Understanding Extreme Atomic Physics at Gbar Pressure

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Spectroscopic measurements of dense plasmas at billions of atmospheres (i.e., Gbar = billions of times the pressure at the Earth's surface) provide tests of the fundamental understanding of how matter behaves at extreme conditions, and by extension, the interpretation of dense astrophysical objects such as white dwarf stars. Developing reliable atomic physics models at these conditions, benchmarked by experimental data, is crucial to an improved understanding of radiation transport in both stars and inertial fusion targets. However, detailed spectroscopic measurements at these conditions are rare, and traditional collisional-radiative-equilibrium (CRE) models,[1] based on isolated-atom calculations and *ad hoc* continuum lowering models, have proved questionable at and beyond solid density, leaving open the possibility for more-accurate methods.

Reported here are x-ray spectroscopy measurements at gigabar pressures using laser-driven implosions. These measurements are used to test a density functional theory (DFT)-based multiband kinetic model (*VERITAS*), which was developed in this work. The *VERITAS* model uses DFT-derived band (atomic level) information to compute the radiative transition rates that can be coupled to the radiation transfer equation to describe the radiation generation and transport processes in a dense plasma. With Cu (as a witness element) doped inside a 30-μm-thick plastic shell implosion, time-integrated and time-resolved Cu K_α emission and 1*s*–2*p* absorption measurements during shell stagnation were performed. These observations are directly connected to the time-dependent atomic ionization balance in the assembled dense plasma. The system is further constrained by integrated measurements of the compressed areal density (ρR), neutron yield, bang time, and ion temperature, allowing the spectroscopic data to differentiate the DFT-based kinetic model from traditional treatments based on isolated-atom calculations and *ad hoc* continuum-lowering models.

DRACO-simulated dynamic plasma conditions was used to investigate x-ray generation and transport through the target using two CRE models (*ATBASE* and *FAC*) and the DFT-based kinetic code *VERITAS*. The predicted time-integrated spectra are compared with the experimental measurements in Fig. 1, in which the x-ray signal is plotted as a function of photon energy (all normalized to the continuum signal level at 7800 eV). The experimental spectra [Fig. 1(b); target is shown as inset in Fig. 1(b)] show both the pronounced K_α emission peaked at ~8042 eV and the 1*s*–2*p* absorption of Cu in the higher-photon energy range of 8100 to 8250 eV. Both the location and amplitude of the emission and absorption features are appropriately captured by *VERITAS* [Fig. 1(a)].

Figures 1(c) and 1(d) show the *Spect3D* simulation results in which either the atomic database (*ATBASE*) or the flexible atomic code (*FAC*) calculations are combined with the Ecker–Kroll and Stewart–Pyatt continuum-lowering models. When these CRE results are compared to experiments, they give a conflicting conclusion about the continuum-lowering model. Namely, the experimental emission and absorption features are qualitatively reproduced by the two CRE simulations of "*ATBASE* + Stewart–Pyatt" and "*FAC* + Ecker–Kroll" in Figs. 1(d) and 1(e) (although the emission peaks are too high), while the other two combinations

