Radiative opacity of high-temperature and high-density gold

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The authors calculate the radiative opacity of gold under conditions representing particle-beam–pellet fusion targets: solid density and a temperature of 750 eV. It is shown that under these conditions the absorption lines form broad bands due to the combined effects of linewidth, electrostatic splitting, and the existence of a distribution of ionization states in the plasma. As a result, line absorption has a dominant effect on the Rosseland mean free path.

I. INTRODUCTION

The irradiation of pellet fusion targets in the break-even regime by intense electron or ion beams involves the production of high-density high- or medium-Z plasmas, at temperatures of the order of 1 keV.[1,2] Under these conditions radiative energy transfer is of great importance. At the high densities involved it can be accounted for by the diffusion approximation, and the opacity is determined by the Rosseland mean free path. The processes contributing to the opacity are the free-free, bound-free, and bound-bound transitions.

In the plasmas studied here the bound-bound (line) contribution is particularly significant. The importance of the bound-bound transitions was first pointed out by Mayer.[3,4] Opacity calculations including these transitions were carried out among others by Cox[5] and by Carson *et al.*[6] The plasma here contains significant concentrations of a large number (typically eight) of ionic species with different degrees of ionization, as determined by thermodynamic equilibrium. This results in a considerable spread of the transition energies between given states. This effect, combined with the effect of linewidth in the plasma and the splitting of multiplets due to electrostatic interactions, results in the formation of smeared broad absorption bands covering the energy range which contributes to the Rosseland mean opacity. If these bands block the dips between the edges of the bound-free absorption cross section curve, the lines should have a large effect on the opacity.

In this work we present a calculation of the opacity of dense hot high-Z plasmas, taking into account free-free, bound-free, and bound-bound transitions. The specific calculations were carried out for the example of gold at solid density and a temperature of 750 eV.

II. MODEL

The ionic composition of the plasma is calculated by solving the Saha equation, which is justified under conditions studied here. A procedure similar to that used by Cohen *et al.*[7] and Parks *et al.*[8] was used. As first approximation the ionic composition was calculated assuming equal partition functions and ionization potentials uncorrected for plasma effects, taken from Carlson.[9] The energy levels were then calculated using the scaled Thomas-Fermi model as suggested by Stewart and Rotenberg.[10] The energies in several representative cases were compared with the more-accurate relativistic self-consistent-field calculations according to Liberman *et al.*[11]; thus, the appropriate scaling factor α used in the scaled Thomas-Fermi model calculations was found. The energy levels were used in a calculation of the ionic partition function by summing over the excited configurations

$$Z=\sum_i g_i e^{-E_i/kT}\,, \tag{1}$$

where g_i is the degeneracy of the configuration and E_i is its energy given by the sum of single-electron energies. The lowering of ionization potentials due to plasma effects is calculated in the ion-sphere approximation[3,12] which is applicable here:

$$\Delta I=\tfrac{3}{2}Z_{\text{ion}}e^2/a_z \tag{2}$$

where $Z_{\text{ion}}e$ is the ionic charge and a_z is the ion-sphere radius. The corrected values of the partition functions and ionization potentials are used to calculate new values of the ionic populations by the Saha equation. From the known weights of the excited configurations it is possible to calculate the average population of each nlj state.

The effect of the free electrons on the transition probabilities and transition energies were neglected here. This effect was studied by Rozsnyai[13,14] who solved the wave equation using the temperature-dependent Thomas-Fermi potential. Stewart and Pyatt[12] have shown that the perturbing free-electron potential essentially influences only those orbitals whose depressed ionization potentials are less than kT. This effect could reduce the transi-

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tion probabilities to these higher-energy states. However, it could be compensated for by the additional width due to bands ocurring in the bound states close to the continuum as suggested by Rozsnyai.[13] We note that the final opacity result here is rather insensitive to the absolute magnitude of the oscillator number (see below).

The known energies and wave functions allow the calculation of the cross sections for the atomic absorption processes. The bound-free cross section for orbital j with principal quantum number n_j and unlowered binding energy E_j is given according to Cohen *et al.*[7] by

$$\mu_{bf}(E)=\begin{cases}0 & \text{if } E_j-\Delta I>E\,,\\ \tau R_\infty E_j^2/An_jE^3 & \text{if } E_j-\Delta I<E\,,\end{cases} \tag{3}$$

where A is the atomic weight, $\tau=4.7617\times10^6$ cm^2/mole. It is assumed here that all transitions above the lowered ionization potential are into the continuum.

