with the Drude-Smith model, it is found that the conducting electrons become localized at lower densities. In addition, the negative derivative of the electrical resistivity on temperature at densities about eight lower than the normal solid density demonstrates that the metal to nonmetal transition takes place in the expanded Be. To interpret this transition, the electronic density of states are analyzed systematically. The absorption spectra are calculated and compared with the simulated results using the detailed configuration accounting model.

17. **Line shape calculations in dense plasmas submitted to a strong magnetic field.**
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The recent development of capacitor-coil targets driven by high power lasers, a technique which allows kilotesla magnetic field generation, opens new frontiers in plasma physics, astrophysics and atomic and molecular physics. In that context, it is important to calculate the spectral line shape of ions in dense plasmas submitted to a large external magnetic field. In dense plasmas where the combined effect of the ion microfield and of the electron broadening is also important, such calculations must go beyond the standard treatment of the Zeeman effect in atomic spectroscopy. Here, we present specific line shape calculations of Lyman lines and Balmer lines (H-like ions) in plasmas submitted to kilotesla magnetic fields. Details of the calculations, which can be extended easily to multielectron ions, are presented. The potential of spectral line broadening as a diagnostic tool of the magnetic field strength in this context, is discussed.

18. **Zeeman effect induced by intense laser light**
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We analyze spectral line shapes of hydrogen-like species subjected to fields of electromagnetic waves. It is shown that the magnetic component of an electromagnetic wave may significantly influence the spectra. In particular, the Zeeman effect induced by a visible light can be experimentally observed using present-day powerful lasers.

19. **Dedale: a NLTE model for radiation-hydrodynamic simulations**
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The modeling of plasmas in non-local thermodynamic equilibrium (NLTE) is central for many applications: the design of hohlraum in the context of inertial confinement fusion, e.g. NIF or LMJ project, the diagnosis of plasma sources through the study of X-ray emission spectra, the estimation of radiative power losses in the divertor of the ITER reactor, the study of photoionized plasmas in astrophysics, and so on.
It is often mandatory to calculate the NLTE radiative properties “on the fly” in the hydrodynamic code, and this requires the use of fast but accurate methods. The CEA radiation-hydrodynamic codes can use different kinds of fast inline NLTE libraries like Radiom [M. Busquet, Phys. Fluids B 5:4191 (1993)] or Nohel [C. Bowen, P. Kaiser, JQSRT 81:85 (2003)]. The Dedale model we are now working on is another approach inspired by models like FLYCHK [H.K. Chung et al, HEDP 1:3 (2005)] and DCA-Cretin [H. Scott, S. Hansen, HEDP 6:39 (2010)]. The stationary collisional radiative rates equations are solved for a set of well chosen Layzer complexes in order to determine the ion populations. The electronic structure is approximated with the screened hydrogenic model (SHM) of More [R.M. More, JQSRT 27:345 (1982)] including relativistic corrections. The radiative and collisional cross-sections are based on Kramers [R.M. More, UCRL-84991 (1991)] and Van-Regemorter [H. Van Regemorter, ApJ 136:906 (1962)] formula, respectively, which allows one to derive simple analytical expressions for the rates. The latter can be improved by using Gaunt factors or tabulations for each process. Special care was taken for dielectronic rates which were compared and rescaled with quantum calculations performed with the Averroés [Peyrusse, J Phys B 33:4303 (2000)] code. The use of the detailed balance for inverse processes ensures to be consistent with the LTE limit, the ion populations becoming in that case exactly Boltzmann factors.

The emission and opacity spectra are calculated with the same approximations as for the radiative rates either in a detailed manner, by summing the transitions between each pair of complexes, or in a more statistical way by summing the one-electron transitions averaged over the complexes. Optionally, nl splitting can be accounted for by: i) computing the oneelectron energies in a WKB approach with a potential reconstructed analytically from the screened charges [P. Pankratov et al., PRA 46:5497 (1992)]; and ii) by evaluating the dipole matrix elements with SHM wavefunctions. It is also possible to improve the spectra by replacing some transition arrays with data tabulated with more sophisticated codes like SCO-RCG [Q. Porcherot, J.C. Pain, F. Gilleron, T. Blenski, HEDP 7:234 (2011)] or FAC [M.F. Gu, Astrophys. J 590:1131 (2003)]. This latter option is particularly interesting for K-shell emission spectroscopy.

The code was used for the neon and tungsten cases in the NLTE-8 workshop, held in Santa Fe in November 4-8, 2013. Some of these results will be presented along with comparisons with Averroés calculations.


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Opacity experiments at the Z facility provide important data for benchmarking opacity models and atomic data. The ability to accurately interpret the data obtained in these experiments increases the confidence in opacity calculations for a variety of astrophysical and laboratory problems. In the experiments, the Z dynamic hohlraum radiation source is used to both heat and backlight material samples. We will present the latest improvements to the simulation codes developed at Prism and how they affect the analysis of the experimental data. In particular, we will discuss angle-dependent radiation boundary condition recently implemented in the radiation-hydrodynamics code HELIOS. This improved modeling capability can potentially be important for studying behavior of plasmas driven by radiation sources that cannot be adequately described as neither directional nor Lambertian. We will also discuss atomic kinetics in radiatively heated samples and the possibility of its deviation from LTE. The effect of such deviation on both hydrodynamic evolution and radiative properties of these plasmas will be addressed.

21. An In-Line Atomic Model for Tin EUV Generation

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Numerical simulation of EUV radiation generation from laser-produced plasmas provides multiple computational challenges. The basic parameters of spatial scale, temporal scale, and laser intensity and wavelength set the physical regime and result in significant resolution requirements. In addition, the tasks of adequately modeling the non-LTE atomic kinetics producing the EUV emission and the transport of the resulting radiation must also be addressed. For a Sn (Z=50) target, the desired 13.5 nm radiation comes primarily from 4f-4d and 4d-4p transitions in Sn4-13+ ions [1]. Detailed data for these ion stages can be systematically calculated [2,3], but the resulting data sets are extremely large and are many orders of magnitude too expensive for use in radiation-hydrodynamics simulations. We describe here the construction of an atomic model that is inexpensive enough to permit in-line use in these large-scale radiation-hydrodynamics simulations while retaining enough detail and coverage to support radiation transport, energetics and spectral simulation. The construction combines detailed, configuration-averaged and screened-hydrogenic data to cover all ion stages. We discuss accuracy and efficiency tradeoffs involved in the various averaging and consolidation methods used to minimize the model size, and present representative results and timings from one- and two-dimensional simulations.

