

CALCULATION OF THE OPTICAL CHARACTERISTICS OF A MULTICOMPONENT MULTIPLY CHARGED PLASMA

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A theoretical model is developed and results of calculations of thermodynamic and optical characteristics of a plasma in the approximation of a radiative-collisional model that allows their calculation in wide temperature and density ranges are reported. Energy levels, ionization potentials, probabilities of transitions are calculated by quantum-mechanical methods in the Hartree–Fock–Slater approximation. For some chemical elements use is also made of extensive experimental spectroscopic information that provides the possibility of determining the energy levels and wavelengths of optical transitions with a high accuracy.

In [1-3] a method of calculating thermodynamic and optical characteristics of a multicomponent plasma is suggested. The method is based on the use of Hartree–Fock–Slater (HFS) self-consistent calculations. The HFS method is used to calculate ionization potentials, energy levels, photoionization cross sections, and other characteristics of atoms and ions. The information obtained is then employed to calculate the ionization composition of a plasma, various thermodynamic functions, and absorption and emission coefficients. This calculation procedure is completely closed, does not rest on any empirical information, and allows quite rapid determination of all necessary thermodynamic and optical characteristics for a plasma of complicated chemical composition with satisfactory accuracy. However, it has a number of serious restrictions: the ionization composition is determined only in the approximation of local thermodynamic equilibrium (LTE), and in calculation of the absorption and emission coefficients only the continuous spectrum (photo- and bremsstrahlung spectra) is taken into consideration.

The procedure for calculation of plasma characteristics suggested below is a substantial extension of the methods of [1-3]. In the present work the ionization composition of a plasma and level populations are calculated within the framework of a radiative-collisional model (RCM) on the basis of balance of the collision and radiation processes in the plasma. Moreover, in calculation of the absorption and emission spectra numerous line transitions are taken into account. The contour of a spectral line is calculated with allowance for all the main mechanisms of broadening.

Among the collision processes impact electron ionization, triple recombination, and collision excitation and de-excitation are taken into consideration. The radiation processes considered are comprised of spontaneous discrete transitions, photorecombination, and dielectronic recombination. Strictly speaking, it is also necessary to include radiative mechanisms of excitation in the balance, i.e., discrete transitions in lines and photoionization. Then the problem is no longer local: the ionization composition of the plasma and the level populations will be determined not only by the local values of temperature and density but also by the entire radiation field in the plasma volume. In this case, it is necessary to solve a combined system of kinetics equations and radiative-transfer equations. The present authors have restricted their consideration to an account only of collision processes of excitation. Sometimes the approximation of an escape factor can be used, where radiative-excitation processes are taken into account approximately in resonance lines.

For moderate and heavy elements one more mechanism of ionization, namely, of the resonance type, can be very important. Light elements have a large difference in energy between the valence and inner shells. For this reason it will suffice to take into account only ionization from the valence shell. For heavy and moderate elements

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a distinctive feature is the presence of completing shells with similar energies. For instance, in the Fe atom the valence shell is $4s^2$, but the inner shell $3d^6$ only slightly exceeds it in energy. In this case, a new channel for ionization can appear: $3d^6 4s^2 - 3d^5 4s^2 nl - 3d^6 4s + e$. Here, at first the $3d^6 - 3d^5 nl$ transition proceeds, whose energy exceeds the ionization potential, and then self-ionization decay occurs, which represents an efficient ionization channel. Such ionization channels are most typical of the group of iron and rare-earth and heavy elements. In some cases, the rate of resonance ionization can be 1–1.5 orders of magnitude higher than the rate of ionization from valence shells.

Calculation of the cross sections and rates of inelastic electron scattering (collision excitation and ionization) is a rather complicated quantum-mechanical problem. The accuracy of its solution depends mainly on the type of approximation used. The most accurate calculation models, such as the method of strong coupling, are extremely time-consuming and are used, as a rule, only in reference calculations carried out for light elements. In practice, the Born approximation for atoms and the Born–Coulomb approximation for ions are most commonly used. In some cases, a more accurate version is adopted: calculation in the Born or Born–Coulomb approximation followed by renormalization of the cross sections to the K -matrix [4]. But even these methods are rather time-consuming and therefore simpler empirical relations such as the Bethe, Van Regemorter, and Meve formulas are frequently used. In [4], the applicability of these formulas is explored quite thoroughly and we follow these recommendations.

