P1:40 Collisional - radiative model DESNA for atomic spectra calculations of non-LTE plasmas in a wide range of plasma parameters

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Calculated absorption and emission spectra of plasma are required for many applications connected with emitting multicharged ion plasma for interpretation of experimental data, plasma diagnostics and spectroscopy, and some other tasks. Earlier we presented a collisional-radiative model for the calculation of ionization composition and excited level populations [1]. The main purpose of this report is to present a new, more general and extended, simple and exact enough model DESNA. The DESNA model is intended to calculate such optical characteristics of nonequilibrium plasma as emission and absorption spectra, mean opacities, and radiation energy losses.

I.   Main equations

For modeling of the atomic spectra except for properties of a substance (cross sections and probabilities of various processes) it is necessary to know the charge–state distribution and the excited levels populations of all ions. In general, a change with time of a population of each level can be described by the differential equations, which take into account the populating and depopulating processes for the given energy level n of ion Z. We assume that the plasma is ionized strongly enough, so it is possible to account only for collisions with electrons, without consideration of the collisions of heavy particles (atoms and ions). Besides, we consider the distribution of electrons throughout the velocities to be the Maxwell distribution. We consider a homogeneous optical transparent plasma with the given temperature and density. Plasma can be both pure or consisting of the mixtures of ions of several chemical elements. The system of the kinetic equations describing the ionization state densities and level populations of ions in plasma, has the form:

$$\frac{dN_Z^n}{dt} = \sum_{E_m>E_n} A_{mn} \cdot N_Z^m - \sum_{E_m<E_n} A_{nm} \cdot N_Z^n + \sum_m C_{mn} N_Z^m N_e - \sum_m C_{nm} N_Z^n N_e + \sum_m W_{mn} N_Z^m +$$

$$+ \sum_{k=1}^{L_{Z-1}} N_{Z-1}^k \cdot (C_{Z-1\to Z}^{ion.}(k,n) \cdot N_e + I_{Z-1\to Z}^{ph.}(k,n)) - \sum N_Z^n (I_{Z\to Z+1}^{ph.}(n,k) +$$

$$+ N_e \cdot (C_{Z\to Z+1}^{ion.}(n,k) + C_{Z\to Z-1}^{th.b.}(n,k)N_e + R_{Z\to Z-1}(n,k) + D_{Z\to Z-1}(n,k))) +$$

$$+ \sum_{k=1}^{L_{Z+1}} N_{Z+1}^k \cdot N_e \cdot (C_{Z+1\to Z}^{th.b.}(k,n) \cdot N_e + R_{Z+1\to Z}(k,n) + D_{Z+1\to Z}(k,n))$$

(1)

$$\sum_{Z=1}^{Z_{nuc.}+1} \sum_n N_Z^n = N_i \text{ - condition for preservation of the number of ions,}$$

(2)

$$\sum_{Z=1}^{Z_{nuc.}+1} \sum_n (Z-1)N_Z^n = N_e \text{ - condition for the plasma quasi-neutrality,}$$

(3)

Here $Z = \overline{1, Z_{nuc}}$ (Z=1 for the neutral atom), $Z_{nuc.}$ is the nuclear charge;

$n, m = \overline{1, L_Z}$. L_Z is the number of excited levels for ion in charge state Z. The value L_Z is defined by lowering of the ionization potential;

N_Z^n, the population of level n with energy E_n for ion Z;

N_i, the ion concentration;

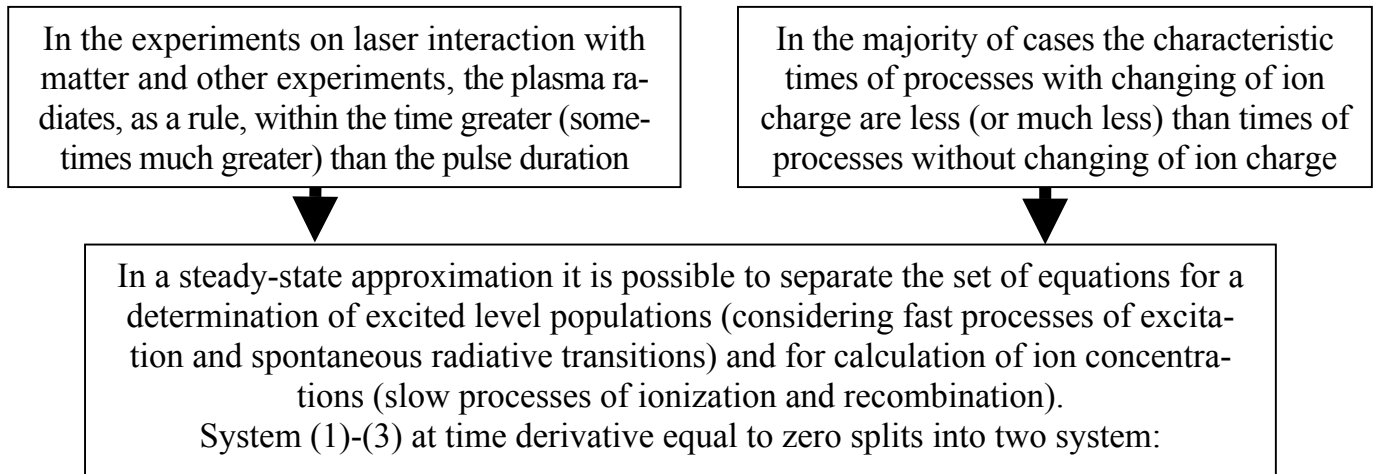A_{mn}, the probability of spontaneous radiative transition from upper level m to lower level n;

C_{nm}, the rate of collisional excitation (or deexcitation) from level m to level n of ion Z;

W_{nm}, the rate of photopumping by external source of radiation;

$C_{Z \to Z+1}^{ion.}(n,k)$, the rate of ionization by electron impact of ion in charge state Z with an excited electron on the level n (after ionization there is formed ion $Z+1$ with an electron on the level k);

$I_{Z \to Z+1}^{ph.}(n,k)$, $C_{Z \to Z-1}^{th.b.}(n,k)$, $R_{Z \to Z-1}(n,k)$, and $D_{Z \to Z-1}(n,k)$ - photoionization, three-body collisional recombination, radiative recombination and dielectronic recombination rate coefficients, respectively.

For the case of mixture of multicharged ions the equations like Eq.(1) must be written for population of excited levels of all chemical elements, and it is necessary to sum up the equations (2) and (3) over all compounds of the mixture.

