Super-transition-array calculations for synthetic spectra and opacity of high-density, high-temperature germanium plasmas

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Abstract

The synthetic emission spectra and opacity of high-density, high-temperature germanium (Z=32) plasma from super-transition-array (STA) calculations are presented. The viability of the STA model, which is based on a statistical superconfigurations accounting approach for calculating the atomic and radiative properties, is examined by comparing and contrasting its results against the available experimental data and other theoretical calculations. First, we focus on the emission data. To model the data, the Eulerian radiation-hydrodynamics code FastRad3D is used in conjunction with STA to obtain the STA-required inputs, namely, the time-dependent temperature and density profiles of the Ge plasmas. Consequently, we find that STA results fit the experimental spectrum reasonably well, reproducing the main spectral features of $2p - 3d$, $2s - 3p$, and $2p - 4d$ transitions from the laser-heated germanium layer buried in plastic [High Energy Density Phys., 6 (2010) 105]. However, careful comparison between experimental and theoretical results in the photon-energy regions of $\sim 1.7$ keV shows some degrees of disparity between the two. This may be due to the non-LTE effects and the presence of spatial gradients in the sample. Limitations of STA to model the experimental spectrum precisely is expected and underscoring the difficulty of the present attempts as the model assumed local thermodynamics equilibrium population dynamics. Second, we examine the STA calculated multi-frequency opacities for a broad range of Ge plasma conditions covering the L- and M-shell spectral range. Comparing with a hybrid LTE opacity code which combines the statistical super-transition-array and fine-structure methods [High Energy Density Phys., 7 (2011) 234], impressively good agreement is found between the two calculations. In addition, the sensitivity of the opacity results in various plasma temperatures and mass densities is discussed. The ionized population fraction and average ionization of the Ge plasma are also described. Comparisons of STA results in the observed spectrum and opacity are considerably close while offering the advantage of computational speed and its capability of treating hot and dense high-Z plasmas.
I. INTRODUCTION

In most indirect-drive inertial confinement fusion (ICF) schemes, the production of high-quality thermal X-rays sources inside a hohlraum is of great interest. Production of X-rays comes from the absorption of the laser beams in the hohlraum. Soft X-rays propagating within the cavity between the fuel capsule and the inner walls will be absorbed by the low-Z capsule, rapidly ablating the capsule material. The irradiation also compresses the DT fuel inside the capsule. Compressing a target to ignition conditions is very challenging and is yet to be fully realized in experiments. For example, in addition to soft X-rays, energetic X-rays tend to propagate ahead of the ablation-front and preheat the inner layer of ablator next to the fuel, introducing a sizable density gradients at the boundary between the fuel and ablator. The density gradient excites the growth of hydrodynamic instabilities. A carefully tailored ablator with mid-Z materials can potentially limit this instability effect. The hard X-rays can be absorbed due to the ablator opacity, preventing preheating of the inner plastic layer next to the fuel, suppressing the instabilities (e.g., Richtmyer-Meshkov and Rayleigh-Taylor) along with reducing the mixing of dense cold plasma with the less dense hot spot. It turns out that both germanium and silicon are hopeful choices as dopants in the ablator for the ICF targets. Knowing their optimum concentration is also essential as too much or too little will defeat its purpose. As a result, knowing the opacity and emissivity of Ge (and Si) is highly desirable.

Experimental measurement of the emission spectra of germanium plasma has been reported by Hoarty et al. In , a high-power, Gaussian laser-pulse has been used to create a high-temperature, high-density plasma to study its X-ray opacity and equation of states. Their target sample was composed of a 50/50 mixture (by particle-number) of Ti/Ge in a 50 µm diameter and 0.1 µm thick disc. The Ti/Ge experimental data were recorded using both time-integrated and time-resolved spectrometers, but only the time-integrated spectrum was absolutely calibrated. This latter spectrum recorded the Ge emission intensity in the 1.3–2.5 keV spectral range covering 2p–3d and 2p–4d transitions in charge states up to +29. The germanium plasma conditions were inferred from simulations performed using collisional-radiative code FLYCHK . In order to obtain the best fit between the calculation and experimental spectra, and to determine that the Ge plasma conditions is approximately 800 eV ± 100 eV and 1.0 g/cm³, a set of five calculations at a density 1.0
g/cm\(^3\) and electron temperatures of 700, 750, 800, 850, 900 eV were equally averaged to take into account the effect of temperature.

A comparison between the local thermodynamic equilibrium (LTE) calculations and the measured Ge emission spectrum has also been discussed in the work of Harris et al.\(^3\). Three LTE opacity codes, namely, GRASP2K\(^5\), CASSANDRA\(^6\) and DAVROS\(^7\), have been used to calculate the synthetic Ge emission spectra. Each of these codes has different levels of sophistication in calculating the atomic structures, and hence the atomic properties. In Harris et al, all the LTE calculations have considered both the density and temperature effects. Their best fit between the theory and experiment was obtained by averaging calculations among temperatures from 600–700 eV and densities from 1–2 g/cm\(^3\).