The contribution of the free-free transition to the mass absorption coefficient is given by

$$\mu_{ff}(E)=(Z^2/A\Gamma)(R_\infty/kT)^2\tau(E/kT)^{-3}\,, \tag{4}$$

where Z^2 is the average squared ionic charge number, n_e is the free-electron density, R_∞ is the Rydberg coefficient, and

$$\Gamma=2(2\pi mkT)^{3/2}/h^3n_e\,.$$

The calculation of the bound-bound contribution is based on the energy levels and transition energies calculated as described above. The oscillator strengths required for the evaluation of the line-absorption coefficient were calculated using the wave functions obtained in the scaled Thomas-Fermi model by[15,16]

$$f_{ik}=24.5E_{ik}\kappa\left(\int_0^\infty rR(n,l)R(n'l')\,dr\right)^2\,, \tag{5}$$

where E_{ik} is the energy of transition from i to k in keV. The factor κ depends on the shells participating in the transition and their occupation numbers, and is calculated according to Parks *et al.*[8]

The width of the spectral lines in the situation studied here is dominated by collisions with the plasma electrons and is given according to the one-electron approximation due to Barranger[17] by

$$w=(2/\Gamma)(n^4/Z_{eff}^2)kT\,, \tag{6}$$

where Γ is the statistical factor defined above, and Z_{eff} is the effective nuclear charge.

Each transition in a given ion is associated with an array of lines due to the splitting by the electrostatic interaction of the electrons within the given configuration. The multiplet distribution for the many particle configurations was evaluated by Moszkowski[18] in terms of multiplet distributions of two-particle configurations. The variance Δ^2E of the many particle multiplet distribution for a transition from i to j is given by

$$\begin{aligned}\Delta^2E(N_i,N_j-1,\{N_k\}\to N_i-1,N_j,\{N_k\})\\ =\frac{(N_i-1)(M_i-N_i)}{M_i-2}\Delta^2E(i^2\to ij)\\ +\frac{(N_j-1)(M_j-N_j)}{M_j-2}\Delta^2E(ij\to j^2)\\ +\sum_{k\neq i,j}\frac{N_k(M_k-N_k)}{M_k-1}\Delta^2E(ik\to jk)\,.\end{aligned} \tag{7}$$

Here N_i is the initial occupation of shell i, N_j-1 is the initial occupation of shell j, M is the level degeneracy, k denotes the levels not participating in the transition, and $\Delta^2E(ik\to jk)$ denotes two-particle multiplet distributions variances. The two-electron interaction energy assuming spins j_1 and j_2 which couple to total spin J, is given by

$$E(j_1,j_2,J)=\sum_k(f_kF^k-g_kG^k)\,. \tag{8}$$

Here F^k and G^k are Slater integrals, calculated specifically for each two-particle system treated in the calculation. f_k and g_k consist of Racah coefficients and are also specifically calculated for each two particle configuration. In calculating the multiplet distribution for a given two-particle system, $E(ik\to jk)$ was obtained by first calculating the values of $E(J)$ for both (j_i,j_k) and (j_j,j_k) according to Eq. (8). The variance was then obtained by generating all the allowed transitions between both configurations subject to $\Delta J=0,\pm1$. Thus the two-particle multiplet variances were explicitly derived for each case and used in Eq. (7) in the derivation of the total many-particle variances.

The number of spectral lines for the many-particle multiplets was obtained using the statistical approach of Parks *et al.*[8] In the case studied here the number of lines and their widths are such that the lines in each transition array strongly overlap and form an absorption band. The shape of this band is given by the multiplet distribution curve, the variance of which is given by Eq. (7). Following Moszkowski,[18] the shape of this function was taken to be Gaussian.

The mechanism which determines the actual width of the absorption bands is due to the existence of various degrees of ionization in the plasma. For each transition array the transition energies were calculated as function of the degree of ionization. The range of degrees of ionization considered was determined by the populations calculated from thermodynamic equilibrium. In a given transition array $(j\to k)$ we denote the transition energy in the ith ionization state by ϵ_{ijk}, and the square root of the multiplet variance by $\sigma_{jk} = (\Delta^2 E_{ik})^{1/2}$. We denote the concentration of the ith ionization state by Y_i. The band profile is then given by

$$g_{jk}(\epsilon) = \sum_i Y_i \frac{1}{(2\pi)^{1/2}\sigma_{jk}} \exp\left(-\frac{(\epsilon - \epsilon_{ijk})^2}{2\sigma_{jk}^2}\right). \quad (9)$$

The bound-bound cross section μ_{bb} for the transition $i \to k$ is given by

$$\mu_{bb}(\epsilon) = (\pi e^2/mc^2) h f_{i,k} g(E),$$

where g is normalized such that $\int_0^\infty g(E)dE = 1$.

The total contribution of line absorption is determined by the total effect of such bands associated with each transition.