In the experiments on laser interaction with matter and other experiments, the plasma radiates, as a rule, within the time greater (sometimes much greater) than the pulse duration	In the majority of cases the characteristic times of processes with changing of ion charge are less (or much less) than times of processes without changing of ion charge

In a steady-state approximation it is possible to separate the set of equations for a determination of excited level populations (considering fast processes of excitation and spontaneous radiative transitions) and for calculation of ion concentrations (slow processes of ionization and recombination).
System (1)-(3) at time derivative equal to zero splits into two system:

System for determination of **excited levels populations**:

$$\begin{cases} \sum_{E_m>E_n} A_{mn}N_Z^m - \sum_{E_m<E_n} A_{nm}N_Z^n + \sum_{m \neq n} C_{mn}N_Z^m N_e - \sum_{m \neq n} C_{nm}N_Z^n N_e + \sum_{m<n} W_{mn}N_Z^m = 0 \\ \sum_{n=1}^{L_Z} N_Z^n = N_Z \end{cases} \quad , \quad (4) \qquad \boxed{N_Z^n}$$

iterations

System for determination of plasma **ionization composition**:

$$\begin{cases} N_{Z-1}(N_e C_{Z-1 \to Z}^{ion} + I_{Z-1 \to Z}^{ph}) - N_Z(I_{Z \to Z+1}^{ph} + N_e(C_{Z \to Z+1}^{ion} + C_{Z \to Z-1}^{th.b.} N_e + R_{Z \to Z-1} + D_{Z \to Z-1})) + \\ + N_{Z+1}N_e(C_{Z+1 \to Z}^{th.b.} N_e + R_{Z+1 \to Z} + D_{Z+1 \to Z}) = 0 \\ \sum_{Z=1}^{Z_{nuc}+1} N_Z = N_i \ , \ \sum_{Z=1}^{Z_{nuc}+1} (Z-1)N_Z = N_e \ , \\ \eta_{Z \to ...} = \sum_m \sum_n^{L_Z} \eta_{Z \to ...}(n,m) \cdot N_Z^n / N_Z \ (\eta_{Z \to ...} - any \ of \ rates \ C^{ion.}, I^{ph.}, C^{th.b.}, D \ or \ R) \end{cases} \quad , \quad (5)$$

$\boxed{N_Z}$

II. Expressions for rate of elementary processes

The rates of elementary processes were calculated by means of widely used simple approximation formulae, which give reasonable results in a wide range of plasma temperatures and densities.

The probability of **spontaneous radiative transition** is given by expression [2]:

$$A_{nm} = 4{,}3 \times 10^{13} \frac{g_m}{g_n} \left(E_n - E_m \right)^2 f_{mn}, \tag{6}$$

where f_{mn}, the absorption oscillator strength; g_m and g_n, the statistic weights of lower and upper levels; E_n and E_m, the level energies (in keV).

The rate of **collisional excitation** was calculated on Van Regemorter formula [3]:

$$C_{mn} = 32 \cdot 10^{-8} f_{mn} \left(\frac{I_H}{\Delta E_{nm}} \right)^{3/2} \beta^{1/2} e^{-\beta} \cdot p(\beta), \quad \beta = \Delta E_{nm}/T_e, \tag{7}$$

where I_H=13.6 eV -; $\Delta E_{nm}=E_n-E_m$. Function $p(\beta)$ is the tabulated Gaunt factor [2].

The rate of **collisional deexcitation** can be calculated using detailed balance relation:

$$C_{nm} = C_{mn} \left(g_m/g_n \right) e^{\Delta E_{nm}/T_e} \tag{8}$$

For the rate of **ionization by collision with electron** we have used expression [4]:

$$C_{Z \to Z+1}^{ion} = C T_e^{-3/2} \frac{e^{-u}}{u^\xi} F(u), \quad F(u)= 0.915(1+0.064/u)^{-2}+0.42(1+0.5/u)^{-2} \tag{9}$$

where $u=I_{Z,n}/T_e$; C=3.920·10^{-11} cm^{3}s^{-1}keV$^{1.5}$ and ξ=2.

The **three body recombination** rate coefficient correlates with the rate of collisional ionization via detailed balance relation [5]:

$$U_Z C_{Z \to Z+1}^{ion.} = 2 \left(\frac{m_e T_e}{2\pi \eta^2} \right)^{3/2} U_{Z+1} C_{Z+1 \to Z}^{th.b.} e^{-I_Z/T_e}, \tag{10}$$

where $U_Z = \sum_{n=1}^{L_Z} g_{Z,n} \exp\left(-E_{Z,n}/T_e\right)$, the partition sum for ion Z; I_Z, the ionization potential.

The **photorecombination** rate coefficient is given by the hydrogenic Griem formula [6]:

$$R_{Z+1 \to Z} = 5.20 \cdot 10^{-14} Z \left(\frac{I_Z}{T_e} \right)^{3/2} \sum_{n=1}^{L_Z} \frac{\mu_{Z,n}}{P_{Z,n}^3} \cdot e^{I_{Z,n}/T_e} \cdot E_1 \left(\frac{I_{Z,n}}{T_e} \right), \tag{11}$$

where $P_{Z,n}$, the principal quantum number of level n and ion Z (in calculations we used effective principal quantum number $P_{Z,n}^* = \sqrt{Z^2 I_H / I_{Z,n}}$); $E_1(x) = \int_x^\infty (e^{-t}/t) dt, \ x \neq 0$, the integral exponential function of the second order; parameter $\mu_{Z,n}$ is defined as a relation of the number of vacancies to a full number of electrons in the atomic shell n:

$$\mu_{Z,n} = \begin{cases} 1 - \left(\Delta_0 / 2P_{Z,n}^2 \right), & \text{for the ground state} \\ 1, & \text{for the excited states} \end{cases}.$$

The **dielectronic recombination** rate coefficient $D_{Z+1 \to Z}$ for the processes of the type $A_{Z+1}(\alpha_0) + e \to A_Z(\alpha_1 nl) \to A_Z(\alpha_0 nl) + h\nu$ we calculate by using approximation formula [2]:

$$D_{Z+1 \to Z} = 10^{-13} \beta_d^{3/2} \cdot e^{-\beta_d \chi_d} \cdot A_d \frac{Q_d}{2l_0+1}, \quad \beta_d = \frac{(Z+1)^2 I_H}{T_e}, \tag{12}$$

here l_0, the angle moment of optical electron in the initial state; A_d, χ_d, the approximation parameters; and Q_d, factor depending on transition.

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III. Ionization potential lowering

At high electron and ion densities local electric fields in plasmas can effectively reduce an ionization potential I_Z. For ions of low ionization degree the value of ionization potential depression can be grater than ionization energy of state n (I_Z-E_{Zn}). Hence at some conditions this phenomenon can cause spontaneous ionization of low charged ions (pressure ionization). Ionization potential lowering for the given plasma conditions defines the number of the bound states L_Z.

For accounting of ionization potential lowering effects in model DESNA we used expression from work [7]:

$$\Delta E_Z = \frac{3}{2}\frac{Ze^2}{r_0}\left(\left[1+\left(\frac{R_D}{r_0}\right)^3\right]^{2/3} - \left(\frac{R_D}{r_0}\right)^2\right); \quad R_D = \left[\frac{kT_e}{4\pi e^2\left(N_e + N_i\overline{Z^2}\right)}\right]^{1/2}, \quad r_0 = \left(\frac{3}{4\pi}\frac{1}{N_i}\right)^{1/3} \quad (13)$$

where R_D is the Debye length and r_0, the minimal distance between ions corresponding to dense packing. So, the number L_Z in (1) is the quantity of states for which $\Delta E_Z < I_Z - E_{Zn}$.