Despite the small difference in the emission intensity, the authors showed the GRASP2K computed widths and positions of the spectral features fit the experimental data well. The authors also compared the results from two other opacity codes CASSANDRA and DAVROS with the measurement. Reasonable agreement was reported, albeit the two UTA codes lack in spectral details in comparison to the GRASP2K code. Although CASSANDRA and DAVROS codes do show some differences in some photon-energy regions, their results are broadly similar. This difference was discussed and attributed to the variations of effective potential models used in CASSANDRA and DAVROS in calculating the total ionic energies. The comparison of emission results from LTE and NLTE calculations indicated that the LTE codes gave a temperature of about 20% lower than the NLTE codes.

Recently, we have employed the STA method\(^8\)\textsuperscript{–}\textsuperscript{14} in conjunction with the MIX model\(^15\) to examine the emissivities, opacities, and degree of average ionization for carbon and plastic CH in the warm, dense matter regime. We assessed the quality of our STA calculations by comparing them with other available theoretical calculations as well as experimental data. The STA calculated emissivities, opacities and average ionization for carbon and plastic CH were found to be in good agreement with other theoretical results and experimental data\(^16\). The STA method was designed to analyze unresolved spectra of hot, high-Z plasma in LTE.

In this work, we employ the STA method to study the radiative and atomic properties from high temperature and dense germanium plasma not only to validate the STA results for laser-produced germanium spectra, but to also investigate the temporal variation in density and temperature of the plasma through its emission process. Additionally, we also
want to examine the STA computed multi-frequency opacity, ionized population fraction and average ionization, and compare them with the calculations obtained from the hybrid LTE opacity SCO-RCG code \cite{17} for a wide range of germanium plasma conditions covering the L- and M-shell spectral range. The paper is organized as follows. In Sec. II, we outline the basic concepts of the STA method. In Sec. III, we present and discuss the STA emission spectra, opacity, ionized population fraction and average ionization results in comparison with other theoretical calculations and experimental data. We give some conclusions from this study in Sec. IV. Unless otherwise stated, all quantities are expressed in atomic units. The solid density for germanium is $\rho_o = 5.323 \text{ g/cm}^3$. Lastly, we refer, interchangeably, to STA method as an STA model, or STA code throughout the paper.

II. OPAcity MODEL

For our opacity model, we have adopted the STA method of Bar-Shalom et al \cite{8}. Since its first release, the original STA code has been modified, updated and made more stable. The changes made include new algorithms for better convergence of the computation of the partition functions \cite{18}, better interface between STA and MIX codes \cite{15}, several options to improve the convergence of the balance between bound and free electrons charge densities, a better way to calculate the parametric potential and simplification of free-free scattering \cite{19}, to name a few.

The followings outline the essential concepts of the STA method. A supershell, $\sigma$, is the union of energetically adjacent ordinary atomic subshells, $s \in \sigma$, where $s \equiv j \equiv \{n_s, l_s, j_s\}$ . A superconfiguration (SC) $\Xi$ of a $Q$ electron ion is defined by its supershell occupation numbers $Q_{\sigma}$ and constructed through grouping the neighboring (in energy) ordinary subshells into supershells. Symbolically, the expressions for $\Xi$ and $Q$ are

$$\Xi \equiv \prod_{\sigma} \sigma^{Q_{\sigma}}, \quad Q = \sum_{\sigma} Q_{\sigma},$$

respectively. This implies that the SC is constructed by partitioning the $Q_{\sigma}$ electrons occupying supershell $\sigma$ among the ordinary subshells in all possible ways according to $\sum_s q_s = Q_{\sigma}$,
where

\[ \sigma^Q = \sum_{\sum q_s = Q} \prod_s j_s^{q_s} \]  

(2)

and \( q_s \) are the occupation numbers of the subshells. Each partition of \( Q \) in Eqs. (1) and (2) is an ordinary configuration \( C \equiv \prod_{s} \prod_{s \in \sigma} j_s^{q_s} \). An ordinary configuration \( C \) is a special case of SC in which each supershell contains only one shell. For example, an ordinary configuration:

\[ C = 1s^22s^22p_{1/2}^22p_{3/2}^3, \]  

supershell: \( \sigma = (3s3p_{1/2}3p_{3/2}3d_{3/2}) \) and a superconfiguration:

\[ \Xi = (1s)^2(2s2p_{1/2}2p_{3/2})^7(3s3p_{1/2}3p_{3/2}3d_{3/2})^1 \]  

(3)

is made of three supershells associated respectively with 2, 7 and 1 electrons. Note that a reasonable number of SCs (typically on the order of a few hundreds for mid-Z elements) can already contain a tremendous number of ordinary configurations. Precision for photoabsorption spectra can be improved by subdividing these SCs. An array \( A_{CC'} \) connecting two configurations \( C \rightarrow C' \) can be identified by specifying the initial configuration \( C \) and the electron(s) jumps which lead to \( C' \). Similarly, the array \( A_{\Xi\Xi'} \) connecting two SCs can be identified by specifying the initial configuration \( \Xi \) and the electron(s) jumps which lead to \( \Xi' \).