References:

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.
ICF Related:

22. Measuring Mix in ICF Capsules with High Resolution Spectroscopy

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Mixing of shell material into the central hotspot during implosion is one of the most significant factors impeding ignition on NIF. X-ray spectroscopy of emission from pre-heat dopants in the mixed shell provides a path to diagnosing hotspot mix. Current x-ray diagnostics on NIF cover a broad band on wavelengths with relatively low resolution, allowing for an estimate of total mixed mass. An instrument with high spectral and spatial resolution could provide currently unavailable information on composition and behaviour of mixed material, by measuring Doppler shifts of individual lines emission. Vertical dispersion variant double crystal spectrometers (DCV) have been successfully fielded on high energy density plasma experiments in the past, and provide remarkable spectral and spatial resolution, and a very high signal to noise ratio. Results of ray tracing for a DCV using Ge(333) crystals suggests spectral resolving power >50000, with a peak exposure of ~10 photons/µm². The use of asymmetrically cut crystals would provide spatial magnification, improving spatial resolution, while maintaining high enough exposure on the detector for useful measurements.

23. Radiation influences of high-Z doped ICF capsule on implosion performance

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Radiation from high-Z dopant is believed to suppress hydrodynamic instabilities in an inertial confinement fusion (ICF) capsule and improves implosion performances. However, the radiation also preheats the inner side of the ICF capsule and induces a loss of areal density at the maximum compression. We have numerically analyzed hydrodynamic properties of the high-Z doped capsule and influence of discretized radiation spectra on the solution. Although low-resolution and narrow-range spectra is acceptable for a pure plastic shell, a larger number of energy groups covering a wider range is required for reproducing the implosion dynamics of the high-Z doped capsule.

Plasma Spectroscopy:

24. Creation and Diagnosis of Solid Density Plasmas

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In the past few years, several experiments using Ultra High Intensity lasers (10¹⁷ – 10¹⁹ W/cm²) have demonstrated the possibility to heat a layer of material to very high temperatures (hundreds of eV) with densities close to solid. Studying these plasma conditions is of great importance for the constraint of theoretical models of dense plasma Equations of State (EoS) and radiative opacities. To achieve this goal, plasma conditions (temperature, density, LTE/nLTE) must be well characterized.

We will show results of experiments performed on ELFIE laser facility at the LULI Laboratory and simulations of these experiments obtained from PIC, hydro-rad and atomic codes. Experimental data coupled with these simulations illustrate the difficulties and problems that occur in characterizing the plasma conditions: temporal gradient, spatial gradients, hot electrons, LTE/nLTE. Indeed, great Care must be taken in analyzing the results. Once these difficulties are overcome, a new avenue for the use of radiative properties in a new thermodynamic regime will be opened that will greatly benefit understanding in this challenging regime.

25. X-ray spectroscopy of well-characterized Al and KBr plasmas, in non local thermodynamic equilibrium (NLTE) conditions

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The X-ray emission of mid- to high-Z plasmas in NLTE conditions is particularly complicated to model. Benchmarking simulations is necessary, and the aim of this study is to measure NLTE emission under well-characterized hydrodynamic conditions. The issue of our experiments is to obtain measurements of emission and hydrodynamics parameters to constrain the hydrodynamic calculations and minimize the free parameters to be introduced in the atomic physics calculations. These measurements will be made with the help of independent diagnostics, namely time-resolved Thomson scattering, SOP, VISAR and interferometry.

We studied laser-created plasmas of KB and Al obtained by the irradiation of solid targets (thin foils or dots). The experiment took place at the LULI2000 laser facility. We used a frequency-doubled pump beam of 1.5 ns pulse duration, wavelength of 0.53 µm, focalized on a 200 µm dot, at about 10¹⁴ W/cm² intensity on target. These measurements will be compared with a previous experiment on the same elements, and with numerical calculations.
Advances in the understanding of high-energy-density plasmas (HEDP) depend on new well-diagnosed experiments, in particular, spectroscopic diagnostics and imaging. These cutting-edge experiments require state-of-the-art modeling capabilities. One of the traditional methods of studying the experimental observables is the post-processing of hydrodynamics simulations. SPECT3D is an application that uses hydro data to generate synthetic observables such as space-resolved and space-integrated spectra, wide-band and monochromatic images, time-gated images, streak spectra, etc. The hydrodynamic simulations can be performed by the code HELIOS-CR, which is a 1-D radiation-hydrodynamics code with an inline collisional-radiative model, or a variety of other 1-, 2-, and 3-D codes. Alternatively, a set of experimental data can be directly analyzed in an attempt to solve an inverse problem and deduce the conditions of a radiating plasma without relying on hydrodynamics models. Values of common interest (average plasma temperature, density, optical depth), can be readily obtained by comparing experimental data with the results of PrismSPECT spectral calculations. We will discuss the latest improvements to all these codes as well as VISRAD, which is a 3-D thermal radiation and CAD code that simulates the reflection, emission and absorption of light radiation throughout a complex system of surfaces. We will demonstrate their application for different classes of HEDP experiments.

Modelling Spectra from High Density, High Temperature non-LTE Plasma

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Experiments on the HELEN and Orion lasers at AWE have proved successful in measuring the spectra from high density, high temperature, plasma. The plasma in these experiments is generated by heating a target, deeply buried in plastic with a picosecond laser. The evolution of the target with time has proved difficult to model as the short timescales can produce large non-LTE effects. The Aurora code has been developed to model the spectra from these experiments; the final aim is to produce a code that is fast and robust enough to run inline in a radiation-hydrodynamics simulation. This paper shows the latest developments in the code and comparisons to experimental data.