The suggested procedure for calculation of the cross sections and rates of collision excitations consists structurally of several levels. For transitions from the ground and first excited states of light elements ($n = 1, 2$) the most accurate approximations are used, namely, the Born approximation, the Born–Coulomb approximation, and the Born–Coulomb approximation followed by renormalization to the K -matrix with the use of data of [4] partially supplemented by calculations of the authors for some elements. For transitions between highly excited levels the Van Regemorter formula is usually used, in which the cross section is efficaciously expressed in terms of the oscillator strength of the corresponding dipole radiative transition. The accuracy of cross section calculations in such empirical relations is ~ 1.5 (usually overestimated). It should be noted that unlike radiative transitions, collisional multipole transitions are not negligibly small. Moreover, transitions of the $ns - n_1 d$ type are often stronger than dipole $ns - n_1 p$ transitions. In the present work the role of such processes was not investigated; this will probably be the subject matter of further investigations. It is pertinent only to note that the systematic excess of calculated excitation cross sections over experimental ones can, to some extent, compensate the neglect of multipole processes. It should also be noted that the role of the latter is of greatest importance for heavy elements. This is determined, first, by the large set of quantum numbers of the total orbital and spin momenta L, S and, second, by the substantial deviation from the scheme of $L-S$ coupling. For light elements, account for multipole transitions is of lesser importance. We do not provide the collision excitation and ionization formulas in explicit form, they are available in [4, 5].

To calculate the probability of a spontaneous transition, use is often made of simplified formulas. In the present work there is no need to use them, since the required oscillator strengths are preliminarily calculated by the HFS method. This is true to an even greater extent for calculation of photorecombination cross sections and rates. A typical approximation in calculations of photorecombination rates is the Kramers formula. It should be noted that the latter is a hydrogen approximation and describes well the photorecombination cross sections for transitions to highly excited states. Here a photoionization cross section is characterized by an inverse cubic dependence on the energy of the quantum. There are a number of examples where such a dependence fits very badly (qualitatively and quantitatively) the behavior of the photoionization cross section of the atom. For instance, the presence of a broad maximum, in the absorption cross section far from the threshold is characteristic of atoms of nitrogen, oxygen, and inert gases. In this case, use of the Kramers formula can lead to serious errors. We use this formula only for highly excited states. For the ground and first excited states photorecombination rates are found by integration of the numerical values of the corresponding cross sections obtained by the Milne formula from photoabsorption cross sections. The latter are calculated in the HFS approximation.

An important radiative process is dielectronic recombination. As a result of inelastic scattering, an incident electron is captured by a bound orbit, thus causing excitation of an atomic electron. Further radiative transition of

the atomic electron to the initial state implies a recombination event. It should be noted that dielectronic recombination is a complicated process with numerous facets. In particular, completing channels of spontaneous transition of the excited atomic electron, completing self-ionization channels, and some other processes can be of importance. We restricted ourselves to accounting for dielectronic recombination in the approximation of the Burgess integral formula [4], which has proved to be good in a number of calculations. Only for some cases was allowance made for additional channels of transition of the atomic electron and self-ionization. Thus, for instance, for the oxygen atom in dielectron recombination the atomic electron can experience the excitations $2s^22p^4-2s^2p^5$, $2s^22p^4-2s^22p^33s$, $2s^22p^4-2s^22p^33d$. In the latter case, in the stabilization $3d-2p$ of the atomic electron the powerful competing channel $3d-3p$ occurs.