IV. Sources of atomic data

The rates of elementary processes must be calculated before solution of the systems equations (4) and (5). An great amount of atomic data on the energies of excited levels, transition probabilities, and oscillator strengths for multicharged ions of different chemical elements are needed for the calculations. The calculations of such data is a very difficult task. So for creation of new databases on necessary atomic data for different elements, their adaptation for specific format and tasks of DESNA model and for further using of these databases we used a compilation of the available data from different sources (full list of similar databases with hyperlinks can be found in [15]):

TOPBASE [8]-[10]. Energies $E_{Z,n}$; the data on f_{mn} and A_{nm} were taken for optically allowed transitions with ΔS=0, |Δℓ|=1

NIST Atomic Spectra Database [11]. Energies $E_{Z,n}$; the data on f_{mn} and A_{nm} were taken for optically allowed, intercombination and forbidden transitions with |ΔS|=0, 1; |Δℓ|=0, 1, 2

MCHF/MCDHF Atomic Data Collection [12]. The data on f_{mn} and A_{nm} were taken for allowed, intercombination and forbidden transitions with |ΔS|=0, 1, 2; |Δℓ|=0, 1, 2; for two-electron transitions

CHIANTI: A Database for Astrophysical Emission Line Spectroscopy, NRL [13]. Some data were taken for *Ar* and *Ti*

BIBL: spectral bibliography database, Institute of Spectroscopy, RAS [14]
Search of scientific papers with data on f_{mn} and A_{nm}.

Quantitative characteristics of ion levels scheme in model DESNA (at July 2003)

Element, Nuclear charge		Number of levels/ transitions	
H	1	45	254
Be	4	226	1571
C	6	631	6950
N	7	935	11516
O	8	1391	18043
F	9	1411	21108
Mg	12	2453	46901
Al	13	2524	48519
Si	14	2680	54520
Ar	18	5189	127336
Ti	22	1064	8417
Cu	29	166	389

V. Model for calculation of atomic spectra

In the field of high enough temperatures, the main contribution to the emission comes from bremsstrahlung, recombination, and line radiation losses. The formulae for calculation of spectral absorption coefficient (in cm^{-1}) and spectral emissivity (the density of radiative power in a single spectral range emitted in a single angle - dimensionality W/(cm^3/eV/steradian) look as follows:

$$k_\varepsilon = \sum_{a,Z}\sum_m\sum_{n>m} \sigma_{mn}^{bb}(\varepsilon)N_{a,Z}^m\left[1 - \frac{N_{a,z}^n}{N_{a,Z}^m}\frac{g_m}{g_n}\right] + \sum_{a,Z}\sum_{n'}\sigma_{Z,n}^{bf}(\varepsilon,T_e)N_{a,Z}^n + \sum_{a,Z}\sigma_Z^{*ff}(\varepsilon,T_e)\cdot N_e$$

$$j_\varepsilon = 5\cdot10^{12}\cdot\varepsilon^3\left\{\sum_{a,Z}\sum_m\sum_{n>m}\sigma_{mn}^{bb}(\varepsilon)N_{a,Z}^n\frac{g_m}{g_n} + \sum_{a,Z}\sum_{n'}\sigma_{Z+1,n}^{fb}(\varepsilon,T_e)N_{a,Z+1} + \sum_{a,Z}\sigma_Z^{ff}(\varepsilon,T_e)\cdot N_e\right\}$$

$$(14)$$

where $\varepsilon=h\nu$ is the photon energy; $\sigma_{mn}^{bb}(\varepsilon)$, the cross section of absorption in line at transition from level m to level n; $\sigma_{Z+1,n}^{fb}(\varepsilon,T_e)$, the effective photorecombination cross section of ion $Z+1$ to level n of ion Z; $\sigma_{Z,n}^{bf}(\varepsilon,T_e)$, the effective photoabsorption cross section from level n; value $\sigma_Z^{*ff}(\varepsilon,T_e)$ characterizes effective bremsstrahlung cross section; and $\sigma_Z^{ff}(\varepsilon,T_e)$, the effective inverse bremsstrahlung cross section. Only levels with $I_{Z,n}<\varepsilon$ are included in summation over n for free-bound and bound-free transitions.

The quasi-classical Kramers expressions [16] were used for calculations of **bremsstrahlung and recombination processes** cross sections (with correction on stimulated emission):

$$\sigma_Z^{ff}(\varepsilon,T_e)=\sigma_Z^{Kr}(\varepsilon,T_e)\cdot\left(1-e^{-\varepsilon/T_e}\right); \quad \sigma_Z^{*ff}(\varepsilon,T_e)=\sigma_Z^{Kr}(\varepsilon,T_e)\cdot e^{-\varepsilon/T_e}$$

$$\sigma_Z^{Kr}(\varepsilon,T_e)=\frac{4}{3}\sqrt{\frac{2\pi}{3m_ekT_e}}\frac{e^6h^2}{m_ec}\frac{Z^2}{\varepsilon^3}N_i$$

$$(15)$$

$$\sigma_{Z,n}^{bf}(\varepsilon,T_e)=\frac{64\pi}{3\sqrt3}\left(\frac{\varepsilon_\Gamma}{\varepsilon}\right)^3\frac{\alpha\cdot a_0^2}{Z^2\cdot\left(P_{Z,n}^*\right)^5}\cdot\left(1-e^{-\varepsilon/T_e}\right); \quad \sigma_{Z+1,n}^{fb}(\varepsilon,T_e)=\frac{32\pi}{3\sqrt3}\alpha^3\frac{\varepsilon_\Gamma^2}{\varepsilon\left(\varepsilon-\varepsilon_\Gamma/n^2\right)}\frac{a_0^2}{n^3}\cdot e^{-\varepsilon/T_e}, (16)$$

where a_0 is the Bohr radius; $\alpha=1/137$; $\varepsilon_\Gamma = Z^2I_H$.

Cross section of **bound-bound** absorption is given by formula [16]:

$$\sigma_{mn}^{bb}(\varepsilon)=\frac{\pi e^2}{m_ec}f_{mn}\Psi(\varepsilon),$$

$$(17)$$

where $\Psi(\varepsilon)$ is the line profile normalized to unity. A simple model for calculations of the line profiles with accounting for Doppler Γ_D, collisional Γ_C, and natural Γ_R widths looks as follow (values of Γ in keV):

$$\Psi(\varepsilon)=\frac{1}{\pi}\frac{\Gamma/2}{(\Gamma/2)^2+(\varepsilon-\Delta E_{mn})^2} \; ; \quad \Gamma=\sqrt{(\Gamma_R+\Gamma_C)^2+\Gamma_D^2}$$

$$\Gamma_R = \frac{4\pi}{3}\frac{e^2}{m_ehc^3}\cdot(\Delta E_{nm})^2 \; ; \; \Gamma_D = 2\sqrt{ln2}\cdot\frac{\Delta E_{nm}}{c}\sqrt{\frac{2kT_e}{M}} \; ; \; \Gamma_C = 6\cdot10^{-10}\cdot N_i^{1/3}\cdot\sqrt{\frac{kT_e}{M}}\cdot$$

$$(18)$$

where M is the atomic weight of element. For comparison with experiment an instrumental broadening can be included in this model.

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VI. Summary
Collisional-radiative model DESNA[*] - present state

What is   D   E   S   N   A ?

DEtailed configuration accounting

Emissivities, **E**quations of level kinetics

Steady-state approximation, **S**pectra

Nonequilibrium, **N**umerical code

Atomic data

Absorption coefficients

*Also, Desna is the river near Moscow

Plasma:	**Multicharged ions:**	**Considered processes:**
☑ Homogeneous	☑ All ionization states from neutral atom to fully ionized ion	☑ Spontaneous radiative transitions;
☑ Isotropic		☑ Collisional excitation and deexcitation;
☑ Stationary		☑ Ionization by electron impact;
☑ Optically transparent	☑ Detailed structure of ion levels with splitting on LS terms	☑ Three body recombination;
☑ Mixture of multicharged ions of several elements		☑ Radiative recombination;
		☑ Dielectronic recombination.