Radiative Transport:

Spectral Modeling of a Semi-Infinite Slab—a Boundary Layer Problem

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To perform a radiation driven HEDP experiment on a target of moderate density ($\rho<\rho_0/100$) for which LTE conditions are desired, the target must be prepared by immersing it into a Planckian radiation field, $B$, where the total radiation energy density is described by Stefan’s law ($ER=aT^4$). Some HEDP experiments, due to constraints imposed by the radiation source, can only illuminate the target from one side, such as the opacity experiments being performed at the Sandia-Z facility. The goal of this work is to assess the conditions that lead to non-LTE behavior in semi-infinite plasmas. Assessing regimes for which an LTE plasma exists, albeit in an ideal geometry of a semi-infinite slab, is important in improving our understanding for these types of experimental platforms. To solve self-consistently the radiation field with the atomic kinetics, a new code, NORA, has been developed. This model employs many of the techniques developed by Mihalas and Auer in the complete-linearization method for modeling stellar atmospheres[1,2]. A general description of the self-consistent model and the atomic model will be presented as well as a description of spatial and material conditions that lead to non-LTE plasmas in single sided illuminated platforms.

References:
Serial femtosecond X-ray crystallography of protein nanocrystals using ultrashort and intense pulses from an X-ray free-electron laser has proved to be a successful method for structural determination. However, due to significant variations in image quality from pulse to pulse only a fraction of the collected frames are actually used in the reconstruction. Experimentally, the X-ray pulse shape is not known and can vary with every shot. This study describes how the pulse shape affects the damage dynamics, which ultimately affect the resolution and biological interpretation. The instantaneously detected signal varies during the pulse exposure due to the pulse properties, as well as the structural and electronic changes in the sample. Radiation damage processes were simulated using the radiation transfer plasma code CRETIN. Pulses with parameters typical for X-ray free-electron lasers were considered: pulse energies ranging from $10^7$ – $10^8$ J/cm$^2$ with photon energies from 2 to 12 keV, up to 100 fs long. Radiation damage in the form of sample heating that will lead to a loss of crystalline periodicity and changes in scattering factor due to electronic reconfigurations of ionized atoms are considered here. The simulations show large variations in the radiation damage processes due to differences in pulse shape. These variations cause significant differences in recorded diffraction pattern and will affect reconstruction.


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The 3-D view factor code VISRAD is widely used in designing high energy density physics (HEDP) experiments at major laser and pulsed-power facilities, including NIF, LMJ, OMEGA, OMEGA-EP, ORION, and Z. It simulates target designs by generating a 3-D grid of surface elements, utilizing a variety of 3-D primitives and surface removal algorithms, and can be used to compute the radiation flux throughout the surface element grid by computing element-to-element view factors and solving power balance equations. Target set-up and beam pointing are facilitated by allowing users to specify positions and angular orientations using a variety of coordinate systems (e.g., that of any laser beam, target component, or diagnostic port). Analytic modeling for laser beam spatial profiles for OMEGA DPPs and NIF CPPs is used to compute laser intensity profiles throughout the grid of surface elements. VISRAD includes a variety of user-friendly graphics for setting up targets and displaying results, can readily display views from any point in space, and can be used to generate image sequences for animations. We will discuss recent improvements to the software package and plans for future developments.

32. A Hybrid Model for radiative transfer in Laser-ablated Plasmas

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Plasmas created by Laser ablation are expected to be used as an efficient media for the generation of short-wavelength light. However, an accurate prediction of the plasma that can range from low to high density is difficult because conventional numerical models are constructed to describe only a specific range of electron density. In particular, the appropriate form of the equations will change due to radiative transfer, depending the optical transparency of the media. We have developed a hybrid model for the radiative transfer to predict the emission and resultant dynamics of the laser-ablation plasma.

X-Ray Sources & XFELs:

33. X-ray Thomson scattering of shocked carbon foam on the Z-accelerator

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For the first time, a space-resolved x-ray Thomson scattering (XRTS) spectra from shocked carbon foam was recorded on the Z-accelerator. The large electrical current produced by the Z-accelerator was used to launch an Al flyer plate to 25 km/s. The impact of the flyer plate on a CH$_2$ foam target produced a shocked state with an estimated pressure of 0.75 Mbar, density of 0.5 g/cc, and temperature of 4.3 eV. Both unshocked and shocked portions of the foam target were probed with 6.2 keV x-rays produced by focusing the Z-Beamlet laser onto a nearby Mn foil. The data comprises of three, spatially distinct spectra that were simultaneously captured with a single spectrometer. These three spectra provide detailed information on the following target locations: the laser spot, the unshocked foam, and the shocked foam. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy’s NNSA under contract DE-AC04-94AL85000.

34. Intensity Dependent Transmission of X-FEL pulses in Aluminum


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The intensity dependent transmission of an x-ray free electron laser (X-FEL) pulses at the below K-absorption edge of aluminum is explored at the SXR beamline of the Linac Coherent Light Source. In this photon energy range, the well-known high transmission has been described by the relatively low L-shell absorption cross sections. However, when intense X-FEL pulses were tuned at the K-shell, the resulting x-ray transmissions show significant differences. In this contribution, X-ray intensity and photon energy dependent transmission data of aluminum foil obtained using a photodiode of SXR beamline as well as the collisional-radiative simulations using SCFLY code will be presented. The difference in transmission could be ascribed to the resonant absorption channel including K-electrons, which is newly opened up by high intensity of x-rays.

35. The average atom model combined the hypernetted chain approximation applied to warm dense matter

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We have combined the average-atom model with the hypernetted chain approximation (AAHNC) to describe the electronic and ionic structure in the warm dense matter regime. On the basis of the electronic and ionic structures, the x-ray Thomson scattering (XRTS) spectrum is calculated using the random phase approximation (RPA). The electronic structures are described by using our average-atom (AA) model, and at the same time, the effects of other ions on the electronic structures are considered using the integral equation of fluid theory. The ionic structures are obtained through the hypernetted chain approximation (HNC), where the ion-ion pair potentials are calculated using the modified the Gordon-Kim (GK) model based on the electronic density distributions. And the electronic and ionic structures are given using the self-consistent field method. The XRTS spectrum is calculated according to the Chihara formalism, where the scattering contributions are divided into three components: elastic, bound-free, and free-free. Comparison with the results of other theoretical models and experiments shows the XRTS spectra obtained are very good agreement, thus the AAHNC model can give a reasonable description of the electronic and ionic structures in the warm dense matter regime.

