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A comparison of theory and experiment for high density, high temperature germanium spectra

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ABSTRACT

This paper compares results from theoretical predictions to experimental emission data from germanium obtained on the HELEN laser at AWE. The aim of the comparison was to test opacity predictions of highly stripped, medium Z elements, a regime which has received relatively little attention due the difficulty of achieving conditions near LTE at high temperatures. The data show emission from the 2p–3d and 2s–3p transitions from a layer of germanium buried in plastic and heated by the HELEN CPA beam. Predictions of spectra constructed using data generated by the grasp2K atomic structure code coupled to Saha–Boltzman population dynamics were compared to the experimental emission. It was found that the grasp2K calculations match the position of all the features in the experiment well, but non-LTE effects in the experiment make it unreasonable to expect a match to line strengths. Two opacity codes, CASSANDRA and DAVROS, were benchmarked against the grasp2K simulations. It was shown that the major difference in the two opacity codes is due to different approaches to calculating total ion energies. For this reason the DAVROS line positions are significantly more accurate than those of CASSANDRA.

1. Introduction

The comparison of opacity predictions to experimental data is an important method of validating theory and model implementation. Experimental methods which produce spectra representative of LTE are well established, but these can only access a limited regime of temperatures and densities. To date most experimental opacity measurements have taken place at well below solid density and a few hundred eV. Experiments which heat microdot samples buried in plastic with a short pulse beam are being developed on the AWE HELEN laser [1]. These experiments are able to access temperatures in excess of 500 eV and densities above one tenth of solid. This new technique gives the opportunity to compare models to experiment in a higher temperature/density regime. It is hoped that this will provide rigorous tests of the approximations and numerical models in the codes and bring to light modeling deficiencies. This paper compares simulations to experimental data produced by short pulse heated emission from the germanium L-shell spectrum.

2. Experiment

Experiments using samples of pure Ge and Ge mixed with Ti were performed on the AWE HELEN laser [2]. The targets consisted of a microdot buried in plastic and were heated by the HELEN short pulse beam. Germanium emission spectra were recorded in the 1.3–2.5 keV spectral range, covering 2p–3d, 2s–3p and 2p–4d transitions, with charge states up to 29^{+}. An example of a spectrum from pure Ge is shown in Fig. 1. Approximate target conditions were estimated using radiation–hydrodynamics simulations of the samples, which were then refined by comparing the emission to synthetic spectra. In the mixed germanium and titanium sample the plasma conditions were inferred from the titanium spectra by comparing the measurements of line ratios and widths to titanium spectra predicted by the FLY code [3]. In the pure germanium samples the conditions were inferred by comparison to simulations performed using the FLYCHK code [4].

From these simulations the plasmas were estimated to be at a density of 1 g/cc, with an electron temperature of 800 eV ± 100 eV. In the FLYCHK simulations the radiation temperature was assumed to be zero as the radiation–hydrodynamic simulation predicated a radiation temperature much cooler than the electron temperature. This is due to the fact that the sample is heated by electrons, which are liberated from the plastic by the laser, rather than radiation. The collisional–radiative simulations showed that as electron density is increased the effective ionisation temperature converges towards the electron temperature and the sample can achieve near LTE conditions. However, simulations using the FLYCHK model indicate that LTE was not achieved at the densities of these experiments.

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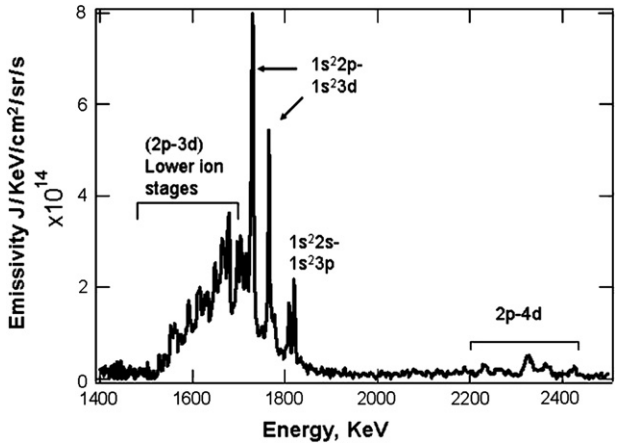

Fig. 1. Experimentally measured time integrated emission from Ge plasma.

3. Detailed spectral model

To aid the design and initial analysis of this experiment a detailed spectral model was created. This model used energies and oscillator strengths generated by the grasp2K [5] code and an ion population distribution given by Saha–Boltzman statistics. Configurations with 2–9 bound electrons and a maximum of one electron in the M-shell or N-shell were calculated. The calculated intensity distributions were broadened by Doppler widths and by the spectrometer instrument function, which was approximated by a Gaussian of 3 eV FWHM.

