HARTREE–FOCK–SLATER CALCULATIONS ON PLASMA PARAMETERS.

PART 1. SPECTRAL CHARACTERISTICS

B. N. Bazylev, L. V. Golub, G. S. Romanov,
and V. I. Tolkach

UDC 533.9

A model is proposed for calculating plasma optical parameters; the calculated spectral absorption coefficients for various elements are compared with published values.

Plasma physics research involves not only measurements but also simulation, which can give a more detailed picture and indicate which processes affect the measured parameters. However, an adequate simulation would be impossible without a knowledge of the thermodynamic and optical characteristics over wide temperature and density ranges, which can be derived from calculations on models.

There are difficulties in simulating plasma thermodynamic and optical parameters; it is necessary to process a large volume of spectroscopic data: energy levels, oscillator strengths, ionization and recombination cross sections, and so on.

Light-element parameters are usually calculated from the observed atomic characteristics [1, 2], but that information is incomplete for many elements, particularly highly ionized atoms, and in that case, one uses various quantum-mechanics methods: semiempirical quantum-defect techniques [3, 4] (very limited application), the self-consistent Hartree-Fock method [5, 6] (very laborius), or combinations of them [7-9]. In all those models and associated software, one needs a large spectrocopic data bank. The approach involves an enormous amount of effort, which increases sharply as the spectroscopy becomes more complicated (elements with open d and f shells or high z), and the probability of subjective errors increases. Research has been done on computerized data banks for such atomic characteristics [10], but this does not eliminate the manual work involved in inputting the data, for which a farily large volume of preparatory work is also required. Also, the number of elements currently covered by the bank is limited. These deficiencies mean that calculations on plasma properties cannot be done readily, particularly for plasmas with complicated compositions or elements with high z. One needs a new type of program for calculating plasma parameter,s where the minimum effort and shortest run times are combined with calculations over wide ranges in parameters and composition, even at the expense of possible reduction in accuracy.

Here we describe a model and software suite meeting these requirements; the minimal amount of input data is required: plasma element and mass compositions, relevant temperature range, photon energies and densities, and spectral group boundaries. Self-consistent field calculations give a data bank, from which one can calculate the ionic compositions of equilibrium plasmas and generate tables giving the thermodynamic aznd optical characteristics.

1. Spectroscopic-Characteristic Calculation. Routine derivation of ionization potentials, energy levels, and photoinization cross sections is best based on the Hartree-Fock-Slater HFS method, in which the energy levels correspond to electron configurations. That approximation describes the structure of a highly charged ion well. For neutral atoms and ions with low charges, the electrostatic interactions are strong, so the one-electron HFS levels describe the actual term structure with an accuracy of about 10% (the disadvantage can be eliminated by using observed potentials at energy levels). The accuracy in calculating inner-electron energies is usually much higher.

Sevchenko Applied Physics Institute, Lenin Belorussian University, Minsk. Translated from Inzhenerno-Fizicheskii Zhurnal, Vol. 58, No. 6, pp. 1012-1017, June, 1990. Original article submitted May 20, 1989.

0022-0841/90/5806-0795$12.50

The HFS equations represent a self-consistent system with approximate incorporation of the exchange interaction [11]:

$$\left(\frac{d^2}{dr^2}+\frac{2Z(r)}{r}+V_{\text{ex}}(r)-\frac{l(l+1)}{r^2}-\varepsilon_{nl}\right)\Psi_{nl}=0,$$

$$\frac{Z(r)}{r}=\int_r^\infty (Z_0-\int_0^{r_1}\rho(x)\,dx)/r_1^2 dr_1;\quad V_{\text{ex}}=-\frac{3}{2}\left(\frac{3}{\pi}\rho\right)^{1/3}, \tag{1}$$

$$\rho(x)=\sum_{nl}\Psi_{nl}^2(x).$$

The HFS equations do not incorporate how the energies ε_{nl} are dependent on the total momenta L and S, which substantially simplifies solving (1), which can be done interatively, during which one determines $Z(r)$, $V_{\text{ex}}(r)$, the eigenvalues, and the bound-electron wave functions. The excited-state wave functions and eigenvalues are calculated in the resulting Z(r) and $V_{\text{ex}}(r)$, and one similarly determines the wave functions in the continuous spectrum Ψ_{El} for a given energy E.