To evaluate the STA moments (i.e., the total intensity, the average energy, and variance) and SC average rates, one needs expressions for the populations of the configurations and super configurations. Assuming local thermodynamic equilibrium, all the configurations described by a SC \( \Xi \), the population of any array of levels \( i \) can be expressed through the Saha-Boltzmann’s law, \( U_Q/U = N_Q/N \), where \( N_Q \) and \( N \) are the partial and total ionic number density, respectively, and \( U_Q \) and \( U \) are their corresponding partition functions. For example, for an ion with \( Q \) electrons, the partition function of the SC \( \Xi \) can be expressed in terms of a summation over all levels \( i \) of all configurations \( C \), i.e.,

\[ U_\Xi = \sum_{C \in \Xi} \sum_{i \in C} g_i e^{(E_i^{(0)} + \delta E_\Xi^{(1)} - Q\mu)/kT}, \]  

(4)

where the sum of configuration statistical weight is given by the sum of product of binomials

\[ \sum_{i \in C} g_i = \sum_p \prod_{s \in C} \binom{g_s}{q_s}, \]  

(5)
each partition $p$ is a set of $q_s$ generating an ordinary configuration $C$ and $g_s = 2j + 1$ is the statistical weights corresponding to shell $s$. We also have the relations $\sum_{s \in \sigma} q_s = Q_\sigma$ and $E_i^{(0)} = \sum_{s \in \sigma} q_s \epsilon_s$, where the latter quantity is the zeroth order energy. The SC energies can be written as

$$E_{\Xi} = \delta E_{\Xi}^{(1)} + \sum_{\sigma} \sum_{p} \sum_{s \in \sigma} q_s \epsilon_s,$$  \hspace{1cm} (6)$$

where $\delta E_{\Xi}^{(1)}$ is the SC first-order average energy correction (see Eq.(86) in Ref.[12]), $\epsilon_s$ the monoelectronic energy and $\sum_p$ means a summation over all the terms of the partition function of $Q_\sigma$ (i.e. the number of ways to distribute $Q_\sigma$ electrons in the different subshells of $\sigma$). It should be noted that it has been demonstrated in Ref.[8, 12], that with a modified set of statistical weights and supershell occupation numbers, the STA moments and the non-LTE average transition rates can be expressed in terms of generalized partition functions.

The STA method or code was based on an ion sphere model in a chemical picture of Liberman’s model [20] by considering the plasma as consisting of multi-charged, multi-ionized atoms with free electrons shared among all ions. For a given atom with a set of the temperature and the density of interest, the code first solves a finite-temperature Thomas-Fermi-Dirac equation [21, 22] and using the solutions in terms of relativistic wave functions provides the average ionization charge state $\bar{Z}$ self-consistently with the free electrons in the ion sphere. A parametric potential [23] has been used to describe the bound electrons as it simplifies and yet captures the changes of the electronic potential for each ion stage [24]. The STA code, in the first iteration, starts by loosely defining very broad supershells, similar to that of the average atom model approach [8]. The SCs are then constructed with these supershells. The moments of the STA transitions are then computed and the resulting spectra are obtained by adding up all the STA contributions. Then, in the next iteration, the supershells are split to optimize the corresponding SCs and this procedure repeats itself until the converged spectra are achieved. The potential for each SC is also progressively refined, the STA recomputed, and finally, the UTA moments [25] are incorporated in the spectral-opacity calculation, as part of the obtaining accurate STAs’ widths and energies.
III. RESULTS AND DISCUSSION

In this study, the FastRad3D code is used in conjunction with the STA opacity code to model the experiments of Hoarty et al [2]. In this case, it is used to calculate the time-dependent temperature and density profiles of the Ge plasmas required by the STA as inputs. FastRad3D is a three-dimensional, Eulerian-based radiation-hydrodynamics code that is used primarily to simulate laser-matter interactions in the context of inertial-confinement-fusion experiments. The code couples models of hydrodynamics, laser deposition, thermal conductivity and various equations of state to a multi-group diffusion model for radiation transport and has been tested extensively against various theoretical benchmarks and laboratory results. Additional details about the FastRad3D code can be found in Ref. [26].

In the work of Hoarty et al [2], the emission spectrum is from a 0.1-µm Ti/Ge disc irradiated by a high-intensity (i.e., $10^{17} - 10^{19}$ W/cm$^2$), 0.5 psec FWHM Gaussian laser pulse. Under such conditions, we hypothesize that the laser energy is deposited in the target in a small volume and over a very short period of time ($\sim$ a few psec) so that the heating is nearly isochoric. Since the total energy deposited depends upon the net absorption of the extremely high-intensity laser pulse — which was not specified in Hoarty et al for the displayed Ge spectrum — we performed a series of simulations that began with different absorbed energies. If all of the energy was absorbed in $1/2$ psec at $1.0 \times 10^{18}$ W/cm$^2$, this would correspond to 500 kJ/cm$^2$ absorbed in the target. We found correspondence with the temperatures reported by Hoarty et al (e.g., 0.5–1.0 keV) for absorbed energies about an order of magnitude less (e.g., corresponding to absorbed intensities of $\sim 10^{17}$ W/cm$^2$).