☞ Non-LTE (or collisional-radiative equilibrium CRE), both collisional and radiative processes are included

☞ Ionization potential lowering is included

} DESNA model is suitable for calculation of atomic spectra and other properties of multicomponent plasma in a **wide range** of plasma conditions:
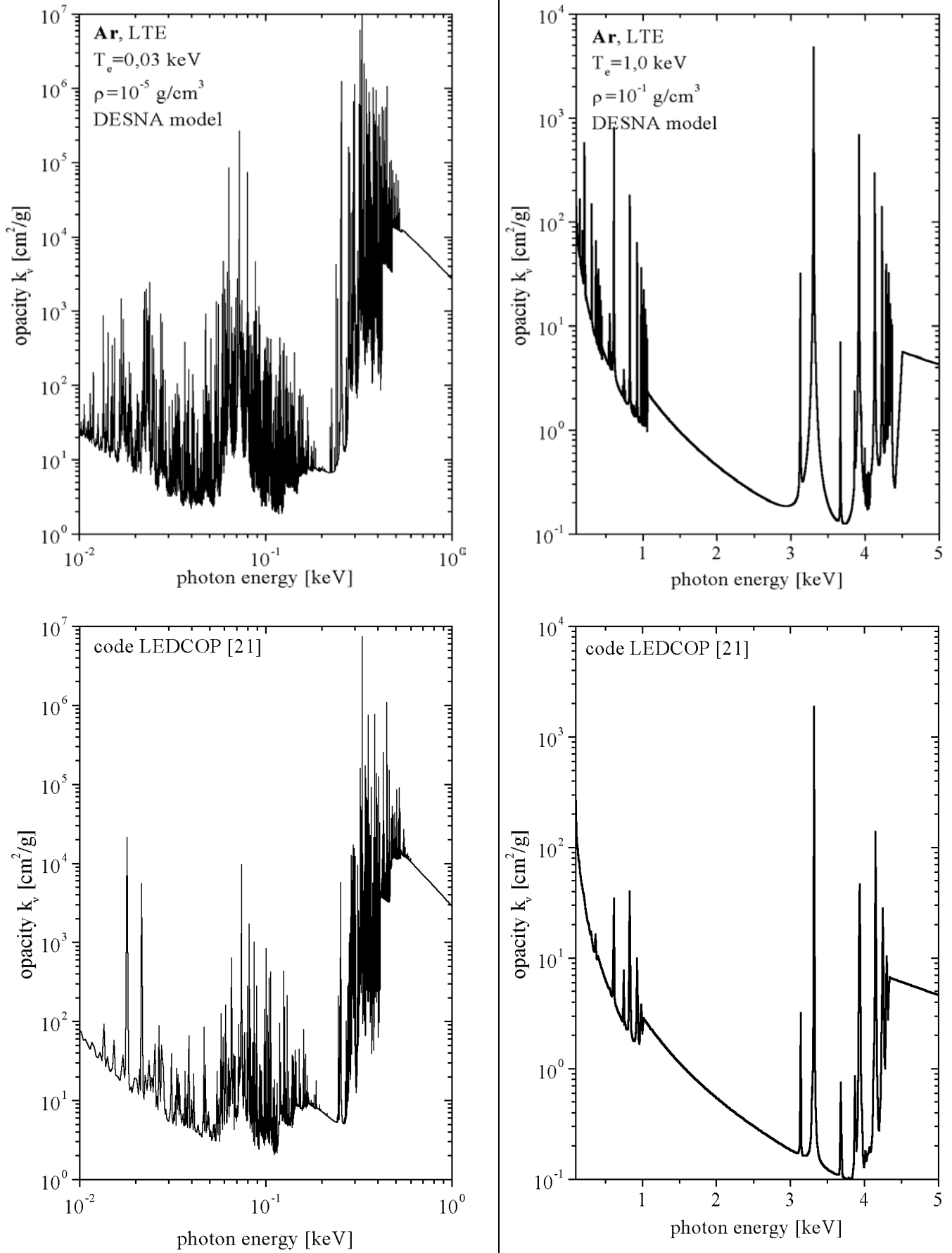$T_e=(10^{-2}eV?\div)1$ eV$\div$10 keV
$\rho=10^{-6}\div10$ g/cm^3

VII. Plans on the development of DESNA model

⌨   Consideration in the levels scheme of the autoionization states and accounting for the dielectronic satellites;

⌨   Accounting for influence on spectra optical thickness of plasma and self-absorption effects;

⌨   Self-consistent consideration of inverse influence on the population of excited levels and spectra of intrinsic radiation of plasma;

⌨   In some special cases – more precise calculations of spectral lines profiles;

⌨   A quasi-stationary or fully non-stationary solution of kinetic equations system;

⌨   Addition of databases on atomic data for other chemical elements and calculations on new substances, including astrophysical mixtures.

VIII.   Results
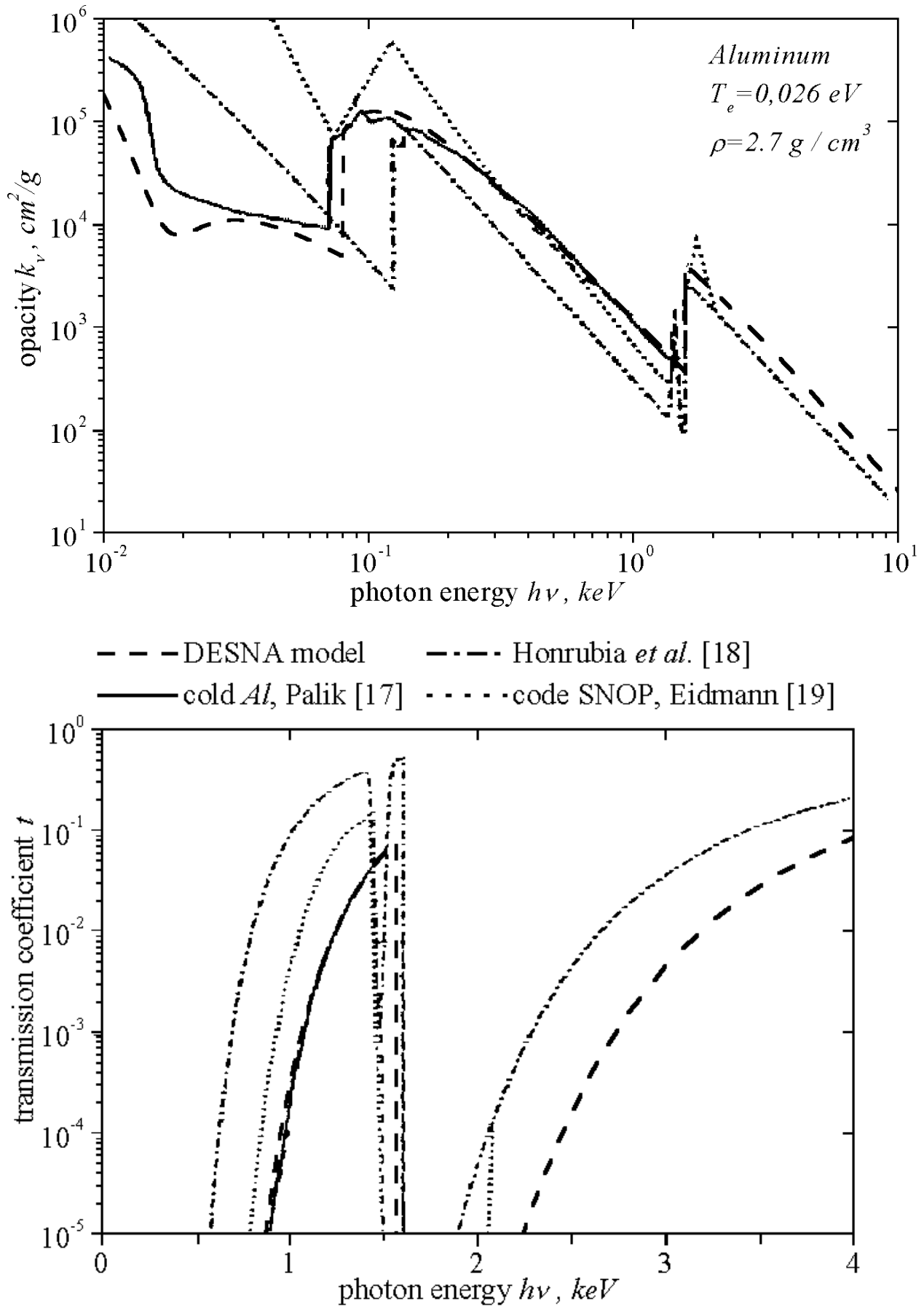
Fig.1 Spectral opacities for aluminum at solid density and low temperature calculated by different authors compared with the experimental opacity of cold aluminum reported by Palik [17] (upper graph) and transmission coefficients for a Δ=25 μm aluminum foil.

