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Predicting Rosseland mean opacities of Aluminum using a difference converging method

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ABSTRACT

A *difference converging method* for *opacity* (DCMo) calculation is suggested to predict opacities and transmissions of metal plasmas at other photon energies that were not measured. The applications of the DCMo to the opacity and transmission calculations of Aluminum plasmas, in the spectral range of $73.5eV \leq h\nu \leq 245eV$ with $T_e = 20eV$, and of $1475eV \leq h\nu \leq 1540eV$ with $T_e = 19eV$, show that: 1) the DCMo correctly reproduce all important absorption structures of the Al plasmas and their corresponding intensities; 2) the agreement between the experimental and the *DCMo* transmissions is notably better than that between the experimental and some other computational transmissions like the ones obtained using OPAL and ATOMIC models.

1. Introduction

The radiative opacity plays key roles in understanding the hydrodynamic behavior of hot dense plasma in stellar physics and inertia confinement fusion (ICF) due to its direct relation with the radiation thermal conductivity. There have been many reliable measurements on opacities of a number of metal plasmas using various experimental techniques [1–15], and many fruitful calculations using different theoretical models and physical approximations [16–46] for about six decades. Since the middle of 1990s, experimental techniques have been available to simultaneously measure plasma temperature, density, and absorption spectrum of ionized hot plasmas [4,5,10,12,13]. Recently, high quality measurement on the opacity of high-Z element at a higher plasma temperature of 85 eV over a wide photon energies of 150 eV to 1200 eV is reported [15]. These accurate experimental measurements not only have supplied many important quantitative data for radiative transportations of some ionic plasmas, but also have made important progresses in verifying opacity models used in theoretical calculations. On the other hand, theoretical simulations on plasma opacities have developed various physical models, such as the average ion (AI) [16,18], the average atom (AA) [27], the unresolved transition array (UTA) [25], the detailed term accounting (DTA) [26], the detailed configuration accounting (DCA) [21,30], the detailed level accounting (DLA) [43] and the super transition arrays (STA) [37]. Although many calculations have generated valuable opacity data that have nice general agreement with measurements, the discrepancies between theoretical models and experiments are still (usually) at 8% to 16%, or even larger until recently. It also often happens that some calculated absorption peak may significantly shift from or be narrower than the measured one. Reasons of such discrepancies, on the computational side, may be mainly due to the incompleteness of the colossal number of complex configurations, the difficulties in correctly determining the energy levels of given ionic structures, and the inaccurately calculating millions of spectral lines of various ionic states and their resulting states couplings. In addition, although one may obtain reasonable opacities using one of the above, or some other, quantum mechanical based theoretical methods, it is still hardly that one may clearly explain the very complicated physical pictures of a multi-ion plasma system just like that one usually do for a simple atomic or molecular collision system.

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Based on the above discussion, one may ponder the opacity calculations in a different approach. Using modern experimental technologies, people can measure the transmissions or opacities in certain frequency (or photon energy) range for a complicated plasma system with reasonably high accuracy and considerable cost. Since the measured accurate opacities obey some valid physical relation, and they contain almost all physical effects and quantum information of ionic structures, electronic configurations and their couplings, one may start from this fact and may search another theoretical method which combines the merits of both the accurate experimental measurements and the advantage of reliable theoretical derivations. With such a philosophy view, one may try to establish an intrinsic physical connection among the opacity data. Such a relation may bridge the unknown opacity with the measured ones. If this relation can be obtained without using any physical models and mathematical approximations, one may use it and a set of measured accurate opacity data to predict the opacities that may not be available or be difficult to obtain experimentally at other wavelengths or photon energies.

In our recent studies, a *difference converging method* (DCM) has been proposed to predict the unknown transitional spectral lines of vibrational diatoms [47], and to predict the unknown differential cross sections (DCSs) of electron scattering from polyatomic molecules [48] respectively. The DCM bridges the unknown transitional lines with the experimental data for the former, while for the latter, it connects the unknown DCSs with the measured ones.

This study proposes a *difference converging method* for *opacity* (DCMo) calculations to predict the Rosseland mean opacities and transmissions from a set of accurately measured data, and applies the DCMo to predict the Rosseland mean opacities and transmissions of Aluminum plasmas at three experimental conditions. In Section 2, the DCMo method will be outlined. Section 3 shows the applications and discussions. Section 4 gives the summary of this study.

2. Theoretical method

To establish a physical bridge that connects unknown opacities with some accurate experimental ones as mentioned above and use it to predict the opacities those may not be available experimentally, this section will: 1) propose a series expansion of the Rosseland mean opacity; 2) find the bridge equation based on this series expansion; and 3) suggest a DCMo method used to predict unknown opacities at other photon energies based on a set of accurately measured opacities using the bridge equation.