Everywhere above, electron collision transitions have been implied. Ionic and atomic transitions can be neglected since their rate is two orders of magnitude lower than that of the corresponding electronic transitions. A special situation develops for temperatures of < 1 eV. In this case, the degree of ionization in the plasma can amount to $10^{-2}-10^{-5}$. The role of electrons can be relegated to the background because of their low concentration, and the principal processes here will be ones with the participation of neutral atoms. Having no possibility of rigorous quantum-mechanical consideration of inelastic scattering of atoms by ions, we restricted ourselves only to rough estimation of it by introducing the factor $\sqrt{m_e/M}$ determined by the ratio of electron and ion masses into the corresponding electron formulas. These effects were taken into account for the rates of collision excitation, de-excitation, ionization, and triple recombination.

A special problem is calculation of the ionization composition and level populations of a plasma. The number of equations in the kinetic matrix corresponds to the number of considered energy levels of all the ions in the plasma. But this entails the following conflict. In calculating absorption and emission spectra, the larger the number of levels taken into consideration, the better, while in solving the system of equations the situation is completely opposite. For a plasma of complicated chemical composition with a high degree of ionization the number of the levels considered can attain several thousand, and one can encounter difficulties in solving systems of algebraic equations of such high dimensionality. In the present work an approximation that makes it possible to circumvent these difficulties is used. It can be assumed that all the ionization and recombination processes proceed through the ground states of ions and atoms, and this will not be a substantial limitation on the model. Populations of ground states substantially exceed those of excited states. Only for some ions are metastable levels slightly competitive. In the approximation adopted the matrix of collisional and radiative transitions will be of block-diagonal form. In this case, the system of algebraic equations for each ion can be solved separately, followed by overall normalization to the number of particles. The system of equations includes the electron concentration, which is also to be determined. The problem is solved by the iteration technique starting from some trial value of the electron concentration. The calculated ionization composition and level populations are used to calculate the thermodynamic functions pressure, internal energy, entropy, etc.

In calculation of absorption and emission coefficients account is taken of photo- and bremsstrahlung processes and transitions in lines. Bremsstrahlung absorption on ions is described quite well by the Kramers formula with the Gaunt correction. At low temperatures one must take into consideration bremsstrahlung absorption on neutral atoms. Methods exist that allow the bremsstrahlung absorption coefficient to be expressed in terms of the elastic-scattering cross section on an atom [6]. The procedure described in [6] is used here. Preliminarily, the elastic-scattering cross sections on an atom are calculated with account for polarization effects. Use is made of a polarization potential of the form $V_p = \beta / (r^2 + r_0^2)^2$. The polarizability β is calculated in terms of oscillator strengths found in the HFS approximation. The photoabsorption coefficient is determined using photoionization cross sections calculated in the HFS approximation. Account is taken of photoabsorption from the inner levels, the ground state, and excited levels up to $n = 10$. To construct a spectrum of continuous absorption a regular logarithmic scale is used. In this case, an energy interval with a magnitude of one order is represented by an equal number of frequency points. This representation is convenient for mapping a spectrum in detail in all its frequency intervals. The emission coefficient under LTE conditions is determined by the Kirchhoff law $\epsilon = \kappa U_p$. The emissivity is proportional to the absorption coefficient multiplied by the Planck function. In the absence of LTE the emissivity is always smaller than the value determined by the Kirchhoff law. It is convenient to introduce a new quantity κ' determined by the

equality $\varepsilon = \kappa' U_p$. It is obvious that we always have $\kappa' \leq \kappa$. Representation of κ and κ' on graphs is very elucidating since it allows one to judge the degree of deviation from LTE in different parts of the spectrum. For instance, in the longwave part of the spectrum, determined by bremsstrahlung absorption and photoabsorption from excited levels, LTE conditions are practically always fulfilled. On the other hand, the correlation between the photoabsorption from the inner shells and the corresponding photorecombination almost never corresponds to the Kirchhoff law. Note that for the inner shells in addition to the balance of the collision and radiation rates it is necessary to take into account the self-ionization processes, which can substantially change the correlation between the quantities κ and κ' , especially for light elements.

