Spectral line intensities calculations For Ne-like argon plasma

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ABSTRACT

Energy level populations and spectral line intensities in plasmas are studied using an advanced uniform approach for the calculation of ion energy levels and elementary processes rate coefficients in plasmas. The spectrum of Ne-like argon for the uniform steady-state plasma is calculated for a wide variation of electron temperature and density. Hence the most efficient lasing at 5 3p-3s transitions with wavelengths 697.6, 860.6, 727.5, 725.7, 670.7 Å should be expected at $10^{19} < n_e < 10^{20}$ cm^{-3} and $T_e \sim 60$ eV. It is shown that at electron densities of $10^{15} < n_e < 10^{21}$cm^{-3} ratios of the strongest 3p-3s line intensities are sensitive to electron density; their dependence on electron temperature is much less pronounced.

1. INTRODUCTION

A significant objective in the development of XUV lasers is to optimize plasma parameters in order to obtain a high efficiency device with small energy consumption. Experiments are aimed to search for plasmas conditions where lasing will be more efficient. In laser produced plasmas [1] [2] laser line intensities are studied with respect to distance from the target, irradiation power, etc. Two problems should be solved to facilitate this research: 1) accurate theoretical predictions of plasma parameters for the lasing effect to be the most efficient; 2) plasmas diagnostics. For many years these problems have been under thorough consideration in connection with other applications. Nevertheless there are still large discrepancies in line intensity calculations by different theoretical approaches. These discrepancies are caused mainly by uncertainties for elementary processes rate coefficients calculations. Therefore, comprehensive analysis for all rate coefficients as well as reasons for possible disagreements between results of different theories should be provided. It is the purpose of our present research to investigate line intensities for Ne-like and Ni-like ions in plasmas using the energy approach in the theory of decaying atomic states based on consistent QED theory. Recently argon plasma was proposed as a possibility for ASE observation. A low temperature capillary discharge can serve as the plasma source for Ne-like argon generation [3] [5]. Our preliminary calculations pointed at some 3p-3s transitions as promising for a laser effect arising from collisionally pumped Ne-like argon[5].

2. LEVEL POPULATION CALCULATIONS

Here a Ne-like argon plasma is considered which is assumed to be uniform and steady-state. Thus for kinetics calculations one needs just rate coefficients for Ne-like argon

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electron collision excitations and radiative decay probabilities for this ion. The first 37 levels are included in the kinetics. Collisional excitations are accounted for just from the ground state. In this preliminary calculation we ignore the collisional mixing of Ne-like argon excited states since we have shown that this approximation is valid for electron densities in the range n_e 10^{17}. The collisional mixing of excited states becomes essential at $n_e \sim 10^{19}$ and will be accounted for in our forthcoming calculations. The ions of adjacent states of ionization are not included in the kinetics. Such a simplified kinetics consideration allows one to clarify the dependence of the key features of line intensities on plasma parameters. It is also a convenient way to compare different theoretical results for line intensities.

We have analyzed in detail [6-8] the radiative decay probabilities for the Ne-like sequence by comparing them with other theorical calculations and with experiments. In Table 1 the energy levels and radiative characteristics for Ne-like argon are given. Levels numbering and state specifications are given in the first two columns. Our theoretical energy levels are presented in the 4th column. These energy level positions were calculated with a method that accounts for higher order perturbation theory corrections [10]. In the 3rd column the experimental energy levels are listed [9]. The comparison shows agreement in limits of a few hundred cm $^{-1}$ for all states with the exception of the 15th and the 27th states. The 5th column gives the radiative decay probabilities into the ground state $3p^6 1S_0$ for each state. The 3-d and 5-th levels can serve as low active levels since their decay into the ground state are rapid enough to provide inversion populations of $2p^5 3p$ levels. The 6th column gives the lifetime characteristics for each level. The 7th column lists the dominating decay channel among all possible 3-3 or 2-2 transitions; i.e. the order number of lower lying state into which the transition probability is of the largest value. In the 8th column the branch coefficient for the dominating decay channel is given. It shows the percentage of the level population decaying into the dominating channel. The 9th column gives the wavelength for the dominating transition. This consideration gives us a quick method of evaluating laser possibilities for different levels. We consider here the simple kinetics for lasing effect evaluation.

In our recent paper [11] we calculated electron collision strengths and rate coefficients for Ne-like argon and iron. It is shown [11] that collisional rate coefficients are close to their maxima at electron temperature $\sim 0.30 E_{threshold}$ for FeXVII and at $\sim 0.15 E_{threshold}$ for ArXI. Electron collision rate coefficients for argon are ~ 2 times larger than for iron. In our model the population of j-th level is determined by

$$N_j = \frac{n_e N_{gr} C^e_{gr \to j} + \sum_{i>j} N_i A_{ij}}{\sum_{i<j} A_{ji} + n_e C^d_{j \to gr}} \qquad (1)$$

where C^e_{ij} is collisional excitation rate coefficient,

C^d_{ji} is collisional deexcitation rate coefficient,

A_{ij} is radiative transition probability,

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$_{gr}$ designates the ground $^1S_0$ state.