36. Plasma Dynamics in ultra-short relativistic laser-solid matter interactions and synthetic diagnostics using XFELs

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Abundant and complex plasma dynamics are triggered by optical ultra-short high power lasers interacting on solid targets: such as atomic ionization, hot electron generation and transportation, collisions between the charged particles, return current, bulk electron heating, ion heating and acceleration, instabilities etc. Controlling the relative dynamic processes requires modelling of transient, non-equilibrium processes on the atomic scale. We present particle-in-cell simulations which studied enhanced ion heating in buried layer targets [1], ionization dynamics and instabilities. In order to connect the plasma dynamics seen in simulations with experiments we will discuss the role of in-situ synthetic diagnostics that mimic experimental diagnostics. As one key example we propose to use X-Ray Free Electron Lasers for probing laser-driven solid-density plasmas by using the small angle X-ray scattering [2] which allows for femtosecond temporal and nanometer partial-resolution of transient plasma processes. With these techniques, probing fundamental plasma properties will allow for direct comparison to simulations, challenging state of the art theoretical modeling of collisions, ionization, radiation transport and atomic processes.

References:

37. X-ray scattering measurements of shocked matter using LCLS FEL beam

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There has been much effort to measure properties of warm dense matter (WDM) that represents a difficult aspect of matter at extreme conditions, as it is at temperatures above several 1000 K and has pressures in the Mbar regime. In laboratory experiments several thermodynamic properties of WDM have been investigated using shock-wave techniques. However, practical issues with gradients in the temperature and density that occur in shock compressed matter have hindered accurate measurements and have made distinguishing among competing theoretical models quite difficult. Here, we present spatially and spectrally resolved x-ray scattering experiments using the LCLS free electron laser to examine and understand the gradients in the properties of matter under dynamic shock loading. We used toroidally curved Ge 111 crystal for imaging spectrometer resulting in 44 μm spatial resolution. The result will be compared with data from HAPG spectrometer.
X-ray Spectroscopy of Dense Laser-produced plasmas


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Recent results from LCLS show larger depressions of the ionisation potential in strongly-coupled solid-density plasmas at temperatures up to 200 eV, than in hotter (500 – 700 eV), less coupled systems produced with the ORION optical laser based at the AWE in the UK. To date both sets of results have been simulated with approaches based on the zero-dimensional collisional-radiative atomic kinetics codes FLYCHK band SCFLY. Opacity is incorporated into these codes via an escape-factor formalism. A more thorough approach requires a self-consistent treatment of the radiation and the atomic populations within a full 3-dimensional treatment. Such a capacity is included in the CRETIN code, which we have used to produce X-ray spectra for solid-density laser-produced plasmas, and compared with SCFLY.

References:
Temperature determination of mixed Z buried layer targets using time-resolved and time integrated K-shell spectroscopy

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Short pulse laser heated buried layers experiments have been performed with the goal of studying emission characteristics of plasmas with mass densities $\geq 1$ g/cm$^3$ and electron temperatures $\geq 500$ eV. The buried layer geometry has the advantage of rapid energy deposition before significant hydrodynamic expansion occurs. For brief periods ($\leq 50$ ps) this provides a low gradient, high-density platform for studying emission characteristics under extreme plasma conditions. A study of plasma conditions achievable using the Orion laser facility has been performed. K-shell materials were used to determine the range of parameters that may be obtained in this geometry at the Orion facility.

Session 9. Plasma Spectroscopy and Simulations II

Energetic Electrons Driven in the Polarization Direction of an Intense Laser Beam Incident on a Solid Target

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Experiments were performed at the LLNL Titan laser to measure the propagation direction of the energetic electrons that were generated during the interaction of the polarized laser beam with a solid target. The target consisted of a central irradiated wire, two wires positioned above and below the irradiated wire in the vertical direction of the polarization of the incident laser beam, and two wires positioned on the sides of the irradiated wire in the horizontal direction, perpendicular to the polarization direction. The irradiated wire, the vertical wires, and the horizontal wires were of three different materials, for example Ho, Gd, and Dy. The K\textalpha lines from the three materials were recorded by a transmission crystal spectrometer on each laser shot. The relative intensities of the K\textalpha lines from the vertical and horizontal wires were measures of the fluence of energetic electrons driven in the polarization direction and in the perpendicular direction, respectively. The gap between the irradiated wire and the vertical and horizontal wires was varied on sequential laser shots, and the intensities of the K\textalpha lines were a measure of the angular distribution of the energetic electrons propagating from the irradiated wire. It was found that the fluence of energetic electrons was larger in the vertical direction of the polarization as compared to the perpendicular (horizontal) direction. This implies energetic electrons are preferentially driven in the direction of the intense oscillating electric field of the incident laser beam. Analytical modeling of the energy and angular distribution of the energetic electrons propagating from the irradiated wire will be presented.

This work was funded by the Defense Threat Reduction Agency, grant number DTRA-1-10-0077 and by the NNSA-DS and SC-OFES Joint Program in High-Energy-Density Laboratory Plasmas, grant number DE-NA0001840.

Spectroscopic measurements of high energy density plasma and Comparisons to Atomic Kinetics Models.

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Spectroscopic experiments on the Orion laser have demonstrated high electron temperatures up to 2.5keV and electron densities in excess of $10^{24}$/cm$^3$. K-shell spectra from samples of scandium/aluminium and sulphur/europium mixtures, buried in plastic and diamond sheet targets, have been measured using a crystal spectrometer coupled to an X-ray streak camera with 1ps temporal resolution and measured time-integrated with a variety of crystal spectrometers recording onto image plates. The results are presented and compared to modelling using the radiation-hydrodynamics code NYM; the atomic kinetics codes FLYCHK and ALICE, and a coupled PIC/radiation-hydrodynamics model. The implications for the study of spectra from laboratory plasma at the conditions of the solar core/radiative zone boundary are discussed.