Absorption in spectral lines is an important component in the overall energy balance. Under LTE conditions the share of radiation in spectral lines can equal $\sim 50\%$. For a corona plasma this value is commonly much higher. On the other hand, account for radiation in lines encounters a number of difficulties. The continuous-absorption coefficient is a rather monotonic function. It can be averaged in some frequency interval and one can restrict oneself to solving a small number of spectral transfer equations. The situation is different in spectral lines. The contour of a spectral line is a strongly nonmonotonic function. Moreover, different parts of it can have substantially different optical thicknesses, which substantially complicates solution of the radiative transfer equations. A rigorous solution of transfer equations in lines requires a rather detailed frequency resolution of them. However, in a plasma of complicated composition the number of such lines can attain several thousand. In this case, detailed resolution of the contour of each individual line is difficult, and one or several lines are often averaged to get some spectral group. Such averaging is not, generally speaking, rigorous, but nevertheless it is frequently used. It is more correct to employ another approach. Spectral lines in which a major part of the energy is transferred (commonly these are resonance lines) must be resolved quite thoroughly with respect to the contour, while the others can be averaged to form groups. The procedure of evaluating the importance of one line or another is rather subjective, and it depends mainly on the particular formulation of the gasodynamic problem. Perhaps, no universal approach exists, and optical characteristics should be calculated individually for each particular problem.

Within the framework of the approach developed by the present authors there are several versions. Absorption in spectral lines can be accounted for using a regular logarithmic scale. Here, instead of the frequency coefficient of absorption on individual points of the contour it is convenient to use the integral over it in some frequency interval. This approach allows evaluation of radiation transfer in weak lines with good accuracy. In resonance lines, it is necessary to calculate the contour of each of the lines more thoroughly since this can exert a pronounced influence on the radiation balance in the system. In the present work, provision is made for detailed calculation of the contours of a number of lines and creation of a special frequency scale that allows a regular scale for continuous absorption to be used in combination with individual scales for the strongest lines. This approach made it possible to improve substantially the accuracy of solution of transfer equations (including two-dimensional equations) with optimum expenditure of computer time.

A separate problem is calculation of the widths of spectral lines and construction of the spectral contour. Here, it is necessary to take into consideration all the basic mechanisms of broadening. Among the latter are the Doppler, radiative, and Stark types of broadening. At low temperatures resonance broadening is also of importance, as is Holtsmark broadening for hydrogen-like ions. All the enumerated mechanisms of broadening of spectral lines were considered within the framework of the approximations described in [7, 8]. The necessary quantum-mechanical characteristics (energy levels, oscillator strengths, etc.) were found from HFS calculations. Usually it is rare that in a plasma a single kind of profile occurs, and therefore it is necessary to perform convolution of several kinds. Most commonly this is the Voigt profile, i.e., convolution of Doppler and Lorentz ones. In this case, it is no longer described by an analytical function. In the present work calculation of tables of Voigt profiles was performed for a wide range of Doppler and Lorentz widths, which allows absorption in lines to be calculated for any temperatures and densities in a plasma. As mentioned above, under certain conditions Holtsmark broadening must be taken into account. In this case, it is already necessary to perform convolution of three types of profiles, which is a nontrivial calculation procedure. In actual practice, however, it is always possible to take into account only the two of them with the largest widths. This reduces to three situations: Voigt, Lorentz–Holtsmark, and

Doppler–Holtsmark profiles. For all the types mentioned we calculated tables that allow calculation of profiles with satisfactory accuracy for all actual situations in a plasma.