The absorbed laser energy is deposited uniformly (i.e., constant energy per electron) throughout the sandwich target. The energy was deposited primarily into the electrons because the initial, *impulsive* heating [27] was deemed to be due to hot electrons from either direct inverse bremsstrahlung heating and/or supra-thermal electrons due to laser-plasma instabilities. As the electron-ion thermal equilibration time near-solid density is very short ($\sim$ psec), the target ions quickly equilibrate to the electrons. The evolution of the target consisted primarily of anisotropic expansion modified somewhat by the radiative cooling (for example, our simulations show that in the first 10 psec after heating the target loses $\sim 25\%$ of its initial energy to radiation). In other words, the laser deposition occurs on a time scale that is much shorter than the hydrodynamics response time and modeling such
“hyper-fast”, initial dynamics poses a serious challenge for any radiation hydrodynamics codes. Consequently, we make an *ansatz* of instantaneous depositing the initial energy into the plasma electrons in FastRad3D in order to estimate the ensuing density and temperature profiles of the target.

A. Emission: theory versus experiment

The intensity $I(\nu, T_e)$ of an emission spectrum, defining in units of $W/(\text{keVcm}^2\text{sr})$, can be expressed as

$$I(\nu, T_e) = S(\nu, T_e)(1 - e^{-\rho\kappa\nu L}),$$

(7)

where $S(\nu, T_e)$ is known as the source function, that is, the ratio of the emissivity $\epsilon_\nu$ to opacity $\kappa_\nu$, $\nu$ is the frequency of the photon, $\rho$ is the mass density of the target matter, $T_e$ is the temperature of the plasma and $L$ size of the target.

In order to construct the time-integrated STA emission spectrum $I(\nu, T_e)$ shown later in Fig. 2(a) and Fig. 3 we have performed several FastRad3D calculations varying the laser-absorbed intensity of $\sim 10^{17}$ W/cm$^2$. We find that the best fit for our case is at $0.8 \times 10^{16}$ W/cm$^2$. The corresponding spectra are shown in Fig. 2(b). Each spectrum corresponds to the plasma in a particular conditions (i.e., density and temperature) at a particular time. The time evolution profiles of the plasma density and temperature are presented in Fig. 1(a).

Deducing from this time-evolution information of Fig. 1(a), we figure out how much time the plasma spends at a particular density and temperature to help us to construct the relevant histogram shown in Fig. 1(b). Consequently, we arrive at an expression for the time-integrated spectral intensity ($I_f$) as a sum of contributions from multiple time-weighted intensities ($I_i$) over the “cooling” period $t_{\text{total}}$:

$$I_f = \sum_{i}^{N} (\Delta t_i/t_{\text{total}}) \times I_i,$$

(8)

with the maximum number of time-snapshots in this case is $N = 13$. The histogram basically gives the statistical weights (or probability) of the plasma-condition over the plasma cooling period. The statistical weight ($\Delta t_i/t_{\text{total}}$) can be obtained by first determine the $\Delta t$. For example, $\Delta t_1 = (0.5 \times (0.7-0.5) + 0.5) - 0.0$ psec = 0.6 psec, $\Delta t_2 = (0.5 \times (0.9-0.7) + 0.7) - 0.6$
FIG. 1: (Color online) (a) FastRad3D computed plasma temperature and density profiles as a function of plasma-evolution time. The vertical-dotted-line indicates the time snapshot, which is given in the legend of Fig 2(b). (b) Statistical weight \((\Delta t/t_{\text{total}})\) at each \(\Delta t\) corresponding to a particular plasma temperature and density. We choose \(t_{\text{total}} = 5.75\) psec. The sum of all the statistical weights amounts to 1.0.

psec = 0.2 psec, and so forth, and hence their corresponding statistical weights are simply \(\Delta t_1/t_{\text{total}} = 0.6/5.75 = 0.104\), \(\Delta t_2/t_{\text{total}} = 0.2/5.75 = 0.035\), and so forth. Note that we chose the cut-off time to be at \(t_{\text{total}} = 5.75\) psec since we found the spectral contributions from later times, namely, \(t = 6.0\) and 7.0 psec, to be relatively insignificant.

It is informative to compare STA results with those from other LTE opacity codes. In
FIG. 2: (Color online) (a) Comparison of simulated emission from GRASP2K and STA codes. The LTE GRASP2K calculation, digitized from Ref. [3], includes contributions from plasma between 600–700 eV and 1.0–2.0 g/cm$^3$ to model the affect of both temperature and density effects. (b) The “time-resolved” STA emission spectra that contribute to the total or “time-integrated” emission spectrum.

Fig. 2(a), we have the STA computed spectrum superimposed onto the result from LTE opacity code GRASP2K [2, 3, 5]. GRASP2K is a general-purpose relativistic atomic structure package based on a fully relativistic multiconfiguration Dirac-Hartree-Fock method. It performs detailed term accounting (DTA) calculations to produce energy levels and oscillator strengths which can then be used to construct a spectrum using Saha-Boltzmann statistics. The code is well-known for its accuracy in determining the line positions and widths, and has been considered by many atomic physicists as a standard for benchmarking. However, if GRASP2K is similar to the HULLAC [28] in the sense that it is an “isolated-atom” code, which does not take into account the density effects by allowing for the ionization potential
depression, its results in this case can be less accurate.