Analysis of X-Ray Nike Spectra from Highly-Charged High-Z Ions*

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We present measurements and interpretation of x-ray spectra from hot plasmas of high-Z ions produced with the KrF Nike laser operating at the Naval Research Laboratory. The spectra of laser-irradiated foils of heavy elements such as Au, Pt, Hf, and others were recorded at the power density of $2 \times 10^{14}$ W/cm². The use was made of two spectrometers, namely, a wide-band convex-crystal survey instrument and a narrow-band high-efficiency spectrometer using a spherical crystal. The main characteristics of the spectrometers and sample spectra will be presented.

Simulations of the measured spectra were performed using the collisional-radiative code NOMAD. The atomic data including level energies, radiative and autoionization transition probabilities, and collisional cross sections were calculated with the relativistic Flexible Atomic Code. A typical simulation would include about six ionization stages with a total of ~30,000 atomic levels. The effects of ionization potential lowering and plasma opacity were taken into account as well.

Atomic Code. A typical simulation would include about six ionization stages with a total of ~30,000 atomic levels. The effects of ionization potential lowering and plasma opacity were taken into account as well.

The synthetic spectra will be compared with the measured data. The strongest identified spectral lines belong to Ni-like ions; there are also satellites from lower ionization stages as well as lines from Co-like ions. The typical values of electron temperature and density derived from comparisons are on the order of 2000 eV and $10^{21}$ cm⁻³.

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Modeling of plasma through reliable electron-impact cross-sections

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Dominant processes involved in plasma modeling are the electron impact processes. Despite the large body of literature on inert gases and various W ions, there is in general serious lack of excitation cross section data for their various fine-structure transitions [1-3]. Also the growing demand of electron-atom/ion collision data can’t be met solely through experimental measurements.

Due to the complexity involved in dealing with the fine-structure transitions the theoretical data used for plasma modeling have been obtained from empirical or simple classical methods that are not reliable. Consequently, reliable fine-structure cross sections are required to be calculated using fully relativistic theory and then incorporated into the collisional-radiative (CR) model for low and high temperature plasma modeling [3].

There is need to develop CR models for both inert gases and tungsten plasma. Inert gases are added in trace amounts to various plasmas for diagnostic purposes, known as trace rare gas optical emission spectroscopy (TRG-OES). Tungsten is of great interest in fusion engineering as a potential plasma-facing material in magnetic confinement devices.

In the presentation, a CR model that we have developed for argon and krypton plasma will be discussed where we have incorporated detailed fine structure excitation cross sections calculated by us using fully relativistic distorted wave (RDW) theory [3, 4]. For tungsten ions, we have applied our RDW method to study electron impact excitations of 3d–4p and 3d–nf (n = 4–8) transitions from the M-shell of the Zn-like W⁴⁺, Cu-like W⁵⁺, Ni-like W⁶⁺ and Co-like W⁷⁺ ions [5] as well as $n=2\rightarrow3$ transitions from L shell of the ground state in Mg-like W⁴⁺, Na-like W⁵⁺, Ne-like W⁶⁺, F-like W⁶⁺, O-like W⁷⁺ ions [6] relevant to high temperature fusion plasma. Different results along with the theoretical details will be presented.

References:

Thursday, October 2nd

Session 10. Ionization Potential Depression

A plea for a reexamination of ionization potential depression measurements

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Experiments at the Linac Coherent Light Source determined the ionization potential depression (IPD) in dense plasmas by measuring the Ka fluorescence associated with K-shell holes created by the x-ray free-electron laser. The analysis of the experimental spectrum found a significantly larger IPD than predicted by the widely used Stewart-Pyatt model. It is shown, however, that a more accurate treatment of atomic levels than used in the analysis has additional channels reducing the threshold laser energy for creating Ka photons without invoking a large increase in the IPD. Thus, it is argued that a simulation of the Ka fluorescence using improved atomic data could impact the interpretation of the experimental results.
Quantum-mechanical calculation of ionization potential lowering in dense plasmas

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The charged environment within a dense plasma leads to the phenomenon of ionization-potential depression (IPD) for ions embedded in the plasma. Accurate predictions of the IPD effect are of crucial importance for modeling atomic processes occurring within dense plasmas. Several theoretical models have been developed to describe the IPD effect, with frequently discrepant predictions. Only recently, first experiments on IPD in Al plasma have been performed with an x-ray free-electron laser, where their results were found to be in disagreement with the widely used IPD model by Stewart and Pyatt. Another experiment on Al, at the Orion laser, showed disagreement with the model by Ecker and Kröll. In this talk, I will present a rigorous and computationally efficient approach to predicting IPDs: a two-step Hartree-Fock-Slater model. Our approach is based on first-principle quantum-mechanical calculations for an atom embedded in a dense plasma, taking into account detailed electronic configurations of plasma ions. I will demonstrate that, in contrast to the Stewart-Pyatt and Ecker-Kröll models, our model successfully describes all available experimental data on IPDs. Calculations within our approach are relatively inexpensive and, therefore, are expected to be applicable for a wide range of plasma conditions, including warm dense matter, planetary science, and inertial confinement fusion.

Ionisation energies in strongly driven matter

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Short-pulse lasers and, particularly, free electron lasers have made it possible to drive dense matter into states far from equilibrium. Such systems might have just different electron and ion temperatures, an imbalance of structural and energetic properties or even electron distributions deviating substantially from the Maxwell-Boltzmann or Fermi distribution in equilibrium. In such cases, the nonequilibrium and relaxation properties will modify almost all system properties. Nevertheless, most modeling capabilities and tools to analyse experimental data rely heavily on temperature-based concepts, thus, neglecting the effects of nonequilibrium distribution functions.

In this contribution, we will demonstrate how nonequilibrium electron distributions can modify the bound state levels in dense, strongly driven matter. Several simulation schemes have shown that solids and gases subject to intense FEL radiation have nonequilibrium states persisting over the time of the measurement. Thus, the atomic physics will be affected as well. We first show this fact within linear response giving modified formulas for the Debye- or Thomas-Fermi-like depression of the ionisation potential. As usual, these results are then combined with the ion sphere model. Strong changes of the effective ionisation energies arise when the electron distribution is shifted. Within some robust assumption of the form of the distribution, we also obtain energy shifts much closer to recent measurements in aluminium than the Steward & Pyatt model, assuming equilibrium distributions. Unfortunately, robust modeling tools for the relaxation behaviour in warm dense matter are lacking and, thus, any agreement with measurements is built on certain assumptions.