For two limit values of electron density one has:

$$\text{If} \quad n_e < \sum_{i<j} \frac{A_{ji}}{C^d_{j-gr}} \quad \text{then} \quad N_j \sim \frac{n_e N_{gr} C^e_{gr-j}}{\sum_{i<j} A_{ji}} \tag{2}$$

$$\text{If} \quad n_e \to \infty \quad \text{then} \quad N_j \sim N_{gr} \frac{C^e_{gr-j}}{C^d_{j-gr}} \sim exp^{-E/kT} \tag{3}$$

Fractional level populations were calculated for 12 values of electron density $10^{11} < n_e < 10^{22}\text{cm}^{-3}$ and for 6 values of electron temperature $T_e = 30, 45, 60, 75, 90, 120\ eV$. The fractional level populations as functions on electron density for 6 energy levels of Ne-like argon are shown at Figure 1 (a,b). Figure 1 (a,b) correspond to 2 values of electron temperature $T_e = 45$ and 75 eV as examples. The conclusion is that at any temperature level populations as functions of electron density are straight parallel curves proportional to n_e in accordance with Eq.(2) until $n^e < 10^{16}$. At larger n_e values, mutual positions of level population curves are changing. Two lowest curves in Figures 1a,1b show fractional level population for 3rd and 5th $2p^5 3s$ [J=1] levels which are low active levels. The group of $2p^5 3p$ levels has very close populations shown at Figure 1 (a,b) with triple curve. The highest $2p^5 3p$ level with J=0 has the largest level population value until electron density $n_e \sim 10^{19}\text{cm}^{-1}$. At this electron density the plateau condition is met (see eq.(3)); since for this level the ratio C^d_{j-gr}/C^e_{gr-j} is almost 2 orders larger than for others levels of $2p^5 3p$ configuration. For these levels the plateau conditions are met at $n_e \sim 10^{20}\ \text{cm}^{-3}$.

Note that at electron densities $n \approx 10^{21}\text{cm}^{-3}$ the inversion population disapears. These conclusions are valid for any electron temperature. It is quite clear that the optimal electron densities are in the range $10^{19} < n_e < 10^{20}\text{cm}^{-3}$ for the lasing effect to be most efficient.

The maxima of fractional level populations increase with electron temperature (see Fig.1 a,b) amounting ~ 0.01 at $T_e \sim 120$ eV. However at a higher temperature the inversion effect becomes less pronounced .

The searching for optimal plasma conditions for lasing are typically based on ionization balance calculations. Presently accurate calculations for ionization balance in plasmas are practically impossible because of great number of rate constants of elementary processes in plasmas. Most of these constants are known with a large uncertainty. Another problem is concerned with a possibility of non-Maxwellian electron distribution in dense plasmas. There is still less studied but very important effect of ions electron shell polarisation by plasma electrons. The problem is that any kind of elementary process with ions in plasmas occurs in the close presence of plasmas electrons, the so called "electron-spectacular". Plasma "electrons-spectaculars" decrease effectively all threshold energies for collisional processes with increasing rate constants; they could also lead to line broadening.

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Typically the evaluation of electron temperature needed to produce a high fraction of definite ions in a plasma is based on experimental results. For moderate Z-values an electron temperature of 0.25 of the ionization potential of the parent ion is enough to produce an abundance of ions with multiplicity larger by one unit. For argon this number is even smaller. We believe that the Ne-like argon ionization stage is the most abundant at the range 30 T_e 75 eV. At higher electron temperatures the ionization equilibrium shifts to F-like ion production. This result was demonstrated by experiments[4].

To obtain accurate values for gain coefficients for a Ne-like argon plasma we need to refine our kinetics calculation :

1) to include electron collision transitions between all excited levels;

2) to investigate the influence of "electrons-spectaclulars" in quasi- bound states on collisional rate coefficients calculations in Ne-like ions; to analyze optimal temperature changes, if this effect is accounted for;

3) to include the states of ions of adjacent ionization stages;

4) to evaluate line broadening due to all collisions and Doppler effect;

5) for a definite plasma geometry account for:

   a) the photon escape factor;

   b) the self trapping (reabsorption) effect for transitions from low active levels to the ground state.

This investigations are now in progress.