Fig. 2(a) also shows that the STA calculated spectrum matches the locations satisfactorily, including the peaks for the $2p - 3d$ and $2p - 3p$ transitions obtained by GRASP2K but provides envelopes to the detailed results for the lower ion stages. This is because the STA approach sometimes cannot resolve spectral features that are simply not made up of single transition, particularly in the case for lower ion stages of $2p - 3d$ transitions, but are coalescences of similar transitions from several ionization stages. In fact, the number of transitions in a feature can be so large that statistical treatments provide a method of determining the spectral feature characteristics. For example, see the discussions of unresolved transition arrays (UTA) by Bauche, Bauche-Arnoult and Klapisch [25]. Under some circumstances, such a statistical approach may overestimate the Rosseland mean opacity because all the gaps between the lines can be overlooked. In any case, it is important to note that the spectrum from the GRASP2K simulations matched the experimental data well and placed the plasma conditions at $1.5 \text{ g/cm}^3 \pm 0.5 \text{ g/cm}^3$ and $600 \text{ eV} \pm 60 \text{ eV}$. On the other hand, result from the non-LTE collisional-radiative equilibrium code FLYCHK also shows a good match to the experimental spectra but indicates $T_e \approx 800 \pm 100 \text{ eV}$ and $\rho \approx 1.5 \pm 0.5 \text{ g/cm}^3$. Given that the results of collisional-radiative FLYCHK calculations also got good agreement with the experimental data lead us thinking that the plasma could lie in this part-LTE, part-non-LTE domains. Of course, additional emission spectra from both CASSANDRA [6] and DAVROS [7] opacity codes for further comparison would also be beneficial. However, we are unable to extract the clean digitized data of CASSANDRA and DAVROS calculations from the published figures [3].

The time-snapshots of different contributions from the final spectra shown in Fig. 2(b) illustrate that the strong emission profile appears between 1.7 and 1.8 keV comes from the initial time $t < 2.0$ psec contributions. On the lower temperature side, the notable emission appears in the $1.5 - 1.7$ keV region comes from the later time $3.0 < t < 5.0$ psec contributions.

Figure 3 displays a comparison between the synthetic Ge spectrum from STA calculation and the measured spectrum in the photon-energy range of $1.3 - 2.5$ keV. In this photon-energy range, the spectrum reveals the L-band transitions. The STA spectrum appeared to be in reasonably good agreement with the experimental data. In particular, the STA reproduces the dominant features of $2p - 3d$, $1s^22s - 1s^23p$ and $1s^22p - 1s^23d$ and $2p - 4d$ transitions depicted in the measured Ge emission spectrum. However, magnifying the
FIG. 3: (Color online) Emission spectrum of germanium. (a) STA calculation versus the experimental data digitized from Ref. [2]. (b) Same plot as (a) but for photon energy between 1.4 and 1.9 keV. Note that the 3-eV instrument-broadening is not considered it appeared to be insignificant to affect the main features of our spectrum.

spectra in the photon energy-range between 1.4 and 1.9 keV for detailed comparison in Fig.3(b) apparently reveals some disparities between the synthetic and experimental spectra. This could mean the presence of spatial temperature and density variations in the sample as well as the non-LTE effects. The limitation of STA to account for these effects and to quantitatively modeling the experimental data is expected and underscoring the difficulty of the present attempts. Besides, the model assumed local thermodynamics equilibrium population dynamics. From this standpoint, the good agreement between the GRASP2K results and experimental data reported in Ref. [3] (e.g., see Figs. 2 and 3) is puzzling and most likely be fortuitous as GRASP2K itself is a LTE model. Furthermore, recent work has also shown these to have a greater effect than was previously thought [29]. In any case, if we were asked to estimate the “time-integrated” plasma conditions, according to our
calculations we say our estimates to be around $\rho \approx 1.7 \text{ g/cm}^3$ and $T_e \approx 690 \text{ eV}$ which are quite close the values reported in Ref.\[3\].

![Graph showing average ionization versus plasma temperature.](image)

**FIG. 4**: (Color online) Average ionization versus plasma temperature. Note that results from GRASP2K and DAVROS are digitized from Ref.\[3\].

In Fig. 4, we further compare the STA, GRASP2K, and DAVROS calculated average ionization versus the electron temperature at a mass density of 2.0 g/cm$^3$. Notice that, in this temperature range, more than two-thirds of Ge are ionized. Raising the temperature from 600 to 700 eV increases the charge state of Ge ions by almost two units. By the way, we have left out the average ionization result from CASSANDRA calculation at 2.0 g/cm$^3$ because the CASSANDRA result is essentially identical to those of DAVROS. The plot also shows that the STA’s average ionization values are very close to that of DAVROS — the difference between the two curves is less than 1%. Alternately, comparing the average ionization values between the STA and GRASP2K models, it is obvious that GRASP2K simulation shows the largest deviation from STA or DAVROS. This difference has been shown and discussed in \[3\] that it was thought that a relatively small number of configurations was used in the Saha-Boltzmann partition function of GRASP2K in determining the average ionization values.

