*31st EPS Conference on Plasma Phys. London, 28 June - 2 July 2004 ECA Vol.**28G**, P-2.019 (2004)*

Calculations of Spectral Opacities for Be-Cu plasmas using STA and Average Atom Models

L.B. Samolovskikh, P.A. Loboda, O.V. Luzganova, D.S. Netsvetayev, V.V. Popova

RFNC-VNIITF, Sneginsk, Russian Federation

Introduction

One of possible designs for an indirect-driven fusion target to achieve ignition at NIF was proposed at Los Alamos National Laboratory [1]. The target makes up the spherical ablator shell with the DT-ice layer on its inner surface filled by the DT gas with a density of 0.3 mg/cm^3. Beryllium with traces of copper is suggested as an ablator material. The target is arranged in a hohlraum fed by time-shaped laser pulses of the NIF facility with the energy of up to 1.4 MJ and peak power of 400 TW. A blackbody radiation temperature in the hohlraum is estimated to be as high as 300 eV.

Presence of copper increases the ablator opacity for X-rays. Excessively small opacity results in preheating of the thermonuclear fuel thus reducing compression efficiency whereas excessively large opacity causes the heating of only a shallow layer being of no use for the compression. Hence, it is necessary to optimize an ablator composition and thickness. According to the LANL calculations, an optimal concentration of copper makes up 0.9%.

Similar thermonuclear-ignition targets were proposed in RFNC VNIITF for the lower laser pulse energies of about 0.3-0.5 MJ expected in the future experiments on the ISKRA-6 laser facility being built at RFNC-VNIIEF [2]. To optimize target design and composition of materials, the modeling of target compression should be done. The target compression simulation requires reliable spectral-opacity data for the ablator. Such opacities arise from the continuum and spectral-line absorption due to free-free, bound-free and bound-bound transitions. Here, the realistic description of line absorption spectra has always been the most challenging task with its contribution to radiative losses and spectral opacities being of principal importance for many problems of high-energy-density-physics.

In highly ionized plasmas containing ions with the small number of bound electrons (1-5), calculations of absorption and emission spectra might be done using a direct accounting of individual spectral lines (e. g. [3]). To calculate the line spectra for the ions with greater number of bound electrons (5-10), when transition lines from different ion states effectively overlap each other, techniques using a Detailed Term Accounting (DTA) and a simplified line shape description were developed [4].

In mid-ionized dense plasmas containing ions with the open M-, N-, O- atomic shells, the number of populated states can be enormous particularly under the conditions of Local Thermodynamic Equilibrium (LTE). To simulate spectra of such plasmas, the only practical way is to use approximate quantum-statistical methods. Some of those are based on various modifications of the Average Atom (AA) model [5], whereas others such as Unresolved Transition Arrays UTA [6] and Super-Transition Arrays STA [7] models imply an effective description of the arrays of overlapped lines corresponding to the transitions between individual ionic configurations or bunches of configurations.

STA model

In the STA model, the arrays of closely spaced or overlapping spectral lines corresponding to specific one-electron transitions $n_\alpha l_\alpha j_\alpha \to n_\beta l_\beta j_\beta$ between the aggregates

of the energetically close configurations, so-called superconfigurations, are described by generalized line shapes. Superconfiguration may comprise either a single configuration, like that one for the UTA model, or some family of configurations selected to provide optimal accuracy and acceptable computer time. Distribution of configurations in the superconfiguration is implied to obey the Boltzmann formula whereas terms of specific configurations are populated proportional to their statistical weights.

The version of the STA model developed at RFNC VNIITF considers the superconfiguration states as the collections of supershells comprising single atomic shells with their occupation numbers: $\Xi \equiv n_1^{q_1} n_2^{q_2} \ldots n_k^{q_k}$. Therefore, one-electron transitions between superconfigurations Ξ, Ξ' are treated as follows:

$$\left(n_1\right)^{q_1} \ldots \left(n_\alpha\right)^{q_\alpha} \ldots \left(n_\beta\right)^{q_\beta} \ldots \left(n_\omega\right)^{q_k} \to \left(n_1\right)^{q_1} \ldots \left(n_\alpha\right)^{q_\alpha - 1} \ldots \left(n_\beta\right)^{q_\beta + 1} \ldots \left(n_\omega\right)^{q_k}$$

Dipole reduced matrix elements are calculated using one-electron wave functions. Effective line intensities are introduced as:

$$D_{\Xi\Xi'}^{\alpha\beta} = q_\alpha \left(g_\beta - q_\beta\right) \times \left\langle n_\alpha l_\alpha \left\| r \right\| n_\beta l_\beta \right\rangle^2 \times \begin{Bmatrix} l_\alpha & j_\alpha & 1/2 \\ j_\beta & l_\beta & 1 \end{Bmatrix}^2,$$

where $g_\beta = 2j_\beta + 1$ stand for the degeneracy of the electron state β and other notations are conventional. Average transition energy $\varepsilon_{\Xi\Xi'}^{\alpha\beta}$ is also evaluated.