However, our present model allows one to draw qualitative conclusions about lasing possibilies for definite lines in a Ne-like argon plasma . According to the generally used expression in a collisionally pumped scheme, gain is

$$\alpha = K * (\frac{\lambda^3 A}{T_i}) * (N_u - g_u \frac{N_l}{g_l}) \qquad (4)$$

That is valid if the broadening of all lines of interest is equal. The preliminary results for relative gain valus are shown at Figure 2. Relative gains are shown as functions of the electron temperature for two values of electron densities: $n_e = 10^{19}, 10^{20}$ eV. 4 transitions are shown at Figure 2; there is also a 5th transition: 10 - 3 at λ - 670.7 Å with a little bit smaller lasing potential. These conclusions partly confirm our previous results for lasing possibility of Ne-like argon in a collisionally-radiative scheme[5] based on a 3-level approximation. The main difference is related to 15-3 (the so called 0 - 1) transition at λ 430.7 Å which appears to be non-effective in the present more detailed consideration.

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3. NEON-LIKE PLASMA DIAGNOSTICS

Theoretical simulations are helpful in the determination of the optimal plasma conditions for lasing. However, special plasma diagnostics should be developed for Ne-like plasmas to test theory and normalize the optimization procedure. There are different methods for plasma diagnostics based on mesurements of dielectronic satellite line intensities with respect to the original resonance line. Typically H-like and He-like spectra of some impurity elements in plasmas are used. For the Ne-like ions the dielectronic satellite spectra of Na-like ions are suggested for plasma diagnostics [12].

Our calculations discovered that a great deal of diagnostic informations could be extracted directly from the Ne-like ions spectrum itself; that essentially facilitates Ne-like plasmas diagnostics. In figure 3 relative line intensities are shown to be dependent on electron density. Intensities of three 3-3 transitions in Ne-like argon normalized by intensity of 15-3 (0 - 1) transition are shown as examples at the electron temperature of 60 eV. Ratios of definite line intensities as well as level populations are sensitive to electron density at $10^{15} < n_e < 10^{22}$ cm^{-3}. Note that they are practically independent of electron temperature.

The ratio of other transitions are sensitive to electron temperature as well as to electron density. In Figure 4 intensities of two 2-2 transitions 29-3 and 29-5 normalized by the 15-3 transition intensity are shown for $T_e = 30$ eV and $T_e = 60$ eV. If T_e increases at $n_e > 10^{18}$ the intensities of both lines increase significantly.

4. CONCLUSION

A consistent theory is developed for accurate calculations of rate coefficients for variaty of elementary processes in plasmas. Our code allows for the use of any time-dependent plasma electron energy distribution. The resulting time dependent populations are calculated through the solution of the system of the ordinary differential equations with starting values corresponding to the concrete physical conditions. Here only asymptotic populations values for steady-state plasma with Maxwellian electrons are presented.

In Ne-like argon plasmas ratios of line intensities do not change with electron density for $n_e < 10^{15}$cm^{-3}. At $10^{15} < n_e < 10^{21}$cm^{-3} ratios of line intensities are sensitive to electron density. Inversion of $2p^5 3p$ level populations disappear at an electron density of $n_e \sim 10^{21}$cm^{-3}. The most efficient lasing at 5 3p-3s transitions should be expected at $10^{19} < n_e < 10^{20}$cm^{-3} and $T_e \sim 60$ eV.

In the absence of enhancement ratios of intensities for the strongest 3p-3s transitions can serve as a tool for plasma electron density diagnostics. Intensities of definite 2-2 transitions with respect to the strongest 3-3 transitions in Ne-like ions are sensitive both to electron temperature and to electron density. Ratios of line intensities shown in Figure 4 could serve for electron plasma temperature diagnostics. Experimental line intensity measurements for uniform steady-state plasmas are important to test the theory.

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Table 1. Energy levels and radiative characteristics of Ne-like argon
A - radiative transition probability to the ground state;
i - the order number of final state of dominating channel for 3-3 or 2-2 radiative transition from n-th level;
branch coefficient is given for the dominating channel;
wavelengths are given for the dominanting channel.