Finally, the Rosseland mean free path is calculated by

$$\Lambda = \int_0^\infty u^4 e^{-u}(e^u - 1)^{-3}\mu^{-1} du, \quad (10)$$

where $u = E/kT$ is the reduced energy and the absorption coefficient μ is given by

$$\mu = \mu_{bf} + \mu_{ff} + \mu_{bb}.$$

The effect of electron scattering on the opacity is negligible in the case studied here.

III. CALCULATIONS

Calculation of the opacity was carried out for the example of gold plasma at a density of 19.0 g/cm^3 and a temperature of 750 eV.

The zero approximation to the equilibrium populations, assuming equal partition functions, indicated a most probable configuration of three electrons outside a full $n = 3$ shell. In the complete calculation including Eq. (1), a complete $n = 3$ shell was assumed and the excited configurations were obtained by allowing the electrons to occupy all $n = 4$ and $n = 5$ states. A more accurate calculation would have to consider ions with a few holes in the $3d$ shell. However, transitions to these levels have little effect on the Rosseland mean in this case. Fluctuations in the number of these holes will cause further smearing of the bands due to configuration broadening. Also, an accurate calculation would have to consider excited configurations with $n = 6$ and $n = 7$ occupied states. This could shift the most probable ionization state by about one charge, but because of the statistical nature of the problem, the effect would be negligible. The distribution of the ionization states is shown in Table I. The average initial state population of electrons consists of 4.7 electrons in the $n = 4$ shell and 2.26 electrons in the $n = 5$ shell.

The initial states of the bound-bound transitions considered here were all the $n = 3$, $n = 4$, and $n = 5$ states while the final states consisted of all $n = 4$ to $n = 7$ levels, subject to the selection rules. Only transitions of $\Delta n = 1$ were relevant to the calculation in this case. All together, 192 transitions were accounted for, and their strengths calculated by Eq. (5).

TABLE I. Abundance as a function of degree of ionization.

Total number of electrons in ion	Fraction of ionic species
31	0.04
32	0.08
33	0.15
34	0.20
35	0.22
36	0.15
37	0.09
38	0.04
39	0.02

The typical spectral line width from Eq. (6) was found to be of the order of 1 eV. The typical width of the many particle multiplet distribution from Eqs. (7) and (8) for the most-probable ion was of the order of 10 eV. The number of lines in a typical transition array in the most probable ion was found to be of the order of thousands. This justifies the absorption band model used for the treatment of transition arrays. The values of σ_{jk} used in Eq. (9) were those derived for the most probable ion. The typical band broadening due to the various degrees of ionization in the plasma was found to be about 50 eV.

IV. RESULTS AND DISCUSSION

The bound-free and bound-bound absorption cross sections are shown in Fig. 1 as functions of the reduced energy $u = E/kT$. The bound-bound

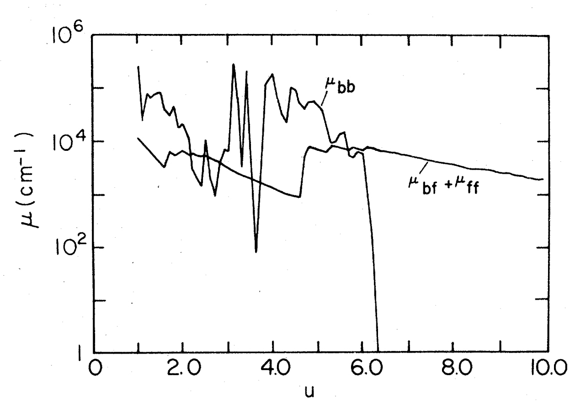

FIG. 1. Photon absorption coefficient as a function of u ($u = E/kT$). μ_{bf} and μ_{bb} denote the bound-free and bound-bound data, respectively.

cross section is observed to be larger than the bound-free cross section in the range of energies which is relevant for the Rosseland mean, and the bound-bound transitions have the effect of blocking the gaps between the important bound-free edges.

The Rosseland mean with the inclusion of the bound-bound transitions was calculated to be

$$\Lambda_{bb,bf,ff} = 0.12 \times 10^{-3} \text{ cm},$$

while the Rosseland mean without the bound-bound transitions is found to be longer by about a factor of 3:

$$\Lambda_{bb,bf} = 0.35 \times 10^{-3} \text{ cm}.$$

This result indicates that in certain regions of the flow in electron beam fusion targets the radiative opacity is dominated by the contribution of line absorption. This effect is due to the formation of broad absorption bands which cover the whole energy range relevant for the Rosseland mean. We note here that by arbitrarily decreasing all the oscillators strength by a factor of 2, the value of Λ decreases by only 13%.

A complete scan of the temperature and density ranges that occur in pellet fusion is required because of the possible sensitivity of the effect to variations in these parameters. For example the width of the absorption bands should depend on the number of electrons outside complete shells, so that the importance of the effect should be studied at temperatures such that this number is small.

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