It was mentioned that in calculation of the ionization composition and level populations processes of radiative excitation and ionization have been neglected since this substantially complicates the problem. Under certain conditions it is necessary to take these processes into account. Thus, for instance, if the plasma has large spatial dimensions, then even at high temperatures the equilibrium shifts from the corona to LTE due to reabsorption of radiation. This effect can be evaluated in the approximation of the escape factor [5] if the plasma is assumed to be quasithermal in some volume. In this case, the effective factor of radiation reabsorption can be calculated, which amounts to a reduction in the role of spontaneous transitions in the kinetic matrix. The value of the escape factor depends substantially on the line contour, the optical thickness at the line center, and the geometry of the plasma region (spherical, cylindrical, or plane). In the limit of large optical thicknesses for simple contours analytical expressions for the escape factor exist. In the present work, calculations of tabular escape factors were performed for a wide range of optical thicknesses (from 0.001 to 1000) for all types of simple contours and Lorentz–Doppler (Voigt), Lorentz–Holtsmark, and Doppler–Holtsmark convolutions, which makes it possible to allow for the escape factor in calculations for an arbitrary type of contours and arbitrary optical thicknesses. A number of calculations carried out shows that account for the escape factor can substantially change the portion of radiation emitted from a plasma.

As mentioned above, the HFS method was used to calculate energy levels, oscillator strengths, and other quantities. It allows calculation of energy levels for closed shells with good accuracy. In cases where the electrostatic splitting is large, the level energy in the approximation of L – S coupling can differ substantially from the energy of the average term in the HFS approximation. For instance, an oxygen atom in the ground state has three terms: 3P , 1D , 1S . Each of them has several fractional parentage states. Thus, the experimental structure of the levels and lines will differ substantially from that calculated in the HFS approximation. Use of calculated data can distort the mode of radiation transfer in the lines and hamper spectral diagnostics. To an even greater degree this problem is typical of heavy and moderate elements. Thus, for instance, the ground state of iron $3d^64s^2$ has 16 terms, some of which even enter the self-ionization spectrum. Furthermore, the spin-orbit splitting already becomes comparable to the electrostatic splitting and must not be neglected. Consequently, for such elements the HFS method is not a good approximation. For such situations provision is made for the use of special corrective data banks. The latter contain, first of all, experimental values of energy levels and a complete accompanying list of all quantum numbers characterizing a given level. This information is taken from a number of published tables of experimental spectroscopic data [9–11]. In calculating level populations and continuous and line absorption coefficients, the calculated value of an energy level is automatically replaced by its experimental value. In the absence of the latter, the calculated value is retained. However, the experimental sources have one serious drawback. For different elements and different ions the degree of completeness of the information differs greatly. For instance, for neutral atoms (especially light ones) and low-charge ions this information is provided in adequate detail. For multiply charged ions it is less detailed and sometimes not at all adequate. In these cases, use was made of calculated data of high quality (a multiconfiguration Hartree–Fock (HF) approximation), and in their absence additional calculations in the HF approximation were made. For multiply charged ions the calculated characteristics served as the basis for corrective data banks. Such banks were created for a number of the most important elements, namely, Be, B, C, N, O, Ne, Al, Si, S, Cl, Ar, Ca, Ti, Fe. The list of these elements was determined by the range of problems in which they were used. Below, some of these problems will be enumerated. Experimental values of oscillator strengths are represented much more meagerly, and therefore for their determination self-consistent calculations (HFS or HF) are most commonly used, which yield good integral quantities. They are necessary for calculation of the oscillator strengths of individual experimental components of lines. For this, use is made of fractional parentage coefficients, $3nj$ -symbols, and other angular characteristics calculated within the framework of the Racah technique [12].

The list of calculations made using the procedure described above is rather extensive. First of all, there are calculations of the optical properties of the earth's atmosphere containing nitrogen, oxygen, and 1% argon. It should be noted that with increasing height, the percentage of these components changes somewhat, which must

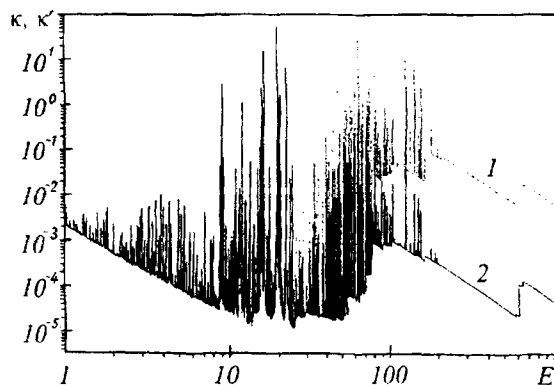


Fig. 1. Absorption and emission spectra of quartz plasma ($T = 10$ eV, $N = 10^{17}$ cm $^{-3}$): 1) absorption; 2) emission. $\kappa, \kappa',$ cm $^{-1}$; $E,$ eV.