n	Level	J	Energy exp [9] (cm^{-1})	Energy theory (cm^{-1})	A n-0 (sec^{-1})	life time (psec)	i	branch coeff. n-i	Wave length $\AA$
1	2s2 2p6	0	0	0					
2	2p3/2 3s1/2	2	2026542	2026504	.13+04				
3	2p3/2 3s1/2	1	2033120	2033273	.50+11				
4	2p1/2 3s1/2	0	2044670	2044390	.0				
5	2p1/2 3s1/2	1	2051880	2052270	.14+12				
6	2p3/2 3p3/2	1	2149320	2149800	.60+05	441	2	.42	814.5
7	2p3/2 3p3/2	3	2169894	2169600	.45+00	460	2	1.0	697.6
8	2p3/2 3p1/2	2	2170923	2170620	.83+07	492	2	.46	692.6
9	2p3/2 3p1/2	1	2176716	2176320	.83+04	481	2	.42	665.9
10	2p3/2 3p3/2	2	2182224	2181790	.16+08	456	2	.50	642.3
11	2p1/2 3p1/2	1	2189330	2188900	.13+05	490	5	.45	727.5
12	2p1/2 3p1/2	0	2192240	2191620	.0	480	5	.55	712.5
13	2p1/2 3p3/2	2	2195230	2194790	.19+08	458	5	.79	697.6
14	2p1/2 3p3/2	1	2196230	2195540	.76+04	462	4	.55	659.8
15	2p3/2 3p3/2	0	2265320	2271360	.0	470	3	.57	430.7
16	2p3/2 3d3/2	0	2349300	2348603	.0	152	9	.43	579.4
17	2p3/2 3d3/2	1	2351420	2350700	.60+10	81	9	.14	572.4
18	2p3/2 3d5/2	2	2355570	2354950	.34+05	158	10	.24	576.9
19	2p3/2 3d5/2	4	2358730	2358660	.87-04	159	7	1.0	529.6
20	2p3/2 3d3/2	3	2361760	2361960	.11+04	154	8	.73	524.0
21	2p3/2 3d3/2	2	2366960	2366990	.24+04	154	8	.27	510.1
22	2p3/2 3d5/2	3	2370655	2371530	.33+04	159	10	.76	530.7
23	2p3/2 3d5/2	1	2381120	2381490	.14+12	7	12	.01	529.4
24	2p1/2 3d3/2	2	2382450	2382700	.45+04	154	11	.51	517.8
25	2p1/2 3d5/2	3	2384880	2385380	.25+04	159	13	.84	527.3
26	2p1/2 3d5/2	2	2385380	2385430	.77+02	159	14	.56	528.7
27	2p1/2 3d3/2	1	2411310	2418700	.32+13	0.3	12	.001	456.5
28	2s1/2 3s1/2	1		2639720	.18+04	51	2	.59	163.1
29	2s1/2 3s1/2	0		2668780	.0	51	3	.64	157.3
30	2s1/2 3p1/2	0		2780200	.0	46	11	.32	169.1
31	2s1/2 3p1/2	1		2781050	.82+10	34	8	.28	163.8
32	2s1/2 3p3/2	2		2783390	.76+04	46	7	.44	162.9
33	2s1/2 3p3/2	1	2791700	2792670	.44+12	2	10	.01	164.1
34	2s1/2 3d3/2	1		2967370	.60+02	38	24	.18	171.0
35	2s1/2 3d3/2	2		2967470	.15+05	38	20	.21	165.1
36	2s1/2 3d5/2	3		2967600	.84+01	39	19	.34	164.2
37	2s1/2 3d5/2	2		2984800	.36+09	38	20	.14	160.5

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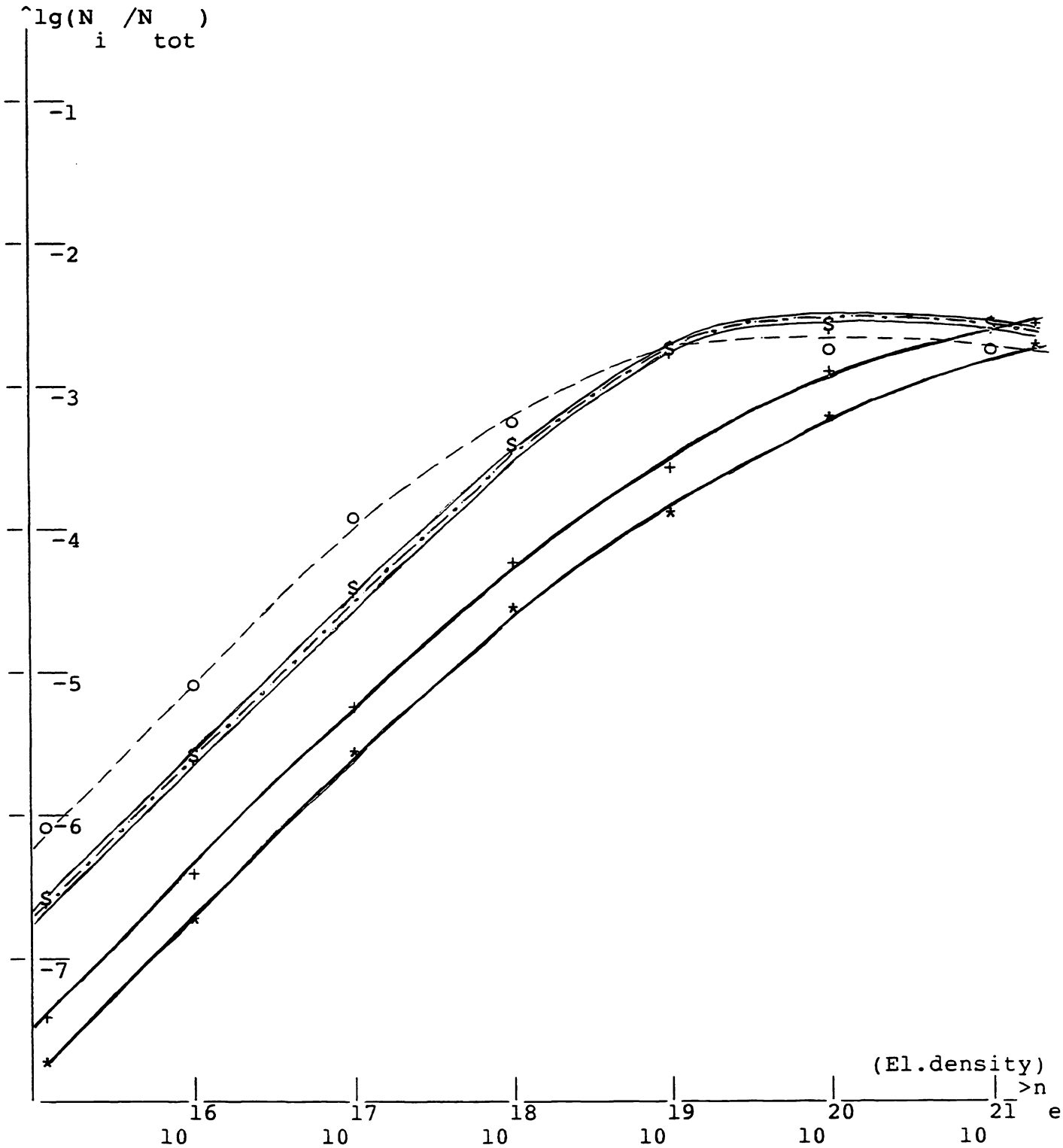