The spectral dispersion of transition arrays come from the energy-dispersion of configuration sets within the superconfigurations. This is described by the Gaussian distributions with the statistical dispersions $\Delta_{\Xi\Xi'}^{\alpha\beta}$ evaluated using the single-electron data from the atomic calculations [6,7]. The resulting dispersion accounting for the Doppler effect is $\Delta = \sqrt{\Delta_{\Xi\Xi'}^{\alpha\beta\,2} + \frac{\mathrm{T}}{\mathrm{AC}^2} \varepsilon_{\Xi\Xi'}^{\alpha\beta\,2}}$, where C is the speed of light. Electron-collisional and natural broadening is taken into account using the Voigt function in the form of:

$\Phi\left(\varepsilon\right) = \frac{1}{\sqrt{\pi}\Delta} K\left(\frac{\varepsilon - \varepsilon_{\Xi\Xi'}^{\alpha\beta}}{\Delta}, \frac{\gamma^{\alpha\beta}}{\Delta}\right)$; $K\left(x, y\right) = \frac{y}{\pi} \int_{-\infty}^{+\infty} \frac{e^{-s^2}}{\left(x - s\right)^2 + y^2} ds$, where $\gamma^{\alpha\beta}$ is the homogeneous width comprising the electron-collisional and natural widths.

Relative abundances $\{c_k^Q\}$ of ionic species of chemical elements $\{k\}$ with the number of bound electrons $\{Q\}$ are evaluated from the Saha equations taking into account degeneracy of free-electron gas at low temperatures and/or high densities. Plasma effects are considered within the simple ion-sphere model by the correction to an ionization potential: $\Delta I_k^Q = 2Ry \frac{< Z >}{R_0}$, where $R_0 = 1.388 \sqrt[3]{\frac{< A >}{\rho}}$ is the mean ion distance and <*Z*> is the average ion charge. Higher terms of partition functions are reduced using the form-factor:

$\tau_k^{\Xi,Q}\left(\rho\right) = e^{-\left(\frac{2 \cdot \Delta I_k^Q}{\left|E_k^{Q-1} - E_k^{\Xi,Q}\right|}\right)^3}$, where $E_k^{\Xi,Q}$ is the superconfiguration energy, $E_k^Q = \min(E_k^{\Xi,Q})$.

A total absorption coefficient due to bound-bound, bound-free, and free-free transitions including the scattering. The bremsstrahlung, the photo-ionization absorption and the Compton scattering is calculated using the Born-Elvert approximation [5], the Kramers approximation [8] and the interpolation presented in Ref. [5], respectively. Opacity is determined as $\chi = \kappa / \rho$.

The STA-model version above was implemented in the SPECTR. To examine the code there was carried out an opacity calculation for an iron in a FeNaF mixture at 0.059

keV, 0.0113 g/cm^3 the same way as in [9]. Results are provided at fig. 1 and in table 1 in comparison with [9] showing the good agreement.

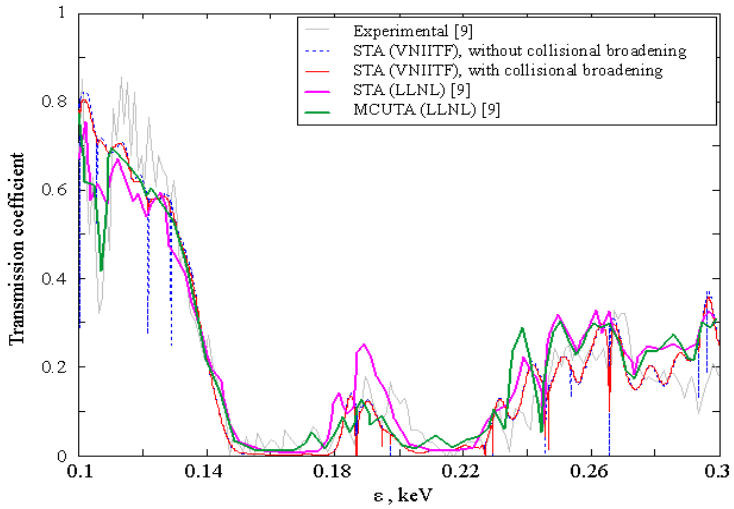


Fig. 1. LTE spectral transmission coefficients for Fe compound in 300 μ layer of mixture of Fe(60.3%), Na(19.85%) and F(19.85%) at 0.059 keV, 0.0113 g/cm^3.

Table 1. Plank and Rosselad mean opacity for iron compound in mixture of Fe(60.3%), Na(19.85) and F(19.85) at 0.059 keV, 0.0113 g/cm^3.