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Fig.2 Calculated in **LTE approximation** spectral opacities of argon plasma for two sets of plasma conditions. Upper plots is the results of calculations by means DESNA model. Lower plots is the results of code LEDCOP [21].
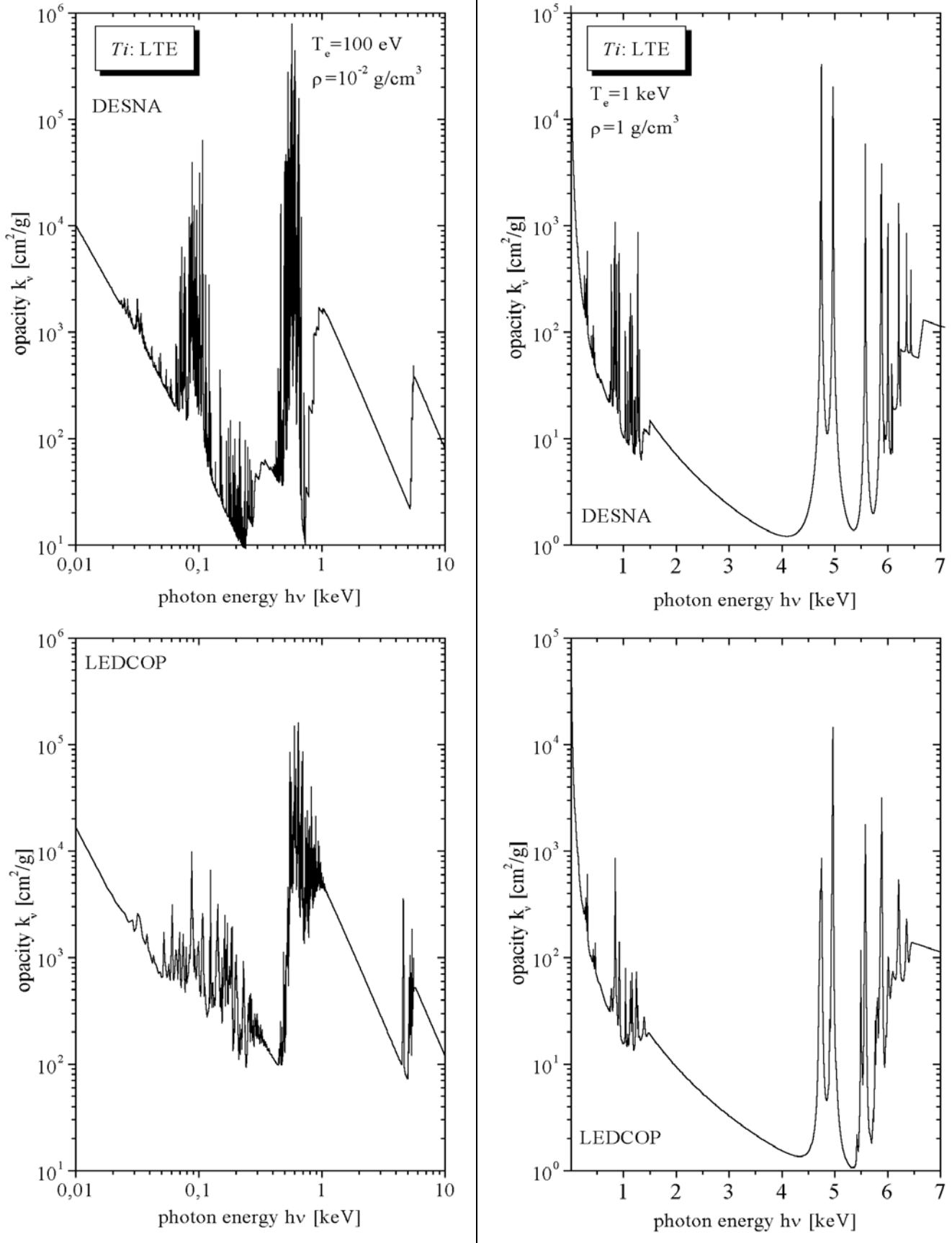
Fig.3 Calculated in **LTE approximation** absorption spectra of titanium multicharged ion plasma for two sets of plasma conditions. Upper plots is the results of calculations by means DESNA model. Lower plots is the results of code LEDCOP [21].
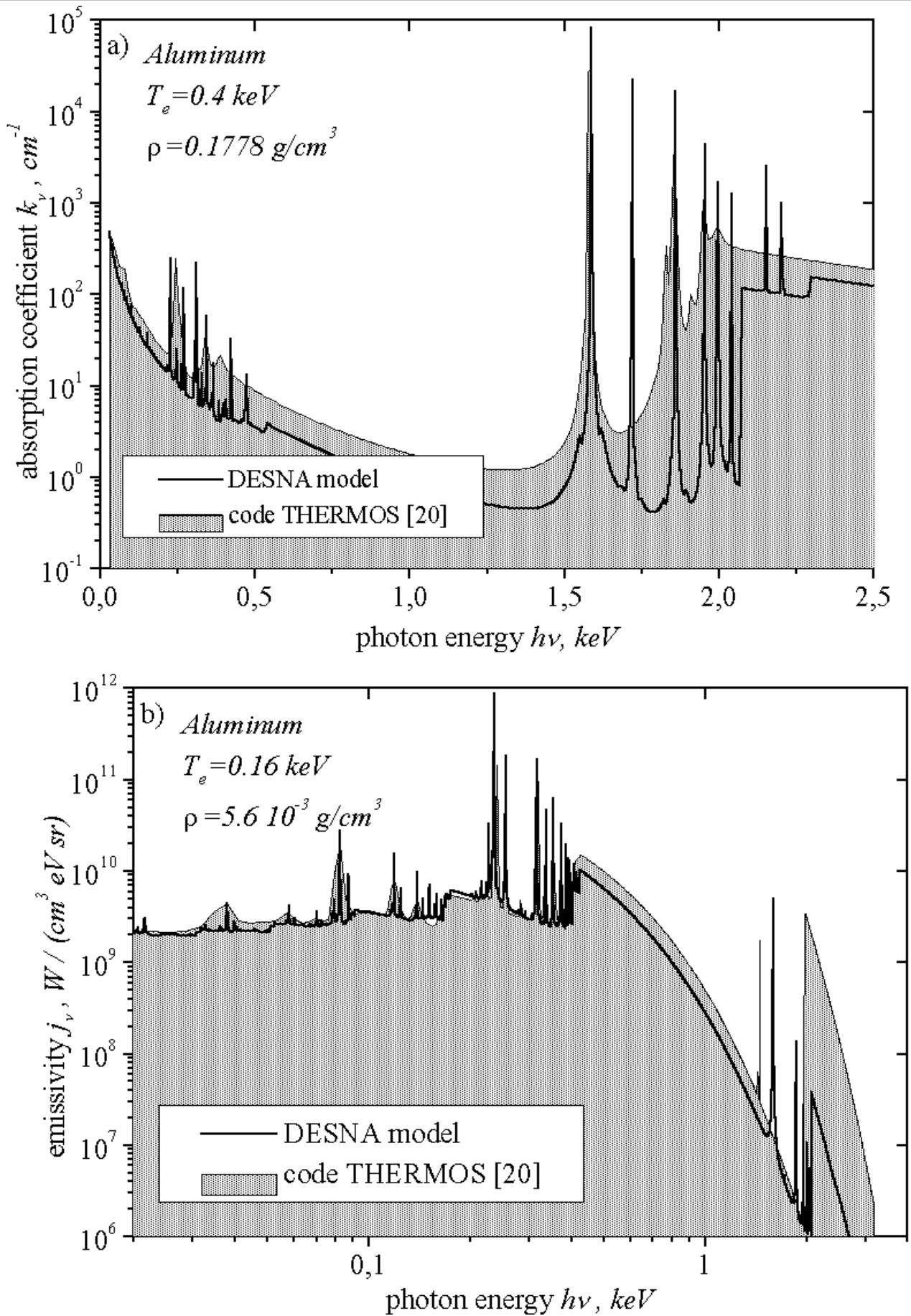
Fig.4 Calculated absorption (a) and emission (b) spectra of nonequilibrium aluminum plasma for different conditions. Comparison with the results of code THERMOS [20] (model of self-consistent field of Dirac-Fock-Slater).