Fig 1 a. Fractional level populations as functions on electron density for Ne-like argon. Te = 45 eV =0.11 Ioniz.Pot.
+ low active level #3 [J=1] (see Tab.1);
* low active level #5 [J=1];
$ high active levels: #6 [J=1], #8 [J=2], #13 [J=2];
o level #15 [J=0].

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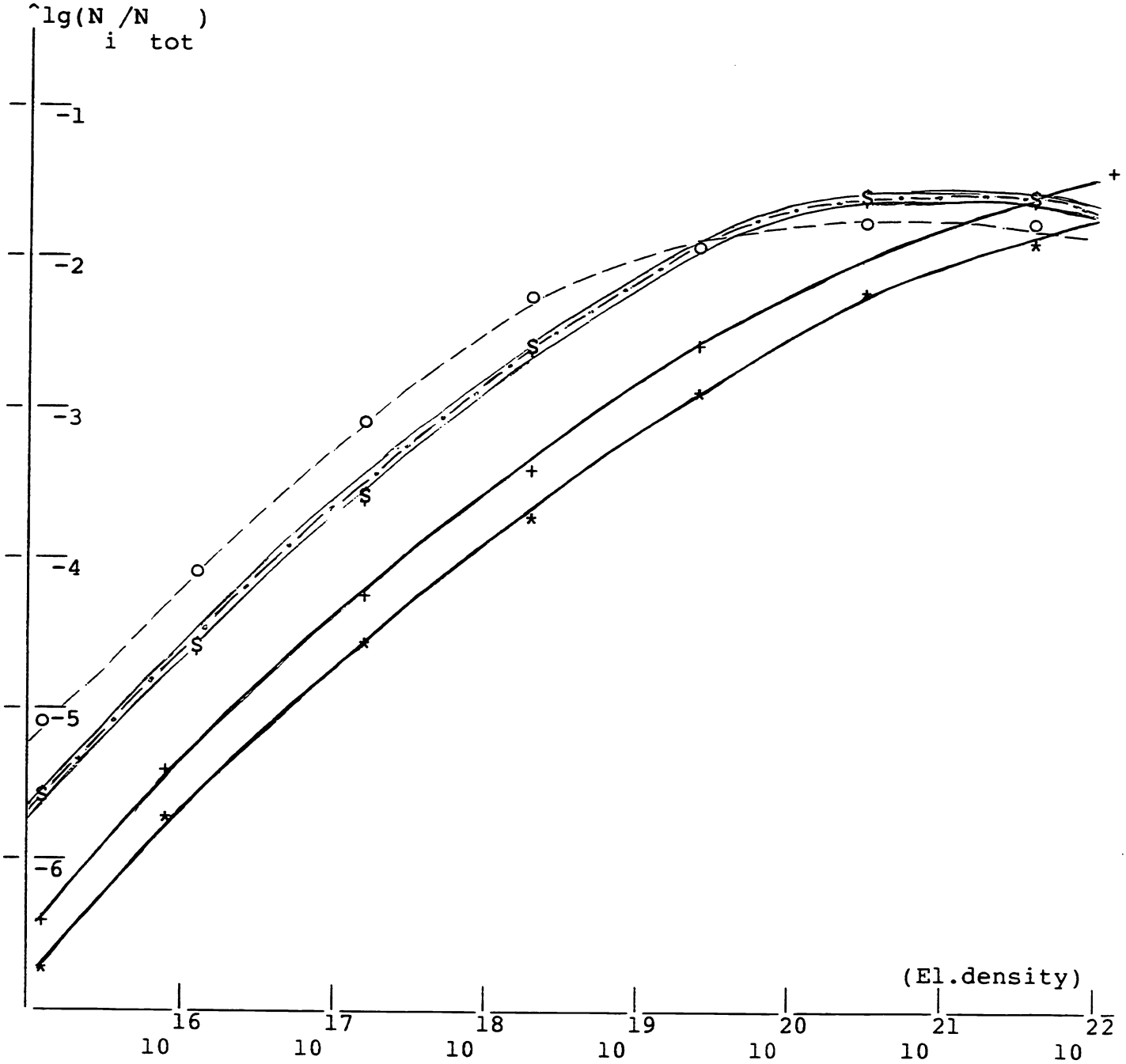