The photoionization cross sections are calculated as lengths:

$$\sigma=8.56\cdot 10^{-19}\frac{\hbar\omega Ry}{I^2}\sum_{l'=l+1}\frac{l_{\max}}{2l+1}MR^2,$$

$$R=\int_0^\infty \Psi_{nl}r\Psi_{El'}dr,\quad E=\hbar\omega-\varepsilon_{nl}. \tag{2}$$

It is necessary to know the shell fillings to sovle (1); in that model, the initial filling for the neutral atoms are derived from experiment, and on transition to the next ion, the electron with the least energy is ionized. The statistical weights for the energy levels are defined by an expression in which the data for g_0 are taken from tables [5]: $g_i=2g_0(2l_i+1)$.

The HFS equations give a data bank containing the ionization potentials, energy levels, photoionization cross sections, and statistical weights for all the ions required in the subsequent calculations.

2. Plasma Ion Composition and Thermodynamic and Optical Parameters. A plasma in local thermodynamic equilibrium has a composition defined by Sakha's equations in the ring approximation for a large canonical ensemble over wide ranges in temperature and density [12]:

$$\frac{N_{i+1m}N_e}{N_{im}}=2\frac{u_{i+1m}}{u_{im}}\left(\frac{m_e kT}{2\pi\hbar}\right)^{3/2}\exp\left(-\frac{J_{im}-\Delta J_{im}}{kT}\right). \tag{3}$$

Here we have incorporate the Coulomb interaction between the ions, which reduces the ionization potentials:

$$\frac{\Delta J_{im}}{kT}=\ln\frac{(1+\gamma/2)[1+(z_{im}+1)^2\gamma/2]}{(1+z_{im}^2\gamma/2)}. \tag{4}$$

The nonideality parameter y is the positive root of the following equation:

$$\gamma^2=\left(\frac{e^2}{kT}\right)^3 4\pi\sum_m\sum_i\frac{N_{im}z_{im}^2}{1+z_{im}^2\gamma/2}. \tag{5}$$

The summation in (5) includes the electron and ion components. The sums in (3) are defined from an expression that contains not only the Boltzmann expression but also the Planck cutoff factor, which eliminates the divergence for $E_{jim}\sim J_{im}$:

$$u_{im}=\sum_j g_{jim}\exp(-E_{jim}/kT)\left[1-\left(1+\frac{J_{im}-E_{jim}}{kT}\right)\exp\left(\frac{E_{jim}-J_{im}}{kT}\right)\right]. \tag{6}$$

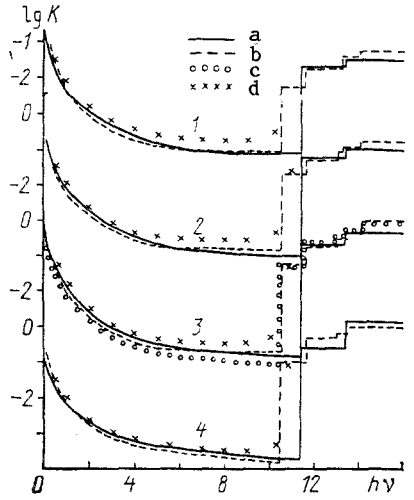

Fig. 1. Continuum absorption coefficients for an air plasma at normal pressure: 1) T = 20,000 K; 2) 18,000; 3) 16,000; 4) 14,000; a) this study; b) [13]; c) [15]; d) [14]; log k in cm^{-1} and hν in eV.

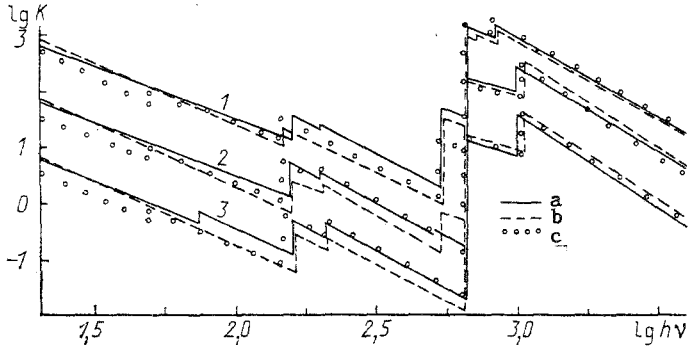

Fig. 2. Absorption by an air plasma at $1 \cdot 10^6$ K: 1) ε = 1, normal density; 2) 0.1; 3) 0.01; a) this study; b) [15]; c) [9]; log hν in eV.