The measured Rosseland mean opacities κ_R satisfy the integral form [24,41,42]

$$\frac{1}{\kappa_R} = \int \frac{1}{\kappa(u)} f_R(u) du \tag{1}$$

where $\kappa(u)$ is the frequency dependent monochromatic opacity, $f_R(u)$ is the frequency-dependent weighting function,

$$f_R(u) = \frac{15}{4\pi^4} \frac{u^4 e^{-u}}{[1-e^{-u}]^2} \tag{2}$$

and u is the dimensionless energy variable,

$$u = \frac{h\nu}{T_e} \tag{3}$$

where $h\nu$ is the photon energy, and T_e is the temperature in energy unit.

The transmission T of radiation through a foil with thickness r and density ρ is directly related to the spectral opacity κ by

$$T(h\nu) = e^{-\kappa(h\nu)\rho r} \tag{4}$$

where the areal density ρr is a constant in g/cm^2 unit during the calculation.

The Rosseland mean opacity κ_R and its logarithmic function had been expanded as some experiential series respectively [49]. In order to build an intrinsic physical bridge among Rosseland mean opacities, one may rationally expand the integral form of the Rosseland mean opacity in Eq. (1) as a, hopefully better, series, and this is done in the Appendix A of the Supplemental Material (SM) [50] of present study. The final form of the series of Rosseland mean opacity given in the Eq. (A10) of the SM is

$$\frac{1}{\kappa_R} = \sum_{i=1}^{M} Y_i \pi_{i,u}(u) \tag{5}$$

where Y_i are opacity constants, and $\pi_{i,u}(u)$ are the expansion coefficients that vary with the frequency variable u (namely with radiation frequency ν and temperature T_e). The form of $\pi_{i,u}$ is reasoned in Eq. (A11) of the SM as

$$\pi_{i,u} = \frac{15}{4\pi^4} \frac{u^{m+i} e^{-u}}{[1-e^{-u}]^{n-1+i}}, \ (m=3, n=2), \tag{6}$$

This expression of $\pi_{i,u}$ may be better than the expansion coefficient of the series of Rosseland mean opacity in Ref. [49] in that it keeps the particular exponential form as the original frequency-dependent weighting function $f_R(u)$ in Eq. (2).

Based on the series expression in Eq. (5), one can go to stage 2), namely use a multi-difference method to derive an analytical formula that bridges the unknown Rosseland mean opacity and a set of measured ones. The detail derivation is given in Appendix B of the SM, and the final expression of the formula given in Eq. (B67) is

$$\kappa_{R_{12}}^{-1} = \sum_{i=1}^{N} l_i \kappa_{R_i}^{-1}, N = 11. \tag{7}$$

The formulae of $N < 11$ may be easily obtained as the ways given in the SM of Ref. [48], and the ones of $N > 11$ can also be derived similarly as the steps in present SM.

The Eq. (7) builds the internal physical relationship among the experimental Rosseland mean opacities. Therefore, one may obtain the unknown Rosseland mean opacity $\kappa_{R_{12}}$ using the Eq. (7) and N known values $(\kappa_{R_i})_N$. In Eq. (7), all expansion coefficients $\{l_i\}$ are known constants and they are ultimately the explicit functions of the expansion coefficients $(\pi_{i,u})$ (as in Eq. (6)) of the Rosseland mean opacity κ_R expressed as in Eq. (5).

The Eq. (7) is derived using the (10 folds) multi-difference method based on the series expression of Rosseland mean opacity in Eq. (5) (namely the Eq. (A10) of the SM). The complicated unknown integral of the Rosseland mean opacity in Eq. (1) is expressed as a series and is converted into simple algebraic computations. The unknown opacity constants Y_i in Eq. (5) can also be evaluated using Eqs. (B7), (B11), (B16), (B22), (B29), (B37), (B46) and (B56) respectively.

Now, we get into stage 3). There are inevitable errors in experimental data, and such errors will be transmitted to the calculated opacities through Eq. (7). The theoretical error $\partial\kappa_{R_{12}}^{-1}$ of the calculated $\kappa_{R_{12}}^{-1}$ might be expressed as

$$\partial\kappa_{R_{12}}^{-1} = \sum_{i=1}^{N} l_i \partial\kappa_{R_i}^{-1} \tag{8}$$

Since it is difficult to know and assess the errors $(\partial\kappa_{R_i}^{-1})'s$ of experimental data, a practical way to have a smaller $\partial\kappa_{R_{12}}^{-1}$ is requiring that the expansion coefficients $l_i's$ are minimums. This property may be used as one of the computational converging requirements.

For a set of N measured data $(\kappa_{R_i})_N$, using Eq. (7) one may evaluate K unknown opacities $\{\kappa_{R_j}; j = 1, \cdots, K\}$ which are not any one of the known data. If there are $m(>N)$ experimental opacities