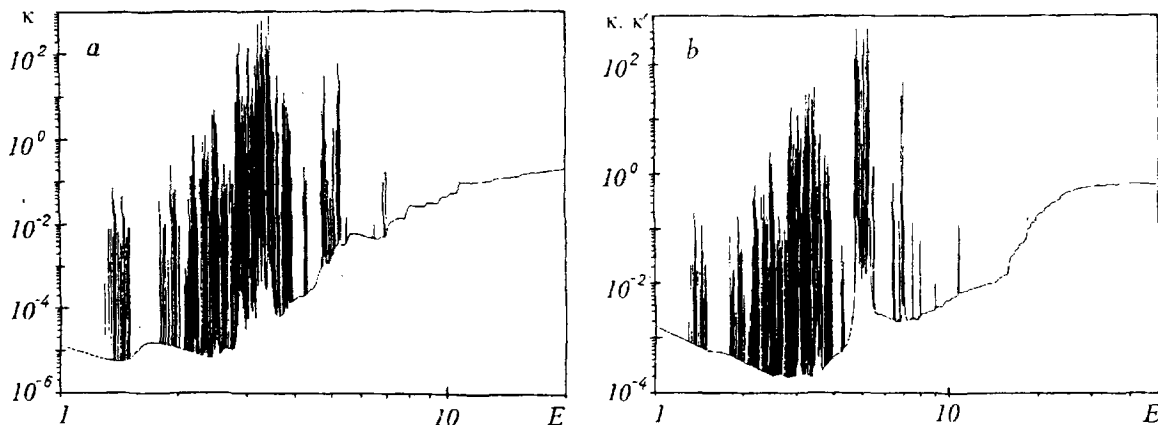


Fig. 2. Absorption spectrum of iron plasma. $T = 0.5$ eV (a) and 1 eV (b), $N = 10^{18}$ cm $^{-3}$.

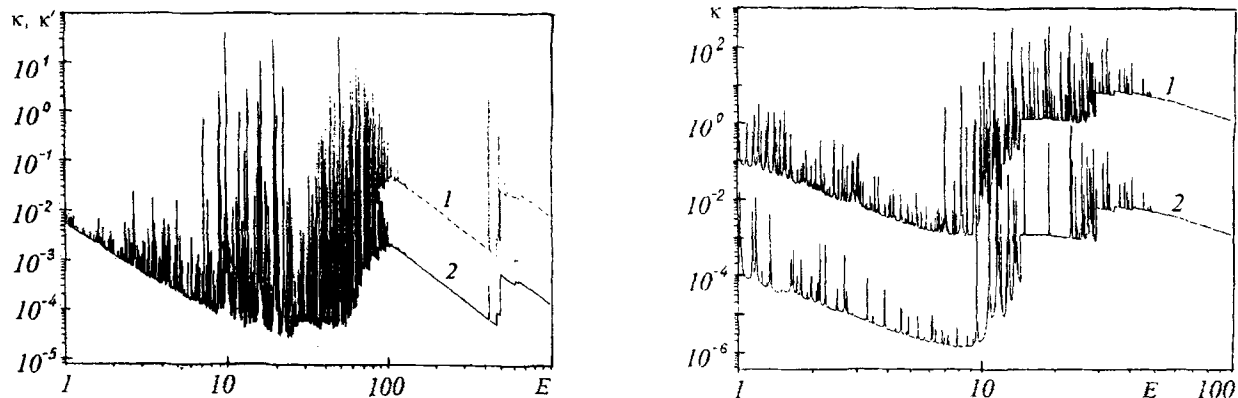


Fig. 3. Absorption and emission spectra of air plasma ($T = 10$ eV, $N = 10^{17}$ cm $^{-3}$): 1) absorption; 2) emission.