Comparison to the experimental data showed that it could not be fit at a single temperature and density, indicating the presence of spatial or temporal gradients in the sample. This is consistent with the conclusions from the non-LTE simulations. The best fit between the experiment and calculation was obtained by averaging calculations between temperatures of 600 eV–700 eV and densities of 1–2 g/cc, see Fig. 2. It can be seen that the positions and widths of spectral features are in agreement with the LTE simulation, but not the intensities. This can be attributed to a combination of non-LTE effects and/or gradients in the sample.

4. Opacity calculations

LTE opacity models that are capable of producing Rosseland mean opacities generally contain approximations to the atomic physics that one would obtain from the grasp2K code, as they must rapidly calculate the spectrum from a large number electronic transitions. The results from two AWE opacity codes were compared to the detailed simulations in order to identify the major sources of error from these extra approximations.

The two opacity codes used in this comparison were CASSANDRA [6] and DAVROS. Both these codes use the local density approximation (LDA) and unresolved transition array (UTA) approximation for computational efficiency, however there are some major differences between the two codes. CASSANDRA obtains configuration energies from a Taylor expansion about the average atom, whereas DAVROS performs a self-consistent field calculation for each ion. The CASSANDRA plasma model is the generalized ion cell (GIC) model [7] whereas DAVROS uses the more usual ion-sphere (IS) approximation. CASSANDRA uses the Mozkowski UTA [8] model, whereas DAVROS uses that from Bauche-Arnoult [9]. CASSANDRA has a simple Stark broadening model [10]; one is yet to be implemented in DAVROS.

The comparison between simulations from the codes, including gradients, and the experiment is shown in Fig. 3. It can be seen that the two UTA codes produce less detailed spectra than grasp2k, but the code predictions are broadly similar. However, if the harmonic mean between 1450 eV and 1850 eV is calculated in this regime, large differences are observed and can be seen in Fig. 4. This implies that the differences between the codes could influence predictions of Rosseland mean and so are worth investigating further.

Some of the major differences in the spectra from CASSANDRA and DAVROS are seen in the spectral lines above photon energies of 1800 eV in Fig. 3 with DAVROS in better agreement with the grasp2k calculation. It was initially thought that these differences were caused different average ionisations predicted by the GIC, IS and Saha–Boltzman models. When the predictions of average ionisation were compared between the three models seen in Fig. 3, it was seen that grasp2K/Saha–Boltzman simulation had the largest deviations, Fig. 5. This is qualitatively inconsistent with the spectral comparisons, indicating that the different ionisation models are not

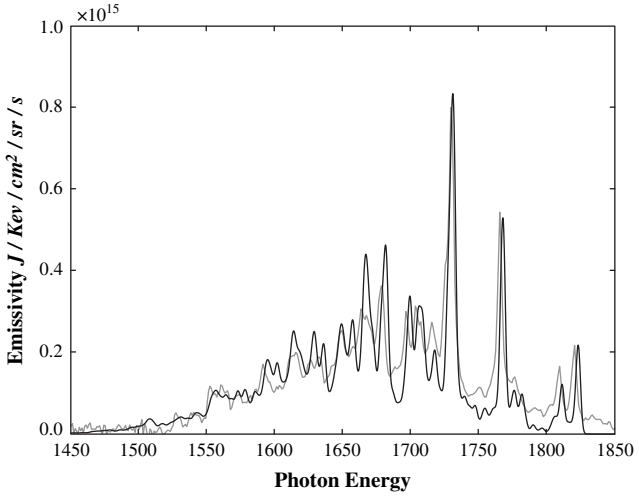

Fig. 2. Comparison of experimental (grey) and simulated (black) emission of Ge 2s–3p and 2p–3d transitions. The simulations include contributions from plasma between 600 eV–700 eV and 1–2 g/cc to model the affect of gradients.

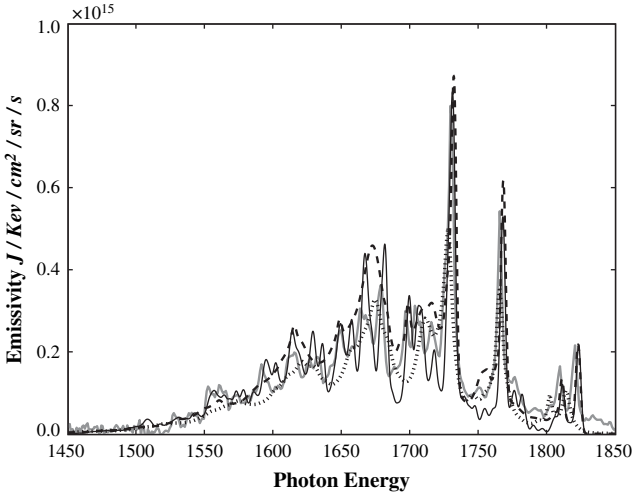

Fig. 3. Comparison of experimental (grey) and simulated emission from grasp2k data (solid black) CASSANDRA (dotted) and DAVROS (dashed) of Ge 2s–3p and 2p–3d transitions. The simulations include contributions from plasma between 600 eV–700 eV and 1–2 g/cc to model the affect of gradients.