Fig 1 b. Fractional level populations as functions on electron density for Ne-like argon. Te = 75 eV =0.18 Ioniz.Pot.
+ low active level #3 [J=1] (see Tab.1);
* low active level #5 [J=1];
$ high active levels: #6 [J=1], #8 [J=2], #13 [J=2];
o level #15 [J=0].

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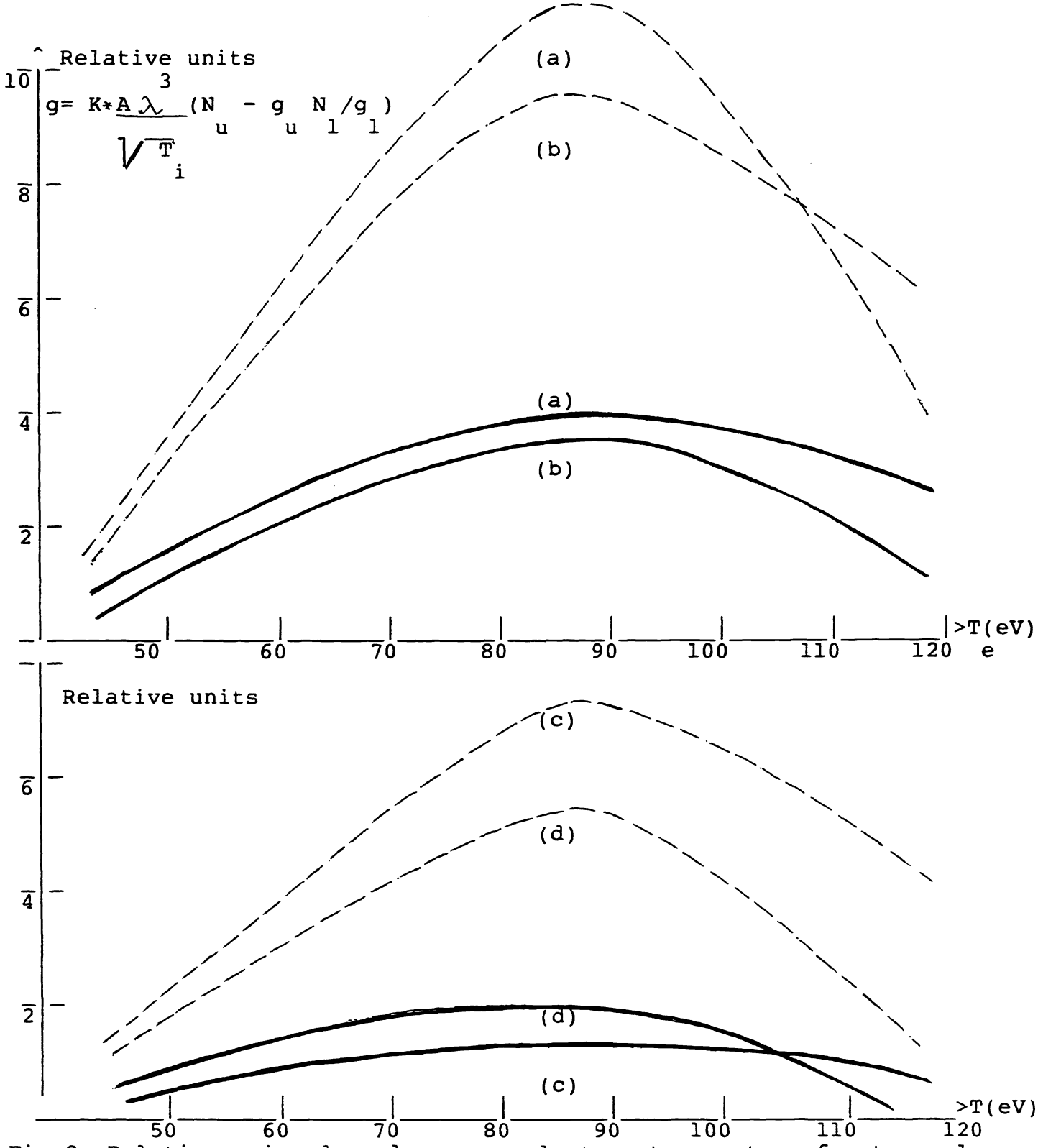