	Plank opacity, cm^2/g	Rosseland opacity, cm^2/g
Experiment (LLNL)	8200 ± 700	4400 ± 600
STA (LLNL)	8431	4630
Monte-Carlo UTA (LLNL)	8226	4525
OPAL/DTA (LLNL)	8188	4100
OPAL/UTA (LLNL)	8257	4255
STA (VNIITF)	8876	4503

Opacity for the beryllium-copper mixture

SPECTR code was applied for calculations of the beryllium-copper mixture opacity essential to describe the fusion ignition target compression (fig. 2). Calculations were made for temperatures from 0.01 keV to 0.36 keV and densities from 10^{-3} g/cm^3 to 10 g/cm^3. Results are given in table 2. The opacity dependence on a copper concentration for the representative ablator temperature and density [2] is provided at fig. 3 (left). It is clear that at copper concentration of 0.9% the copper absorption forms more than half of the Rosseland opacity.

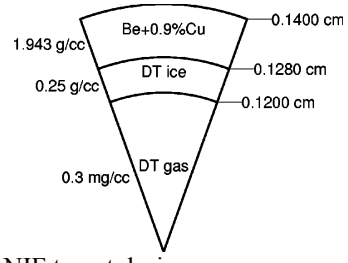


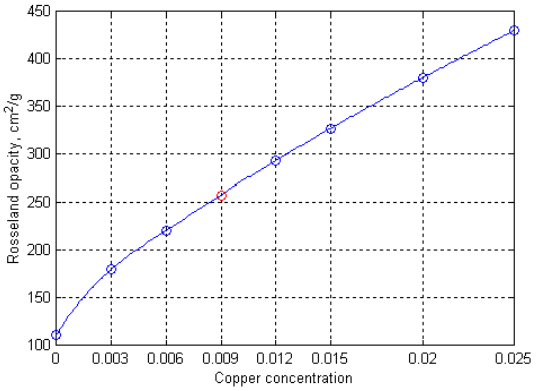
Fig. 2 Indirect driven fusion ignition NIF target design.

Copper ions contribute an essential absorption especially for high-energy (>1 keV) photons for which beryllium is translucent that helps to reach the optimal absorption spectrum suitable for the better target compression and energy gain. This is evident at fig. 3 (right) where one can see the spectral opacity for pure beryllium and the BeCu mixture at 0.1

keV, 0.1 g/cm^3 in comparison with a BeCu mixture calculation by an AA model [5,10]. It is also seen that the STA model gives the finer spectrum structure than the AA model.

Table 2. Rosseland opacity (cm^2/g) for mixture of beryllium (99.1%) and copper (0.9%).

ρ, g/cm^3 \ T, keV	0.01	0.04	0.1	0.25	0.36
10^{-3}	$2.069\cdot10^{3}$	516.9	8.177	$6.927\cdot10^{-1}$	$2.703\cdot10^{-1}$
10^{-2}	$1.000\cdot10^{4}$	$2.916\cdot10^{3}$	66.70	4.286	1.066
10^{-1}	$3.229\cdot10^{4}$	$1.143\cdot10^{4}$	257.6	22.13	9.516
1	$5.803\cdot10^{4}$	$2.681\cdot10^{4}$	929.6	116.6	46.95
10	$1.566\cdot10^{5}$	$3.940\cdot10^{4}$	$3.001\cdot10^{3}$	334.4	114.0



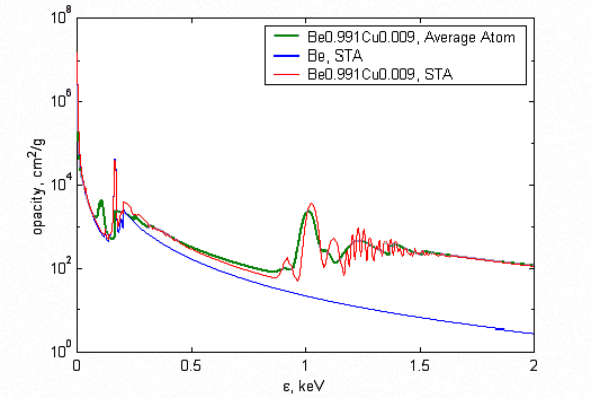


Fig. 3 *Left*: opacity vs. copper concentration at 0.1 keV, 0.1 g/cm^3;
Right: spectral opacity for pure Be and Be(99.1%)Cu(0.9%) at 0.1 keV, 0.1 g/cm^3 by different models.

Conclusion

The STA model version was implemented in the SPECTR code for spectral opacity calculations. Results of the trial task showed to be in a good agreement to experimental facts and calculations by another authors. This technique allows to obtaining more detailed absorption spectra than the AA model whereas only moderate number of superconfigurations is considered to simplify evaluations in comparision with a DTA. Such model is suitable in case of weakly and middle non-ideal plasmas. The model was used for BeCu mixture opacity calculations required to simulate the inertial fusion NIF and ISKRA-6 targets compression. Results would be exploit for the ablator composition and thickness optimization to reach the maximum energy gain.

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