An iterative method has been used to solve (3)-(6); we calculate the ion composition and determine the thermodynamic functions:

$$N_h = \sum_{m=1}^{M} \sum_{i=1}^{z_m} N_{im}; \quad p = kT(N_h + N_e) + \Delta p_c;$$

$$\varepsilon = \frac{3}{2} \frac{kT}{\rho}(N_h + N_e) + Q + \Delta E_c;$$

$$S = 82536 \cdot 10^8 \left[\left(1 + \frac{N_e}{N_h}\right) \left(\ln \frac{(kT)^{3/2}}{N_e} + \ln N_e - \frac{\sum\sum_{m\ i} N_{im} \ln N_{im}}{N_h} + \right.\right. \quad (7)$$

$$\left.\left. + \frac{\sum\sum_{m\ i} N_{im} \ln u_{im}}{N_h} + \frac{\sum\sum_{m\ i} N_{im} \varepsilon_{im}}{N_h kT} + 1.5 \ln A + 10.58 \right] + \Delta S_c.$$

The corrections for Coulomb interaction are:

$$\Delta p_c = \frac{-kT\varkappa^3}{24\pi}; \quad \varkappa = \gamma \frac{kT}{e^2};$$

$$\Delta E_c = -\frac{kT\varkappa^3}{8\pi\rho}; \quad \Delta S_c = -\frac{k\varkappa^3}{24\pi\rho}. \quad (8)$$

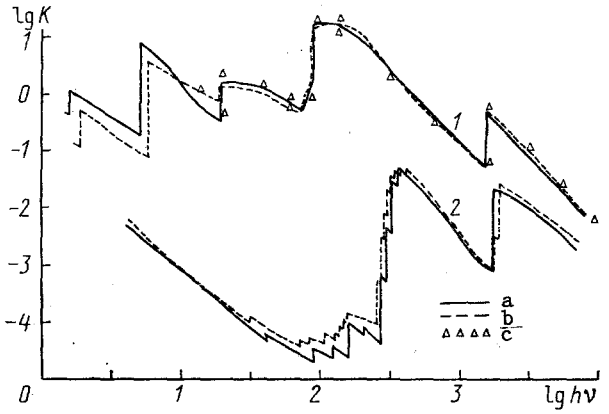

Fig. 3. Continuum absorption for an aluminum plasma: 1) T = 1 eV; δ = 0.1; 2) 31.6 and 0.01; a) this study; b) [7]; c) [16].

The continuous absorption is governed by photoionization and inverse Brehmstrahlung:

$$\varkappa_\varepsilon' = \left(\sum_{m=1}^{M} \sum_{i=1}^{z_m} \sum_{j=1}^{L} N_{im} g_{jim} \exp\left(-\frac{E_{jim}}{kT}\right) \sigma_{\phi jim}(\omega) + \sum_{m=1}^{M} \sum_{i=1}^{z_m} N_{im} \sigma_{bim} \right) \left(1 - \exp\left(-\frac{h\omega}{kT}\right)\right). \qquad (9)$$

The calculations give not only the data bank but also thermodynamic-characteristic tables, absorption coefficients, and mean and mean-group absorption coefficients for Rosseland and Planck weighting functions for given temperature and density ranges.

3. Discussion. We performed calculations for several substances to test the model, in particular air, aluminum, and xenon, for which there are calculations from various models [3-9, 13, 14], most of which are based on spectroscopic measurements for neutral atoms and low degrees of ionization [1, 2], which information is particularly valuable in identifying model features.

Figure 1 shows spectral absorption coefficients for an air plasma at low temperatures (14,000–20,000 K); the calculations agree well with the [9, 13, 15] data at 0-10 eV. Correction for the line flanks in [14] give somewhat stronger absorption, particularly around 10 eV. Above 10 eV, there is satisfactory agreement, although the structures in the photoionization steps differ somewhat. The HFS model gives two steps: the $2p^3$ shell for nitrogen and the $2p^4$ one for oxygen, although experiment gives several photoionization thresholds for the ^4S and ^3P terms. On the whole, the absorption at a temperature of 1-2 eV is described satisfactorily. The accuracy of the HFS model increases with temperature, as Fig. 2 shows from the absorption coefficients for an air plasma at a temperature of about 100 eV at various densities.

Figure 3 gives the absorption coefficients for aluminum plasmas at 1 and 30 eV; for photons above 10 eV, there is good agreement with [7, 16], but at low energies (absorption from excited levels), there are some discrepancies at T ≈ 1 eV. Figure 4 shows xenon plasmas. In [8], measurements were used for the first four ions, where relativistic corrections were incorporated together with the deviations from LS coupling. Nevertheless, there is good agreement with the calculations over much of the spectrum.

Conclusions. The model can be used to calculate ion compositions and continuum absorption coefficients over wide ranges in temperature, density, photon energy, and atomic number.

The characteristic errors usually do not exceed factors of 1.5-2, which is sufficient for most aspects of radiation gas dynamics. Observed ionization potentials for neutral atoms and the first ions extend the model to temperatures of about 1 eV.