Fig.2. Relative gains dependences on electron temperature for two values of electron density: solid line - $n_e = 10^{19}$ cm^{-3}, dashed - $n_e = 10^{20}$ cm^{-3}.

transitions: (a)-(13-5, λ_e=697.6 Å); (b)-(6-3, λ_e=860. Å);
(c)-(11-5, λ_e=727.5 Å); (d)-(8-3, λ_e=725.7 Å);

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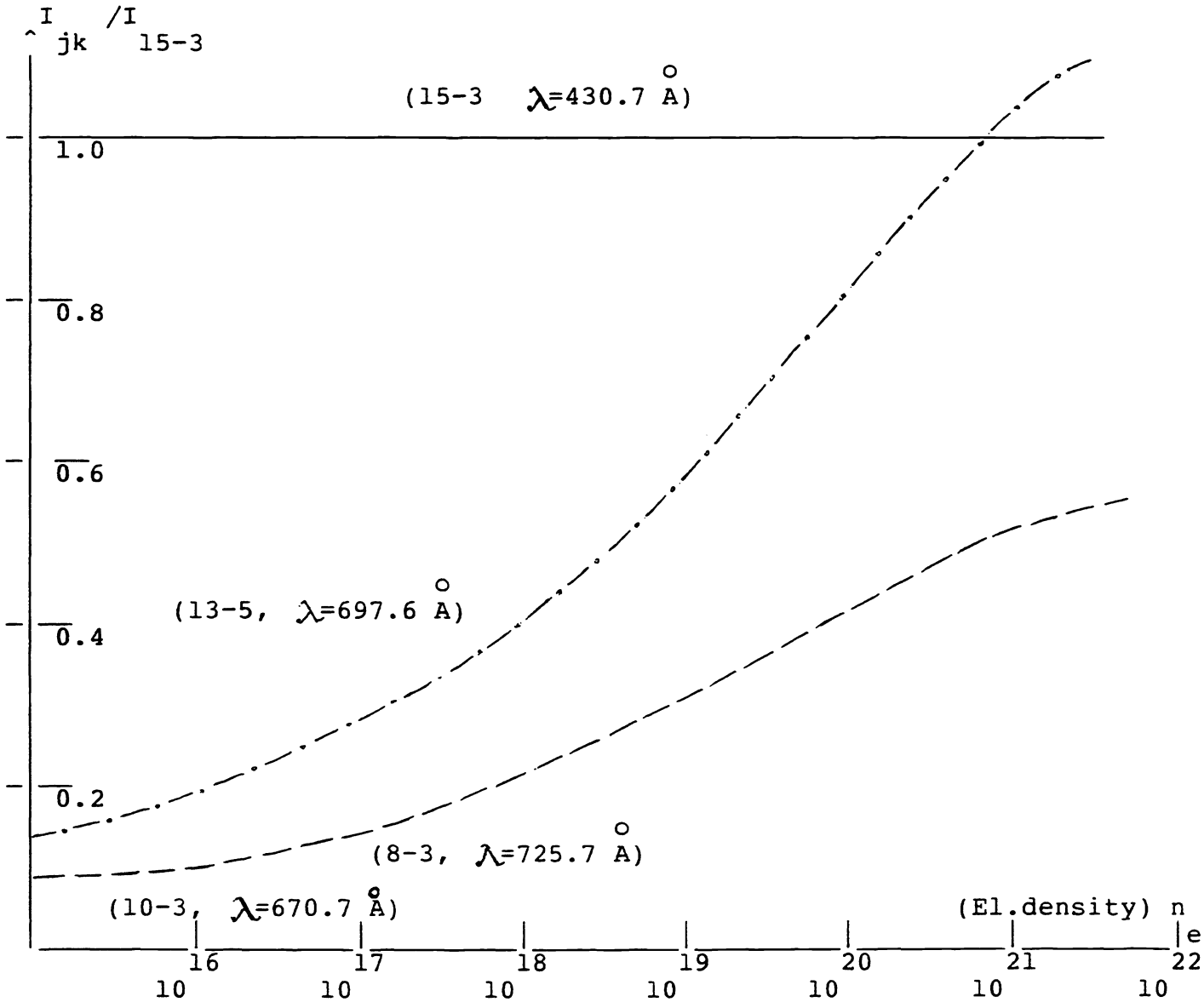


Fig 3. Relative line intensities dependence on electron density at electron temperature T_e = 60 eV for Ne-like argon plasma; for another electron temperatures these intensity ratios are very similar.