Now, concerning the difference observed between the STA and DAVROS. Possible causes may be due to (i) the statistical approximation used in the STA model to amalgamate the similar transitions from several ionization stages and (ii) the use of parametric potential \[23\] in place of the Hartree-Fock potential in our numerical solution of the Dirac’s equation.
FIG. 5: (Color online). Ionization fractions versus the charge states for Ge at various temperatures and densities.

Next, we examine in Fig. 5 the LTE ionization fractions versus germanium charge states at various temperatures and densities. Here we see that within these temperature and density range, indeed, several ionization stages do contribute to the transitions we saw earlier and are keeping with the explanation we offered earlier for the discrepancy. For the case of $\rho > 1.0 \text{ g/cm}^3$, at a temperature of 800 eV the ionization balance appears to be near charge state of 28 with a population fraction of $\sim 0.32$. Similarly, at a temperature of 400 eV the ionization balance moves to a lower charge state and appears to be near charge state of 23 with a population fraction drops to $\sim 0.25$. For the case of $\rho \leq 1.0 \text{ g/cm}^3$, we can see that the ionization balance strongly depends on the temperature and mass density. For example, at higher electron temperature of 800 eV the ionization balance peak-value drops by a factor of 2 and extends over a broader charge states as one moves from 0.1 to 1.0 g/cm$^3$. On the
other hand, at a lower electron temperature of 400 eV the ionization balance peak-value stays roughly the same, but its peak moves from charge state 27 to 24 as one compresses the plasmas (see Fig. 5(a1)-(a3)).

B. Opacity: theoretical models comparison

We now turn to examine density- and temperature-dependent opacity. The Rosseland mean opacity, $\kappa_R$, and Planckian mean opacity, $\kappa_P$, are defined by

$$\frac{1}{\kappa_R} = \frac{15}{4\pi^4} \int_0^\infty \frac{x^4e^x dx}{u(x)(e^x - 1)^2},$$  \hspace{1cm} (9)$$

$$\kappa_P = \frac{15}{\pi^4} \int_0^\infty \frac{u(x)x^3 dx}{(e^x - 1)},$$ \hspace{1cm} (10)$$

respectively, where $x = h\nu/kT_e$, $u(x) = N_A\bar{\sigma}(h\nu)/A$, $N_A$ is the Avogadro’s constant, $A$ denotes the atomic mass number, $\bar{\sigma}(h\nu) = \sigma(h\nu)(1 - e^{-x})$ and $\sigma(h\nu)$ is the total cross-section including all processes like scattering of photon, bound-bound, bound-free and free-free absorptions.

Figure 6 presents the opacity results of STA calculations together with the SCO-RCG calculations at $T_e = 300$ eV, at various mass densities. The plots show a good agreement between the two theoretical calculations. In brief, the SCO-RCG is a LTE hybrid opacity code which combines the statistical super-transition-array approach and fine-structure calculations for intense and spectrally broad transition arrays [17]. Criteria are used to select transition arrays which are removed from the super-configuration statistics, and replaced by a detailed line-by-line treatment. The data required for the calculation of the detailed transition arrays, like Slater, spin-orbit and dipolar integrals, are obtained from the super-configuration code SCO (Super-Configuration Opacity) [30], to provide a consistent description of the plasma screening effects in the wave functions. Then, the level-energies, line-positions, and line-strengths are calculated using the RCG routine of Cowan’s atomic structure code [31].

Figure 6 also reveals two pronounced structures. In addition to the L-band structures with a corresponding photon energy range of $1.1 - 1.6$ keV, one also sees the M-band structures with a corresponding photon energy range of $0 - 500$ eV. The dependence of the opacity on the plasma density is obvious. Because of the depression of the ionization potential as
FIG. 6: The density dependence of the radiative opacity for germanium at electron temperature of 300 eV are shown in (a) STA and (b) SCO-RCG. Opacity ratio of STA to SCO-RCG for the same temperature at $\rho = 0.1 \text{ g/cm}^3$ is shown in (c). The deviation from unity in opacity ratio is likely due to (i) the difference in photon-energy resolution used in the STA and SCO-RCG codes and (ii) the replacement of the superconfigurations by the detailed line-by-line treatment in the SCO-RCG code.

As the density rises, the Inglis-Teller limit [32] in which many spectral lines merge and show a quasi-edge appears to shift to lower and lower photon energies, and slowly disappears into the continuum. It is important to note that although the opacity profiles of Planck and Rosseland means of Ge plasmas have been investigated using the SCO-RCG opacity code by Benredjem et al. [33–37], this is the first comparative study between the SCO-RCG and STA opacity results. In addition to the opacity, we also compare the STA predicted ionization fractions at $T_e = 300 \text{ eV}$ with the results from SCO-RCG calculation for $\rho = 0.1, 0.5$ and
As shown in figure 7, they are nearly identical.