Fig. 4. Absorption spectrum of air plasma calculated in different approximations ($T = 2$ eV, $N = 10^{18}$ cm $^{-3}$): 1) HFS with correction of the spectrum; 2) without correction (κ is reduced 1000-fold).

be taken into consideration. The second important problem, where results of the present work were used, is calculation of the optical properties of the substance of a meteorite or another cosmic body entering the earth's atmosphere. Here, various possible compositions were studied: SiO $_2$, H $_2$ O, Fe, FeO. In investigating the processes of collision of a cosmic body with the earth's surface, it can be important to account for changes in the composition of the soil or the salts in seawater. Some calculations that are of interest as test calculations were also made. For this, calculations of such elements as beryllium, graphite, and aluminum were carried out.

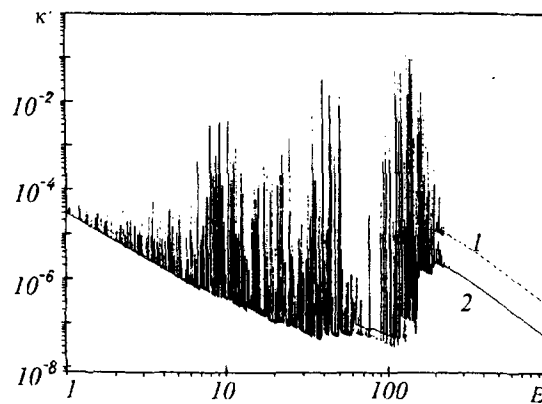


Fig. 5. Absorption spectrum of aluminum plasma in the approximations of a radiative-collisional model and the escape factor ($T = 20$ eV, $N = 10^{16}$ cm^{-3}): 1) with allowance for the escape factor ($l = 5$ cm); 2) without allowance for it.

For the purpose of illustration we provide graphs of absorption and emission coefficients (in representation of the quantity κ') for some chemical elements or mixtures. As already mentioned, the absorption spectrum often has a very complicated structure. This can be exemplified by the absorption spectrum of quartz at high temperatures (Fig. 1). In this case, the spectrum represents overlap of a large number of spectral lines of silicon and oxygen. The same figure gives the quantity κ' . As is seen, in the hard part of the spectrum the emission coefficient is seen to deviate substantially from the Kirchhoff law. Iron plasma has an even more complicated spectrum. Account for electrostatic and spin-orbit splitting of the energy levels for iron ions leads to the fact that the spectrum even becomes qualitatively dissimilar to the spectra of light elements (Fig. 2). In particular, one does not observe the abrupt photoabsorption thresholds with a typical cubic dependence on the quantum energy that are usually inherent to light elements. Figures 3, 4 show absorption spectra of air plasma. One calculation was made with the use of just HFS data, and in the other, experimental data banks were used. Whereas for the continuous spectrum good correlation is observed, the line spectrum differs substantially in the number of spectral lines and their intensity. Figure 5 presents emission coefficients (the quantity κ') for aluminum plasma. In these calculations, a spherical plasma volume with a diameter of 5 cm was arbitrarily taken. As is seen, account for self-absorption in the resonance lines leads not only to a change in the amplitude of these lines but also to a change in the ionization composition of the plasma and, correspondingly, to a change in the photoabsorption.

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NOTATION

n , principal quantum number; L , S , quantum numbers indicating the total orbital and total spin momenta of the electron shell; m_e , electron mass; M , atomic mass; V_p , polarization potential; β , polarizability; r , distance between the electron and the nucleus in the atom; r_0 , mean radius of the atom; ϵ , emissivity; κ , absorption coefficient; U_p , Planck function; κ' , emission coefficient; E , energy of the quanta; T , temperature; N , particle concentration; l , size of the plasma volume. Subscripts: e, electron; p, polarization; P, Planck.

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