_____ intensity for 15-3 transition is assumed to be unit;

----- intensities of two transitions: 10-3, at λ=670.7 Å and 8-3 at λ=725.7 Å are practically equal.

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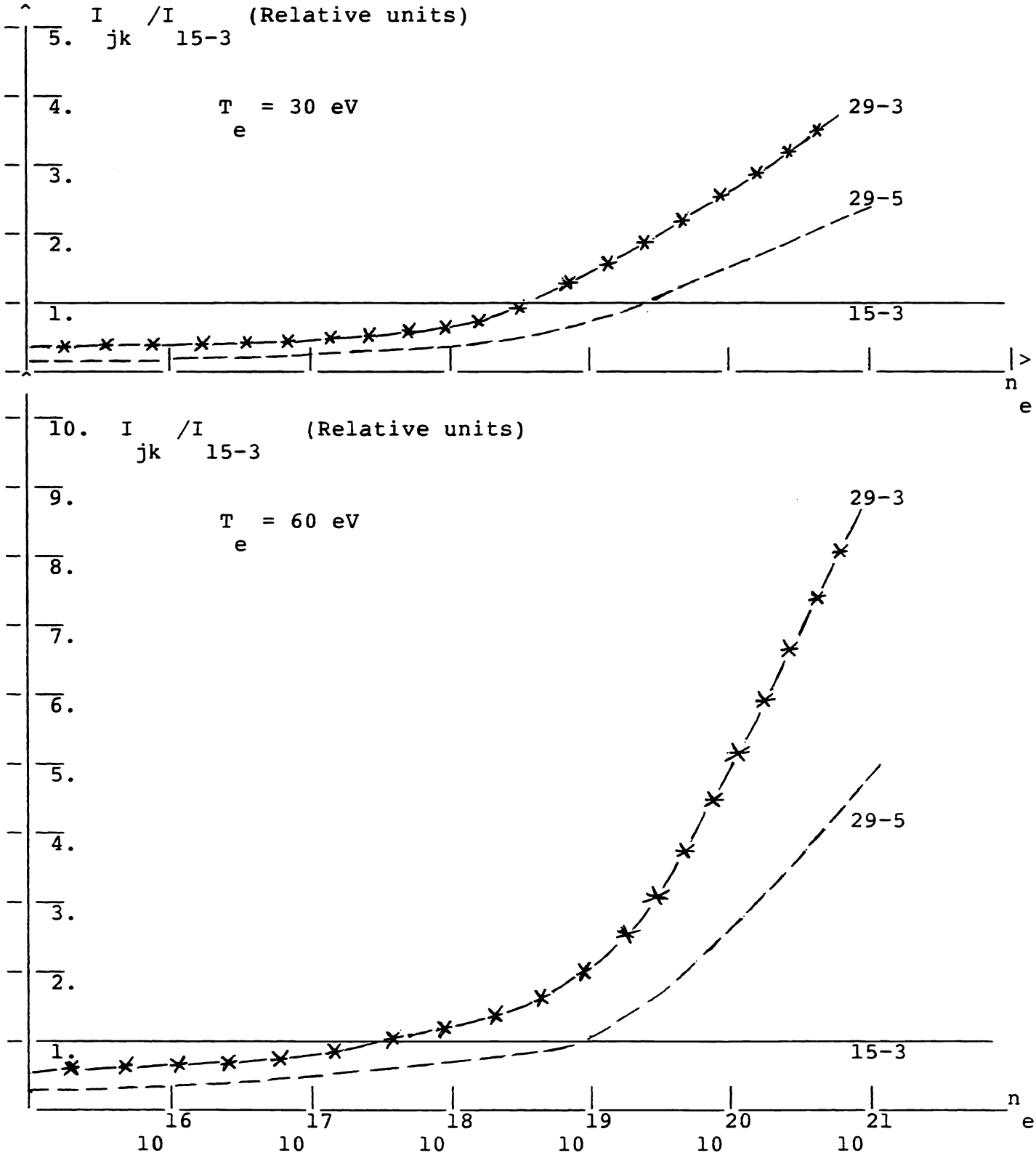


Fig 4. Relative intensities for 2 values of electron temperatures:
_____ 15-3) 2p3/2 3p3/2 [J=0] - 2p3/2 3s1/2 [J=0] (λ=430.7 Å)
-------- 29-5) 2s1/2 3s1/2 [J=0] - 2p1/2 3s1/2 [J=1] (λ=162. Å)
-*-*-*-* 29-3) 2s1/2 3s1/2 [J=0] - 2p3/2 3s1/2 [J=1] (λ=158. Å)
in Ne-like argon plasmas as functions on electron density.

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