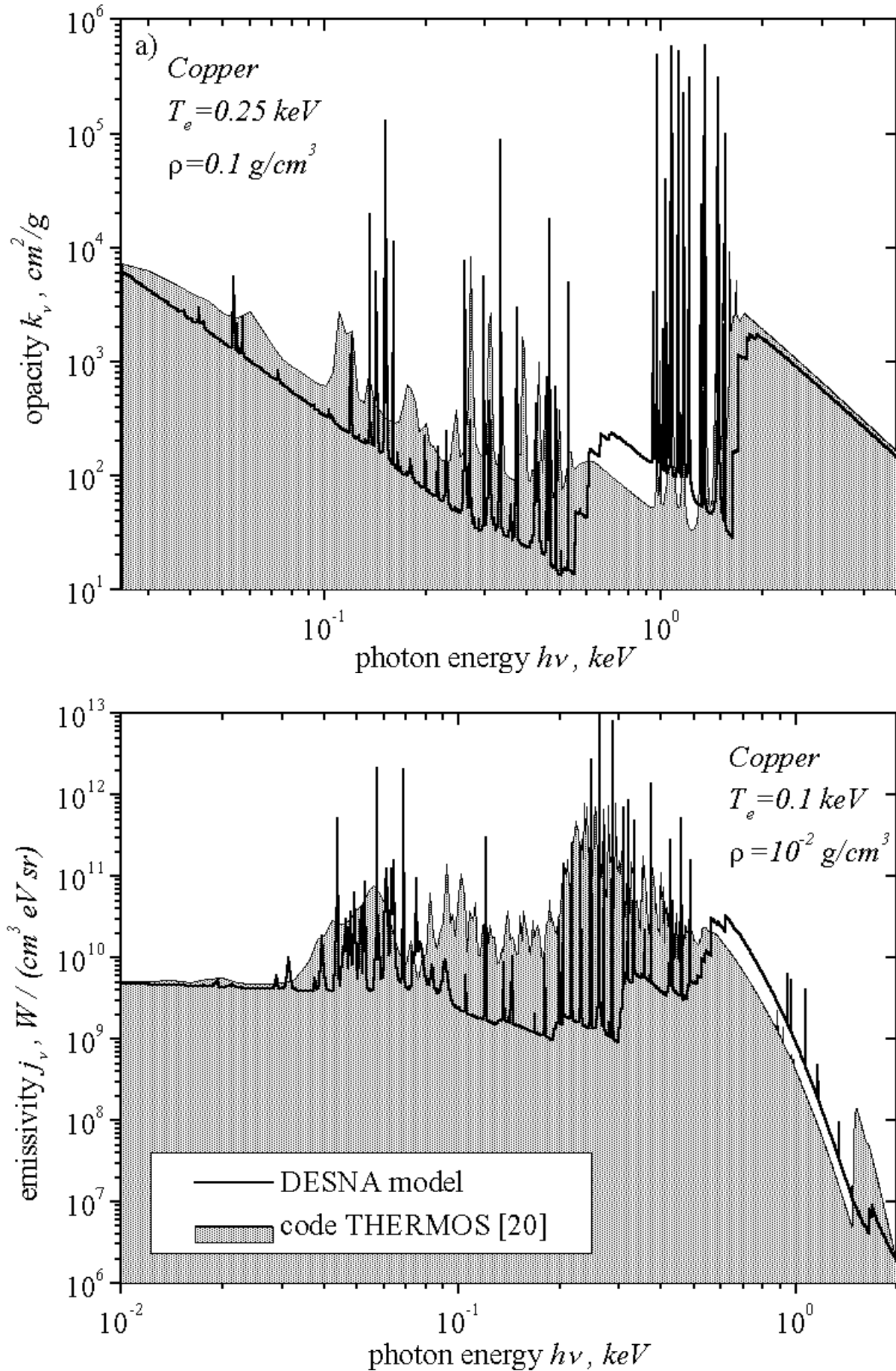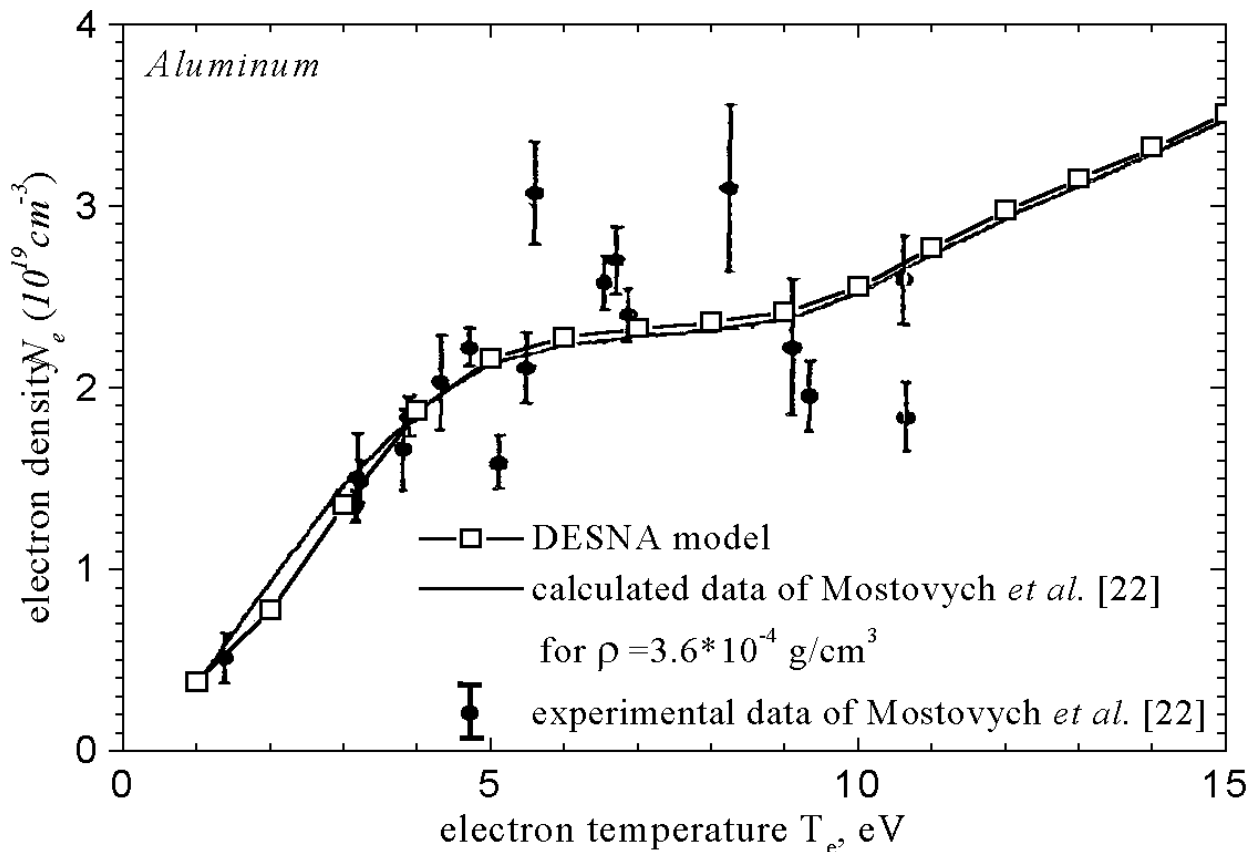
Fig.5 Spectral opacity (a) and spectral emissivity (b) of nonequilibrium copper plasma for various conditions. Thick line – DESNA model, thin line – results of code THERMOS [20].
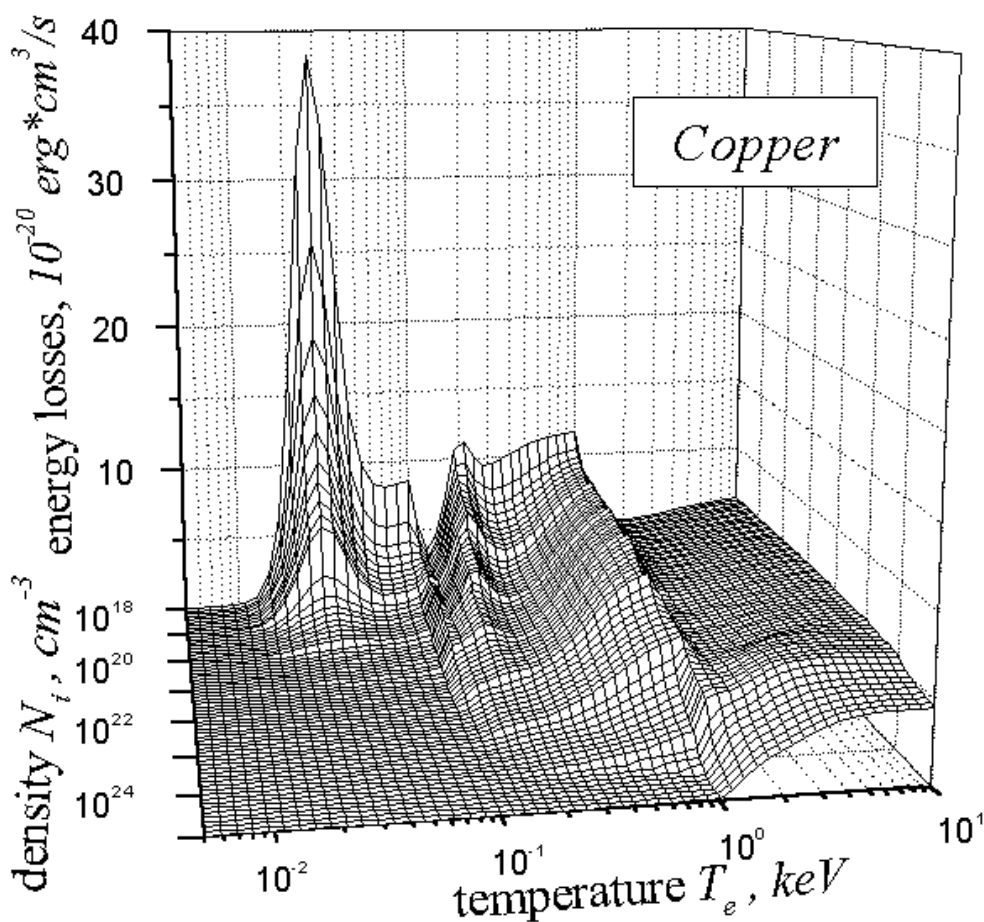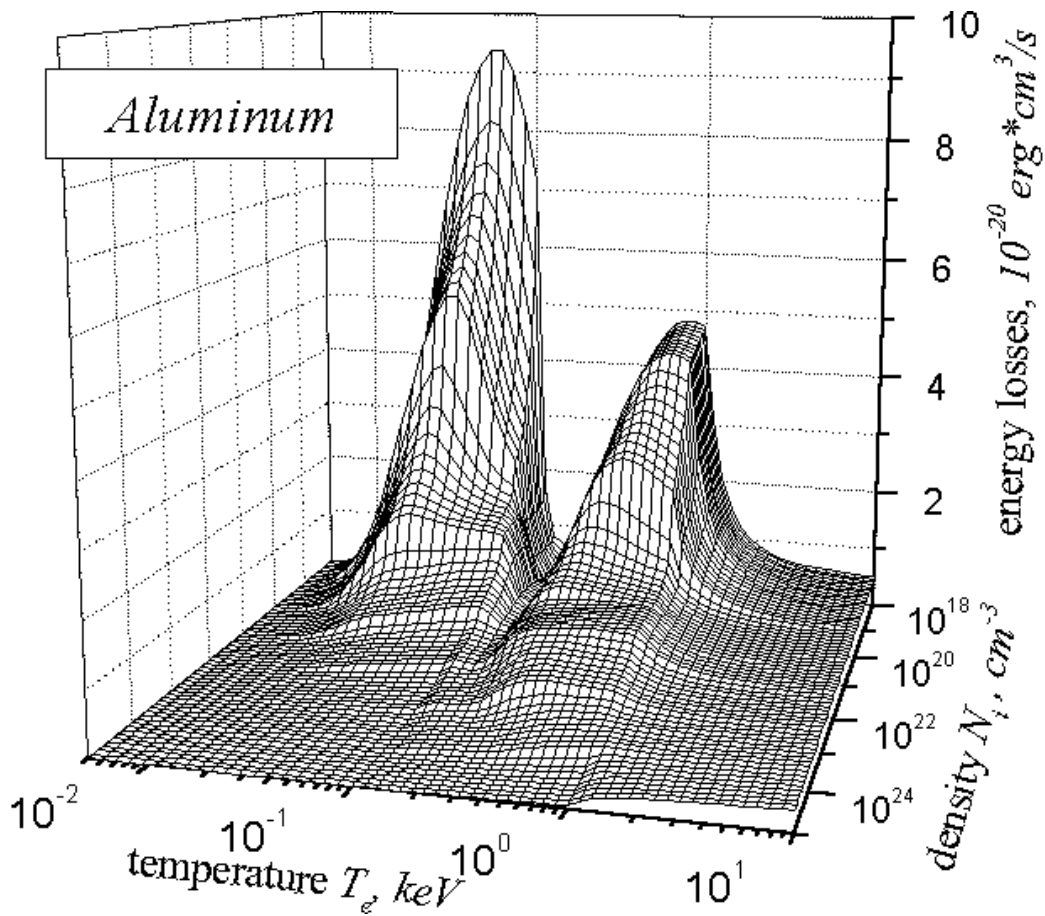
Fig.6 Total line plus continuum energy losses are calculated to one ion and one electron for an aluminum and copper plasmas in a wide range of electron temperature and ion density.
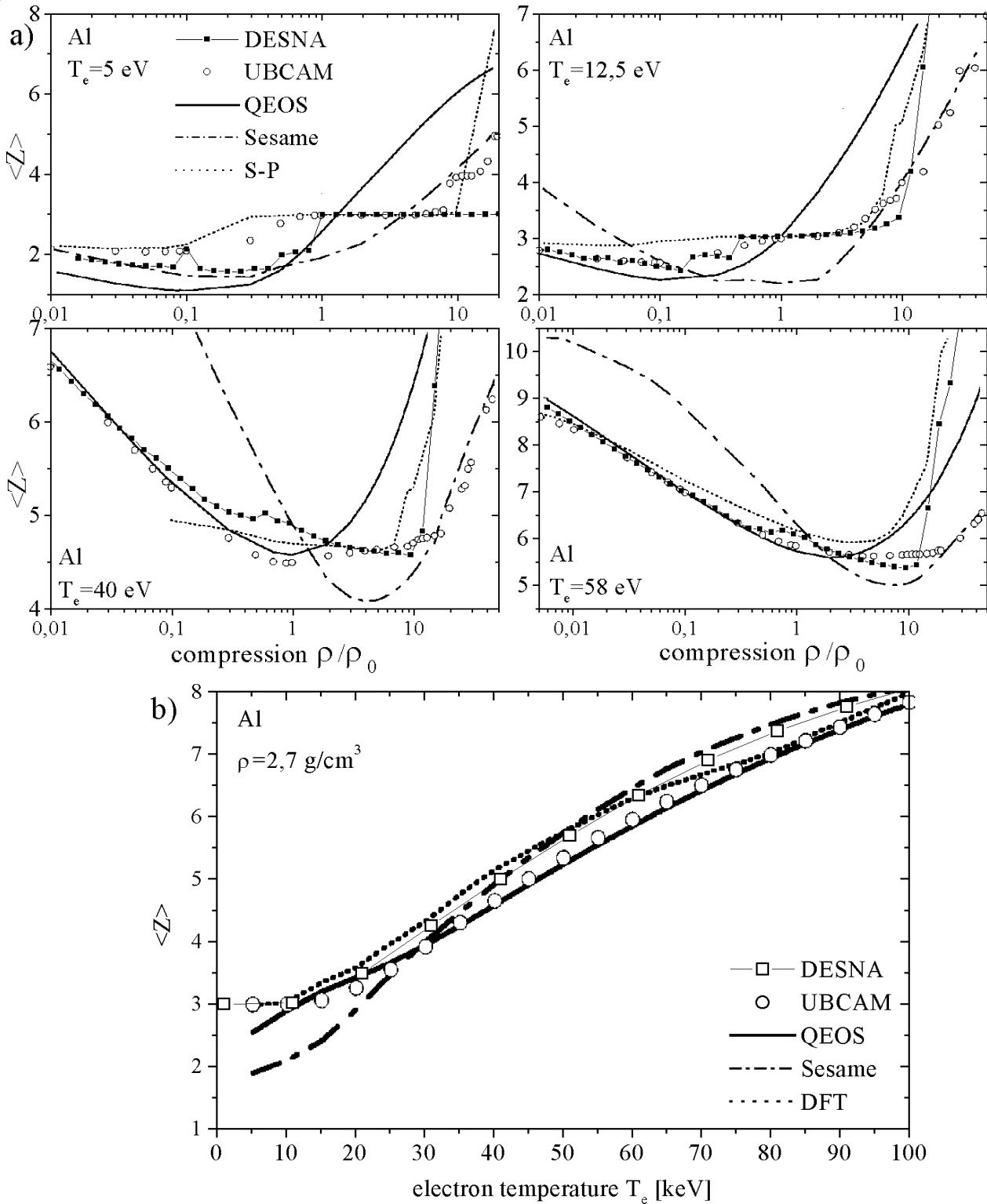
Fig. 7 Average charge of ions in an aluminum plasma as a function of: a) plasma compression ρ/ρ_0 (ρ_0 – density at normal conditions, $\rho_0(Al)$=2,7 g/cm^3) for various temperatures; b) electron temperature at normal density. Comparison of DESNA results with the data of UBCAM – University of British Columbia atomic model (G. Chiu, A. Ng, *Physical Review E*, **59**, 1999, p. 1024); with QEOS data - quotidian equation of state (R. M. More, K. H. Warren, D. A. Young, and G. B. Zimmerman, *Physics of Fluids*, **31**, 1988, p. 3059); with equation of state library Sesame data (Sesame Data Table", Los Alamos National Laboratory, Material Number 23715); calculations results on density functional theory DFT (F. Perrot and M. W. C. Dharma-wardana, *Physical Review E*, **52**, 1995, p. 5352); and calculations of UBCAM authors by using of Stewart and Pyatt formulae [7] (S-P).