Statistical properties of coupled plasmas in the framework of the classical two-component plasma MD simulations.

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Hot and dense plasmas are commonly investigated using classical molecular dynamics. In the more recent developments electron / ion mixtures are considered in MD codes. Such a code, the BINGO-TCP code has been designed with two specific features useful in the framework of high-density plasmas. First, it partially accounts for quantum properties of individual ions, namely the ionization potential, included as a parameter in electron / ion potentials depending on the ion charge states. Second, it involves an ionization / recombination protocol allowing the plasma to reach a stable ion charge distributions [1]. This is implemented by ignoring electron degeneracy and restricts a priori the validity domain of the BINGO-TCP code. Investigations carried out for warm dense matter conditions have shown that depending on the sampled quantity electron degeneracy can be ignored or improved using phenomenological tricks [2]. This approach benefits from all the advantages of molecular dynamics that relies on a minimum set of postulates avoiding a systematic use of the Born-Oppenheimer approximation. The BINGO-TCP code exploits extensive sampling and provides statistical data about structure and dynamics properties of electrons and ions. A straightforward access to the electron dynamics properties of the free electron population in the plasma appears as a net advantage of the method. Applications to Thompson diffusion on Beryllium plasmas are reported as illustration. A second illustration is provided by an investigation of the ionization potential depression in dense aluminium plasmas. Through these examples it appears now that classical MD can be considered for the interpretation of dense plasma experiments including warm dense matter.

References:

Session 11. Ionization Potential Depression

Density functional theory calculations of continuum lowering in strongly coupled plasmas

Sam Vinko
An accurate description of the ionization potential depression of ions in plasmas due to their interaction with the environment is a fundamental problem in plasma physics, playing a key role in determining the ionization balance, charge state distribution, opacity and plasma equation of state. Here I will present a method to study the structure and position of the continuum of highly ionized dense plasmas using finite-temperature density functional theory in combination with excited-state projector augmented-wave potentials. The method is applied to plasmas created using intense X-rays from the Linac Coherent Light Source (LCLS) free electron laser, and shows excellent agreement with recently obtained experimental results. We find that the continuum lowering at intermediate temperatures is larger than predicted by standard plasma models and explain this effect through the electronic structure of the valence states in these strong-coupling conditions.

Density-independent continuum lowering in HDM


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By using the experimental technique described in [1], we have measured - with charge state resolution - the ionization potential depression (IPD) in solid density plasmas from different elements and compounds. The results confirm the stronger depression, as observed in [1], than that predicted by the usual ion-sphere models. The previous results are well reproduced by DFT calculations [2], which explain them in terms of an electron density, which resembles the neutral free atom’s electron distribution, rather than the uniform electron density used in the analytical models. A comparison between the measurements for the elements and their compounds provides strong evidence for the IPD in strong coupling being determined only by the atomic properties of the species of interest rather than by the overall density of the system.

References:

The effect of Anderson localization on pressure ionization

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Average-Atom models of hot dense matter encounter difficulties in describing pressure ionization. The single-electron Schroedinger equation is typically solved in the time-averaged effective potential of an ion, which is spherically symmetric. This produces spectra, which often contain unphysically narrow resonances. Direct application of the Born-Oppenheimer approximation dictates that the instantaneous effective potential should be used instead. This potential contains 3-dimensional disorder due to the random positions of all the other ions. It is well known in the field of condensed-matter physics that the eigenfunctions of the single-electron Schroedinger equation in such potentials are subject to Anderson localization: electrons at energies for which the disorder generates a mean-free-path for elastic scattering which is shorter than the de Broglie wavelength do not propagate freely through the plasma, and are instead exponentially localized. Alternatively, one may employ the sensitivity of the eigenstates to periodic boundary conditions, identifying localized states as those with sensitivities smaller than the mean level spacing, and delocalized states with larger sensitivities. In the context of condensed matter, these two alternatives are known to be equivalent.

So far, the effect of Anderson localization has not been included in average-atom plasma models, even at a qualitative level. This is somewhat surprising, as it is natural to associate bound electrons with localized states and free electrons with delocalized states. Descriptions which address this deficiency, based on solutions of the Schroedinger equation in the spherically symmetric time-averaged effective potential (limited to the volume of a single ion-sphere) were studied. On the basis of these solutions, the abovementioned quantities – the mean-free-path and the sensitivities – were evaluated, and the position of E_{loc}, the energy at which the transition from localized (bound) to delocalized (free) electrons occurs, was estimated. In the process of doing so, it was necessary to revisit the evaluation of the density of states of the plasma, and to employ an appropriate average-atom description of the crossover from discrete bound states at negative energies to continuous free states at positive energies. Quantitative results of numerical studies of the Anderson model of disorder, obtained in the condensed matter context, were applied to the plasma. In evaluating the degree of ionization as a function of density and temperature, it was found that the effects of disorder on the density of states should be taken into account, in addition to the shift of the boundary between bound and free electrons from the standard E = 0 to the more appropriate E =
E_{loc}. For energies very close to E_{loc}, electrons are bound not to a single ion but to a spatial region containing many ions, measured by the localization length, which grows as E_{loc} is approached. The correlation length for delocalized states similarly diverges at E_{loc}.

Session 12. FELS Experiment and Theory I

Modeling of nanoplasmas created from finite-size systems

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In my talk I will give an overview on the recent results of our theoretical investigation how the unique properties of X-ray free-electron laser (FEL) radiation can be employed to create and investigate dense plasmas. I will discuss the applications of molecular dynamics and transport approach to follow the evolution of nanoplasmas created by intense FEL pulses from finite-size systems.