The sensitivity of the opacities to the variation of the plasma temperatures is displayed in Fig. 8. Comparing the opacities at temperatures of 500 and 100 eV, one can see that the opacity at 500 eV displays more complex structures than the one at 100 eV; the variation of opacity with density is also stronger at higher temperatures, at least for the range of density and temperature considered in this figure. These features have been observed and discussed recently by Mondet et al.\cite{33}. The main cause of this is due to the increase of level populations as one increases the temperature. One can also envisage that narrow spin-orbit separation such as between $2p_{3/2} - 3d_{5/2}$ and $2p_{1/2} - 3d_{3/2}$ will evanesce due to the thermal
FIG. 8: The density dependence of the STA radiative opacities for germanium at electron
temperature (a) $T_e = 500$ and (b) 100 eV.

broadening when the temperature is increased and to an increase of level populations. Here
we also notice that the opacity of germanium at 100 eV is higher than that at 500 eV, except
around 1.7 keV. Again, such behaviors are also consistent with the observations of Mondet
et al.\textsuperscript{33}. 

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Finally, it is also of interest to compare the STA Rosseland and Planck mean opacities against the results from SCO-RCG \cite{35}. As shown in Fig. 9, we see that the Rosseland mean opacity results of SCO-RCG and STA calculations are in close agreement. As for the Planck mean opacity, it is shown that STA matches the SCO-RCG points favorably, except at the plasma temperature of $T_e = 200$ eV where the STA value is about 40% higher than the SCO-RCG one. The fact that the Planck value predicted by SCO-RCG at $T=200$ eV is significantly different from the one at $T=100$ eV, but rather close to the one at $T=300$ eV, can be explained by the populations of the different subshells of the M shell (see table II). Indeed, the transitions which have the strongest weights in the Planck and Rosseland means are 3-4, 3-5 and 3-6 transitions (see tables III) and the opacity is proportional to the populations of the initial state. As we can see, the variations of populations of the

\begin{table}[h]
\centering
\begin{tabular}{|c|c|c|c|c|c|}
\hline
$T_e$(eV) & $\bar{Z}_{SCO-RCG}$ & $\bar{Z}_{STA}$ & $\bar{Z}_{AA}$ & $\bar{Z}_{STA}/\bar{Z}_{SCO-RCG}$ & $\bar{Z}_{AA}/\bar{Z}_{SCO-RCG}$ \\
\hline
100 & 15.550 & 15.837 & 15.241 & 1.0185 & 0.9801 \\
200 & 20.780 & 20.965 & 20.804 & 1.0089 & 1.0012 \\
300 & 23.943 & 24.141 & 23.912 & 1.0083 & 0.9987 \\
400 & 26.903 & 27.168 & 26.912 & 1.0099 & 1.0003 \\
500 & 28.609 & 29.093 & 28.693 & 1.0169 & 1.0029 \\
\hline
\end{tabular}
\caption{Average ionization at $\rho = 0.1$ g/cm$^3$.}
\end{table}
$n = 3$ subshells are more important between $T=100$ and $T=200$ eV, than between $T=200$ and $T=300$ eV. This is particularly obvious for the 3s subshell. These population changes impact both the photo-excitation and the photo-ionization contributions to opacity (see table IV). Of course, the 2-3 transitions also contribute to the mean opacities but are not responsible for the discrepancy between SCO-RCG and STA. Table IV shows that the photo-excitation is the dominant contribution to the Planck mean. Moreover, the difference in the STA and SCO-RCG photo-ionization cross sections involves low photon energies which do not affect the mean opacities. The difference between SCO-RCG and STA is mainly due to the photo-excitation (bb) contribution: 1354 cm$^2$/g for SCO-RCG and 2237 cm$^2$/g for STA, at $T=200$ eV (see Table IV). This discrepancy might be attributed to the difference between the Detailed-Line-Accounting treatment used in SCO-RCG (which involves only ordinary configurations except for highly excited states [38]) and the statistical super-transition-array model used in STA code. However, as mentioned above, except for that particular temperature, the results of STA are very close to the SCO-RCG ones, for a much lower numerical cost.

| $T$ (eV) / Subshell | 2s   | 2p   | 3s   | 3p   | 3d   |
|---------------------|------|------|------|------|------|
| 100                 | 2.000| 6.000| 0.927| 2.026| 1.894|
| 200                 | 1.965| 5.771| 0.099| 0.235| 0.286|
| 300                 | 1.448| 3.756| 0.030| 0.078| 0.111|
| 400                 | 0.700| 1.756| 0.015| 0.043| 0.066|
| 500                 | 0.251| 0.646| 0.008| 0.023| 0.037|

TABLE II: Average populations of the different subshells belonging to L and M shells in a germanium plasma at $\rho=0.1$ g/cm$^3$ and various temperatures, obtained from SCO-RCG calculations.

For completeness, we also listed in Table I the average ionization values obtained from our Average-Atom, STA, and SCO-RCG codes at a density of 0.1 g/cm$^3$ at five different temperatures. At this density, across the temperature range, the table shows STA values are consistently and slightly higher than the values obtained from the SCO-RCG calculations, indicating the predictions of a slightly higher electronic densities.
| Transition | Average-atom energy |
|------------|---------------------|
| 3d-4f      | 359 eV              |
| 3p-4d      | 409 eV              |
| 3s-4p      | 434 eV              |
| 3d-5f      | 504 eV              |
| 3p-5d      | 562 eV              |
| 3d-6f      | 583 eV              |
| 3s-5p      | 600 eV              |
| 3p-6d      | 642 eV              |
| 3s-6p      | 685 eV              |
| 2p-3s      | 835 eV              |
| 2p-3d      | 1350 eV             |
| 2s-3p      | 1445 eV             |