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Fig.8 Comparison of calculated on model DESNA and in work [22] electron concentration as a function of plasma temperature with experimental data for an aluminum plasma. Mass density in calculations $\rho=3.6\times10^{-4}$ g/cm^3. Calculations for the nonequilibrium (CRE) plasma.

IX. Conclusions

A collisional-radiative model DESNA has been developed. Comparison of average charge, emission and absorption spectra calculated by means DESNA model with some experimental data and with calculation results of number of other models (including results which are not inserted in this poster) shows that DESNA model gives reasonable results in wide range of temperatures and densities. Model DESNA is suitable for calculations at nonequilibrium conditions (in particular, for LTE or coronal approximations). This peculiarity opens a wide opportunities for using of model in various applications connected with spectra of multicharged ions. DESNA model is intended for calculation of optical properties both pure elements plasma and arbitrary mixtures.

The main limitation of model are connected with using of ready atomic data from outside special databases. Comparison shows that for ions with moderate Z (for example, copper, Z=29) a quantity of considered levels and transitions is not enough to well reproduce all spectral particularities. At present, the quantity of atomic data in available databases for ions with Z>20 (except iron) is extremely low and there is a great necessity in atomic data for multicharged ions of such elements. Some interested methods and models for calculations of atomic data are described in presentations of 35th EGAS.

The results of modeling of some experimental spectra of multicharged ion plasma with help of DESNA model are presented in poster P1:41 (and more detailed description can be found in [23]).

Acknowledgments

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