A Plasma based description of the ultra-fast ionization and structural changes in protein nanocrystals

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As X-ray free-electron-lasers (XFEL) are becoming available to the macromolecular crystallography community, structural determination using small nano-sized crystals will likely become routine. The damage process in nanocrystals illuminated by intense femtosecond X-ray lasers leads to a loss of structural coherence during exposure and a consequential change of the Bragg signal that decreases with increasing resolution. The ultra-intense pulses can ionize every atom in the sample, creating an exotic state of matter with hot free electrons, which ultimately transfer energy into atomic motion, leading to loss of Bragg diffraction. The relevant variable that will influence imaging at high resolution is the incident photon intensity at the sample before the Bragg diffraction is gated, while the rest of the pulse will mainly contribute to background through diffuse scattering. We present a plasma-based description of the ultra-fast ionization and structural changes in protein nanocrystals as a result of photon bombardment from the short intense X-ray pulses, and compare to experiments.

Probing ultrafast, transient plasma dynamics at solid density with X-ray lasers

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Combining high power lasers with x-ray lasers provides unique opportunities to study ultrafast, transient processes in solid-density plasmas. We present simulation studies of probing ionization dynamics, electron transport and heating of solid-density targets driven by high power lasers with state-of-the-art X-ray lasers. We show that a precise understanding of the underlying atomic physics processes is necessary and needs to be implemented in kinetic simulations of the laser plasma interaction. Our results show that albeit the complexity of atomic processes happening during the laser plasma interaction, the very same processes can be exploited to understand the temporal evolution of the plasma.

Saturable absorption of a hard x-ray free-electron-laser heated solid-density aluminium plasma

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High intensity x-ray pulses from an x-ray free electron laser are used to heat and probe a solid-density aluminium sample. The photon energy dependent transmission of the heating beam is studied through the use of a photodiode. The resulting transmission is found to differ significantly from the cold case, however it agrees well with atomic-kinetics simulations. The difference is attributed to variable levels of saturable absorption achieved under irradiation by intense x-rays at different photon energies.

Session 13. FELS Experiment and Theory II

Generalized atomic kinetics to treat heating of solids under short intense XFEL irradiation

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The energy deposition calculation is a key issue to study the warm/hot and dense matter produced during interaction of intense femtosecond XUV/X-ray radiation with solid materials. The pulse is mainly absorbed via photoionization of bound electrons, which means a very different deposition of energy compared to optical lasers, and thus requires a bound electron kinetics treatment. We propose here a generalization of the detailed configuration accounting (DCA) approach, up to the solid state, to treat the heating of the valence band (VB) electrons of solids, under XUV/X-ray radiation. The important solid-state processes involving electrons of the VB (e.g. Auger processes, fluorescence) are linked to the standard isolated atom DCA processes to get a progressive and coherent transition from the cold to the heated solid-density plasma. We account for the degeneracy of the VB electrons with a Fermi-Dirac distribution and by using appropriate Pauli-blocking factors. We used our model to treat the interaction of 75 to 120-eV photons with solid aluminum, with intensities between $10^{13}$ to $10^{17}$ W/cm$^2$ and 15-fs to 150-fs pulse durations (FLASH parameters). In this photon energy range, the main channel of absorption is the photoionization of the 2p shell (with a first 2p edge at 73 eV and a second at 93 eV in the cold solid). First, we report the effect of the shift of the cold edges when heating the VB to constant solid density. Then, we focus on the importance of the different elementary processes included in our collisional radiative model. We found that the effect of Auger decay (which as been linked to the process of 3-body recombination in the heated solid density plasma) and the process of collisional ionization are of great importance for the XFEL absorption. Finally, we present the integration of this 0-dimension model in a 1D decay (which as been linked to the process of 3-body recombination in the heated solid density plasma) and the process of collisional ionization are of great importance for the XFEL absorption. Finally, we present the integration of this 0-dimension model in a 1D Lagrangian hydrodynamic code dedicated to XFEL-matter interaction [see, O. Peyrusse, Phys. Rev. E 86, 036403 (2012)], to study the relaxation of the plasma on larger time scales.

Coherent dynamics of open quantum systems

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We develop a multilevel atomic master equation approach and theoretically investigate coherent dynamics of inner-shell electrons of neon atoms irradiated by a high-intensity X-ray laser. This method combines the processes of coherent dynamics induced by the X-ray laser and incoherent relaxations due to spontaneous and Auger decays. We find that coherence can suppress the multiphoton absorptions of neon in the ultra-intense X-ray pulse, compared to rate equation approach, due to coherence-induced Rabi oscillations and power broadening effects. We study the coherence in ionization processes of neon, and find that multiphoton ionization processes of valence electrons come into play for the strong X-ray laser beam, while sequential single-photon processes of inner-shell electrons dominate the absorption for the present typical experiments with a laser intensity of $\sim 10^{19}$ W/cm$^2$. We discuss possible experimental implementations such as signatures for coherent evolution of inner-shell electrons via resonance fluorescence processes.

Resonant photo-pumping of a hot, near-solid density plasma using an X-ray free electron laser

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The understanding of laser-produced plasmas plays a central role across a wide range of areas interesting to physicists: interstellar media, astrophysics, tokamak impurity studies, and inertial confinement fusion science. Most of the plasmas observed in these various areas are in non-local thermodynamic equilibrium (NLTE), the description of which involves complex and detailed atomic processes. It is non-trivial to identify these processes that are at the core of the population kinetics and atomic physics codes; however, slow progress has been made over the last 40 years. The slowness is mainly due to the lack of a versatile, reliable probe. These issues may be overcome with the recent advent of 4th generation of X-ray light sources, i.e., X-ray free electron lasers (XFEL). The XFELs have exceptionally high peak brightness, short pulse durations, spectral tunability and small spectral bandwidth, making them a perfect candidate to study the dynamics of hot and dense plasma formation and dynamics on the atomic level.