TABLE III: Average energies of the most important transitions involving L and M shells in a germanium plasma at \( T=200 \text{ eV} \) and \( \rho=0.1 \text{ g/cm}^3 \), obtained from SCO-RCG calculations.

| \( T \text{ (eV)} \) | \( \kappa_{\text{SCO}}(\text{ff}) \) | \( \kappa_{\text{STA}}(\text{ff}) \) | \( \kappa_{\text{SCO}}(\text{bb}) \) | \( \kappa_{\text{STA}}(\text{bb}) \) | \( \kappa_{\text{SCO}}(\text{bf}) \) | \( \kappa_{\text{STA}}(\text{bf}) \) | \( \kappa_{\text{SCO}}(\text{total}) \) | \( \kappa_{\text{STA}}(\text{total}) \) |
|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| 100             | 97.24           | 73.47           | 6441            | 6624            | 985.6           | 1012.03         | 7523.84         | 7709.50         |
| 200             | 20.45           | 17.08           | 1354            | 2237            | 142.7           | 122.73          | 1517.15         | 2376.81         |
| 300             | 7.589           | 6.477           | 1389            | 1421            | 68.86           | 63.13           | 1465.45         | 1490.61         |
| 400             | 3.930           | 3.057           | 678.1           | 730.0           | 39.41           | 35.47           | 721.44          | 768.53          |
| 500             | 2.162           | 1.687           | 238.1           | 241.77          | 20.29           | 14.83           | 260.55          | 258.26          |

TABLE IV: Contributions of photo-excitation and photo-ionization to Planck mean opacity in a germanium plasma at \( \rho=0.1 \text{ g/cm}^3 \) and various temperatures obtained with SCO-RCG and STA codes.

IV. CONCLUSIONS

The L-shell emission spectrum of germanium from a disc of 0.1-\( \mu \text{m} \)-thick Ti/Ge mixture (sandwiched in a plastic) irradiated by a high-intensity (i.e., \( 10^{17} \text{--} 10^{19} \text{ W/cm}^2 \)), 0.5 psec laser-pulse has been measured. The conditions of the plasma were inferred from simulations performed using both the LTE and non-LTE opacity codes. The non-LTE collisional radiative FLYCHK code estimated the plasmas to be at a density of \( 1.5 \pm 0.5 \text{ g/cm}^3 \) and an electron temperature of \( 800 \text{ eV} \pm 100 \text{ eV} \). On the other hand, three LTE opacity codes equipped with various levels of sophistication in atomic physics models found the plasmas to be at the same density as FLYCHK but at a lower electron temperature of \( 600 \text{ eV} \pm 60 \text{ eV} \).
Motivated by the work of Hoarty and Harris et al., we used a combination of the radiation-hydrodynamics FastRad3D and STA opacity codes to study their emission data. To model the data, first, we performed the FastRad3D calculations, in one-dimension, to obtain the time-dependent plasma density and temperature profiles of the target. We employed an ansatz in the calculations, which considered an instantaneous energy-deposition into the plasma electrons because the energy-deposition of the laser occurs in a time-scale much shorter than the hydrodynamics response time. The resultant profiles were subsequently used in the STA calculations to obtain the synthetic emission spectra and opacity of hot and dense germanium plasma.

Comparing STA calculated emission spectrum with LTE-GRASP2K results, we obtained reasonable agreement. Our analysis of the partial spectral contributions to the time-integrated emission spectrum also illustrated the sample conditions strongly depend upon the plasma temporal variations in density and temperature. In comparison with the experimental data, STA showed sufficient line-structure to reproduce the major emission spectral features of 2p−3d, 2s−3p and 2p−4d transitions displayed by the experiment.

The LTE-model is commonly assumed to be valid for describing a hot and dense plasma as in LTE, the electrons and ions have high collisions frequency are in equilibrium. However, one cannot simply dismiss the possibility that the photons aren’t in equilibrium with these particles. The disparity between the STA results and experimental data in the ∼1.7 keV regions may be an example of that — the non-LTE effects as well as the presence of the spatial temperature and density variations in the plasma. The limitations of the STA to account for these effects and quantitatively modeling the experimental data is expected, and are underscoring the difficulty of the present approach. Thus, good agreement between the GRASP2K and experimental spectra could be fortuitous, as GRASP2K is an LTE model.

The STA computed opacity profiles, ionization population fractions and average ionization were all compared with the results obtained from the SCO-RCG calculations for various plasma temperatures and densities over the L- and M-shell spectral range. The results from the two theories agree very well. All said comparisons of STA results in the observed spectrum and opacity are considerably close while offering the advantage of computational speed for generating opacity-emissivity database of high-Z plasmas needed for FastRad3D hydrodynamic simulations.

One final remark. Busquet’s RADIOM model [39, 41] for effective ionization temperature
$T_z$ is an appealing and a simple way to introduce non-LTE effects in hydrocodes. Since the experimental emission spectra appears to be in nearing LTE condition, it is of interest and our plan to examine the validity of the RADIOM model by comparing its predictions with the Hoarty’s experiment and results from collisional radiative FLYCHK calculations.

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