NOTATION

r, radial coordinate; Ψ_{nl}, wave function; ε_{nl}, energy eigenvalue; V_{ex}, exchange potential; Z(r), effective charge; ρ(x), electron density; n, principal quantum number; l, orbital quantum number; σ_ϕ, photoionization cross section; σ_b, Brehmstrahlung absorption cross section; $\hbar$, Planck's constant; ω, photon frequency; Ry, Rydberg constant; M, number of equivalent electrons; g, statistical weight; N, number of ions in unit volume; N_e, number of free elec-

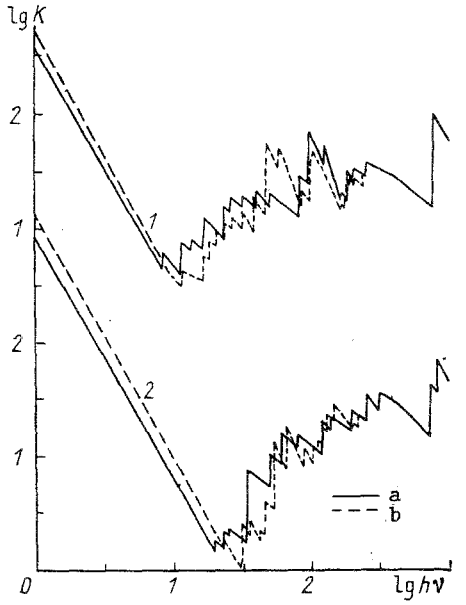

Fig. 4. Absorption by a normal-density xenon plasma: 1) T = 5.33 eV; 2) 9.48; a) this study; b) [8].

trons in unit volume; u, statistical sum for ion; m_e, electron mass; $\bar{e}$, electron charge; k, Boltzmann's constant; T, temperature; J, ionization potential; ΔJ, Coulomb reduction in potential; z, mean ion charge; γ, nonideality parameter; E, level energy; N_h, number of heavy particles; p, pressure; ε_t, specific internal energy; Q, a specific ionization and excitation energy; S, entropy; $\varkappa'_\varepsilon$, spectral absorption coefficient corrected for induced emission; $\varepsilon = \hbar\omega$, photon energy. Subscripts: j, energy level number; i, ionization multiplicity; m, number of element in plasma.

LITERATURE CITED

1. Ch. Moore, Atomic Energy Levels, Vol. 1, NBS, Washington (1949).
2. W. L. Wiese, M. W. Smith, and B. M. Glennon, Atomic Transition Probabilities, Vol. 1, NBS, Washington (1966).
3. D. R. Bates and A. Damgard, Phil. Trans., 242, 101 (1949).
4. A. Burgess and J. Seaton, Mont. Not, R. Astron. Soc., 120, No. 2, 121-151 (1960).
5. I. I. Sobel'man, Introduction to the Theory of Atomic Spectra [in Russian], Moscow (1963).
6. P. O. Bogdanovich, "A program for the numerical solution of Hartree-Fock equations," in: Software for Atomic Calculations [in Russian], Vol. 2, Vilnious (1978).
7. F. N. Borovik, S. I. Kas'kova, G. S. Romanov, et al., Opt. Spektrosk., 52, No. 4, 614-620 (1982).
8. F. N. Borovik, S. I. Kas'kova, G. S. Romanov, et al., The Equation of State and Absorption Coefficients for Xenon, Part 1 [in Russian], Deposited at VINITI, No. 6023-82 Minsk (1982).
9. G. A. Kobzev, Optical Parameters of an Air Plasma at High Temperatures: Continuum: Basic Processes and Calculation Methods [in Russian], Preprint, IVTAN, No. 1-112, Moscow (1983).
10. V. Yu. Bugaev, V. G. Pal'chikov, et al., Preprint, VNIIFTRI, Moscow (1988), pp. 4-19.
11. J. C. Slater, Phys. Rev., 81, 385 (1951).
12. A. A. Likal'ter, Zh. Éksp. Teor, Fiz., 56, No. 1, 240-245 (1969).
13. I V. Avilova, L. M. Biberman, et al., Optical Parameters of Hot Air (in Russian], Moscow (1970).
14. Thermal Radiation Phenomena, Vol. 1, Radiative Properties of Air, IFI/PLENUM, Washington (1969).
15. G. S. Romanov, K. L. Stepanov, S. I. Kas'kova, et al., Absorption Coefficients of High-Temperature Air Plasma, Part 2, Minsk (1988).
16. V. I. Buzdin, A. V. Dobkin, I. B. Kosarev, et al., Thermodynamic and Optical Parameters of High-Temperature Plasmas [in Russian], Deposited at VINITI, No. 52-84, Moscow (1983).