We report on the first experiment that uses a free electron laser to resonantly excite an atomic population in such plasma state. Here, an uncompressed optical laser pulse irradiated an aluminium foil to produce a hot and near-solid density plasma. Then, at different time delay in the plasma evolution, the LCLS X-ray beam resonantly pumped the plasma by selective photo-excitation of an electron in the He-like Al ground state. The energy of the probe photons was tuned to match various excited states up to the
X-ray free electron lasers are creating game-changing science in physics, chemistry and life sciences. Illumination of single biological particles extremely intense and ultra-short X-ray pulse yields high-quality diffraction patterns, although the energy deposited into the sample turns it into a high-temperature plasma. We describe diffraction experiments on single sub-micron particles at X-ray free electron lasers (FLASH and LCLS), made in combination with mass spectrometry measurements to characterise the X-ray-induced fragmentation of the sample. Single diffraction patterns indicate that the particles are intact during the exposure. The ion time of flight measurements give a glimpse on the complicated dynamics generated in a confined plasma by ultra-intense X-ray pulses. We use non-LTE plasma modeling to understand and support our observations.

**Beating the recombination time scale in nanoplasmas induced by X-ray flash diffraction of a biological particles**

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We present a talk to illustrate how the High Energy Density Physics (HED) instrument at the European XFEL [1] will be realized. Following an overview of the current status of XFEls and VUV-FELs, the capabilities planned for the HED instrument will be presented. We have recently published the Technical Design Report for this instrument [2], which also described its time schedule leading to the start of user operations in 2017. With this contribution, we aim at: (1) to provide information to the community concerning a new and unique platform for the study of hot-dense-matter science, and (2) to engage a wider group of researchers who can provide feedback on their future plans, which will assist in improving the High Energy Density instrument design.

**References:**


**XUV High-Order Harmonic probing of XFEL created Warm Dense Matter**

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The extreme ultra-violet (XUV) optical response of warm dense aluminium is a subject of much theoretical interest, yet lacking in experimental data. Recent experimental results pertaining to the optical properties of warm dense aluminium are reported. Thin foils of aluminium were heated with 60 fs pulses of x-rays above the aluminium k-edge at the LCLS. A probe pulse of XUV light from high harmonic generation (HHG) was used to measure optical properties during the transition from a cold solid, to the warm dense regime, and the plasma conditions were inferred from x-ray emission spectroscopy. The short pulse heating mechanism naturally separates the ion and electron temperatures in time, giving a unique insight into the contribution of each to the optical properties. An overall increase in absorption with increasing temperature was observed, in agreement with models, yet the exact values of transmission and rate of absorption are outstandingly difficult to measure experimentally.
heating were not in good agreement. This work is an important indicator for future theoretical approaches, as well as future experiments.

**Resolving ultra-fast heating of dense cryogenic hydrogen**

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Knowledge of thermodynamic properties of matter under extreme conditions is critical for modeling stellar and planetary interiors, as well as for inertial confinement fusion (ICF) experiments. Of central importance are the electron-ion collision and equilibration times that determine the microscopic properties of matter related to reflectivity and thermal conductivity. On a macroscopic scale, these affect the depth of mixing layers in Jovian planets, as well as the formation of a central hot spot and the assembly of a stable thermoneutral fuel layer in ICF implosions. Uncertainties in the transport properties in dense matter limit our ability to accurately model such complex systems. As a versatile diagnostic tool for warm and dense matter states, x-ray scattering was demonstrated on picosecond and nanosecond time scales. With the advent of free electron lasers (FELs) the implementation of volumetric x-ray heating and accurate x-ray scattering on the femtosecond time scale is now becoming possible due to the short FEL pulse lengths (< 300 fs), their unprecedented peak brightness, and the high repetition rate. To investigate dynamic processes of warm dense matter on such short time scales, pump-probe experiments are necessary, where a first pulse generates an excited state that is subsequently probed by a second pulse at well-defined time delays.

We have used the split and delay capability of FLASH to produce two pulses of comparable intensity to volumetrically heat dense cryogenic hydrogen and subsequently probe it by soft x-ray scattering. The total scattered fraction rises to a peak value of 4x10^-6 within 0.9 ps, remaining constant for delays up to 2 ps [1]. This dynamics is reproduced with a Saha model for ionization. In contrast, simulations using a quotient equation of state (QEOS) show quasi-instantaneous heating within the FEL pulse duration of 300 fs [2].

**References:**


**Particle simulation of photoionization by ultra-high power X-ray laser**

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In this work, a molecular dynamics (MD) particle simulation is combined with the atomic kinetics described by a collisional-radiative (CR) model. Various physical processes, such as photoionization and Auger transitions, which occur during the interaction of X-ray free-electron laser with solid Fe targets are included in the particle simulation. The simulation shows similar results to those obtained in recent experiments at X-ray intensities up to 10^20 Watts/cm^2, which may be the brightest X-ray beam in the entire Universe. The MD+CR simulation offers a new approach toward understanding such high power laser interactions with matter.

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**Session 15. Atomic Physics in Plasmas**

**A study of density effects in plasmas using analytical approximations for the self-consistent potential**

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Since the first studies in a stellar atmosphere context, the analysis of density effects in ionized matter has attracted a considerable interest. Several theoretical approaches have developed, most of them being conducted within the ion-sphere or the ion-correlation framework. We have chosen here to use an ion-sphere approach involving a Thomas-Fermi-like description for free electrons, the bound electrons being described by a full quantum mechanical formalism. This allows us to deal with plasmas out of thermal local equilibrium, assuming only a Maxwell distribution for free electrons. Moreover we show that such a theory allows us to obtain accurate and simple analytical approximations for the potential created by free electrons. We estimate preferable to put the emphasis on the plasma potential rather than on the electron density, since the energies and wavefunctions depend directly on this potential. Beyond the uniform electron gas model, temperature effects may be analyzed. In the case of H-like ions, this formalism provides analytical perturbative expressions for the energies, wavefunctions and transition rates. Such expressions can be compared to numerical results obtained with a detailed atomic package, which is also used to describe plasma environment effects for arbitrarily charged ions.

**A New Method for Atomic Physics Calculations**

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A new method for performing atomic physics calculations is presented.[ Hill E.G. JQSRT 140 1-6 (2014) and Hill E.G. JQSRT 147 71-78 (2014 ) ] The method uses Slater determinants to form a subset of magnetic fine structure levels and then recovers quantities familiar from Racah algebra based methods allowing the calculation of the full compliment of energies and rates required for an atomic kinetics model. The method's advantages and competitiveness relative to Racah algebra and its applications, including in an atomic physics/kinetic model ALICE, will be discussed.