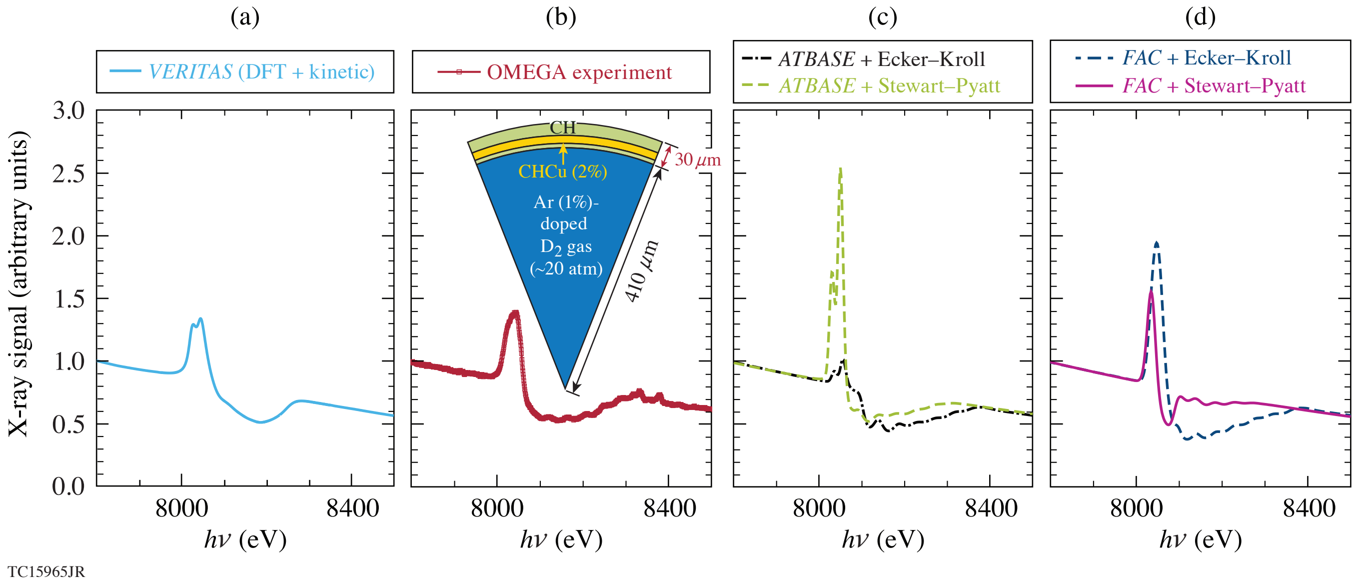

Figure 1
Comparisons of time-integrated x-ray spectra: (a) *VERITAS* DFT model prediction for the time-integrated K_α emission and 1*s*–2*p* absorption signals from a laser-driven implosion with a Cu-doped plastic layer. The model prediction is compared to (b) OMEGA experimental data, (c) CRE model predictions using the atomic database *ATBASE* in combination with Stewart–Pyatt and Ecker–Kroll continuum-lowering models, and (d) CRE model predictions using the *FAC* code with two different continuum-lowering models.

drastically disagree with experiments. This illustrates again the dilemma of the traditional spectroscopic treatment for warm dense plasmas: which *ad hoc* continuum-lowering model works better depends on the atomic physics model that is invoked. The resemblance between the *FAC* + Ecker–Kroll model [Fig. 1(d)] and experiments is likely coincidental since other recent measurements of ionization-potential depression have defied the Ecker–Kroll model. Overall, the DFT-based *VERITAS* model,[2] without invocation of an *ad hoc* continuum lowering model, better resembles the observed x-ray signal in the experiments. Nonetheless, one can see that the *VERITAS*-predicted continuum slope, the K_α-emission amplitude, and the 1*s*–2*p* absorption width are still slightly mismatched with respect to the experiment.

To summarize, a theoretical and experimental study of atomic physics in Cu-doped plastic at several billion atmospheres of pressure has been performed. Overall, a DFT-based approach reproduces many of the emission and absorption features that are observed in the experiment, while traditional plasma spectroscopy treatments show sensitivity to the combination of atomic physics and continuum-lowering models that are implemented. This sensitivity contributes to the present open questions on the validity of *ad hoc* continuum-lowering models. This work indicates the necessity for a self-consistent treatment of dense plasma effects on altering atomic energy levels/bands and their populations at ultrahigh pressures. The DFT-based *VERITAS* approach, with potential future benchmarks using other buried metal and metal-alloy layers, could provide a reliable way for simulating radiation generation and transport in dense plasmas encountered in stars and inertial fusion targets. The experimental scheme reported here, based on a laser-driven implosion, can be readily extended to a wide range of materials in single- and multishell geometries, opening the way for far-reaching investigations of extreme atomic physics and DFT models at tremendous pressures.

This material is based upon work supported by the Department of Energy National Nuclear Security Administration under Award Number DE-NA0003856, the University of Rochester, and the New York State Energy Research and Development Authority.

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2. S. X. Hu *et al.*, Nat. Commun. **13**, 6780 (2022).