STUDY OF VARIATION IN FRACTIONAL ABUNDANCE, EXCITATION RATE COEFFICIENT AND CONTRIBUTION FUNCTION OF SPECTRAL LINE (Λ=340 A$^{\text{O}}$) OF Fe XVI ION AS A FUNCTION OF ELECTRON TEMPERATURE.

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ABSTRACT: Ionization rate coefficient and Recombination rate coefficient, Fractional abundance, the excitation Rate Coefficient and Contribution function of iron ions are fully determined by electron temperature. Fractional abundance of ion of charge z can be determined by taking ratio of Density of ion of charge z to the summation of density of all possible ionized states. The excitation Rate Coefficient, the fractional Abundance and electron density decide the intensity of spectral line. The spectral line intensity is proportional to the contribution function. The Contribution function can be found by taking product of fractional ion abundance and its excitation rate coefficient of upper state of transition emitting the spectral line in consideration. In present work the fractional abundance, excitation rate coefficient and Contribution function of spectral line (λ =340 A$^{\text{o}}$) of Fe XVI ion as a function of electron temperature are computed and are studied by presenting graphically.

KEYWORD: Ionization rate coefficient, Recombination rate coefficient, the excitation Rate Coefficient, Fractional Abundance, Contribution function, Electron Temperature.

1. INTRODUCTION

It is well known that energy states of atoms and ions in the plasma are populated by electron collisions and depopulated by collisions of ions with slow electrons. Besides the collisional processes the atomic and ionic states are populated and depopulated due to some radiative processes also.

Electrons passing through the plasma transfer their energy to the plasma particles by two types of collisions i) Elastic collisions ii) Inelastic collisions.

In elastic collisions the transfer of kinetic energy of electron in to the kinetic energy of the plasma particles (atoms or ions) takes place. In this process the kinetic energy of the colliding particles is conserved.   This type of collisional process is responsible to the heating of the plasma particles to some extent. In fact the second type of collision i.e. inelastic collisions are mainly responsible for the excitation of atoms and ions in the plasma. Any collision in which the internal energy of excitation of a particle is changed is referred to as inelastic collision. In this type of collision the kinetic energy of electron is converted into potential energy of colliding plasma particles and the plasma particles get

excited. These particles in excited states either transfer their energy back to the electron or they undergo a transition giving radiative emission. The rate of transfer of energy from the electrons to the plasma particles may be written as,

$$\frac{dE}{dt} = N_g C_e N_e E_c + \sum_j N_{gi} N_e C_{in} E_j - \sum_j N_{gi} N_e C_{dex} E_i \quad (1)$$

where N_g is number of gas particles. C_e is coefficient of elastic collision. E_c is energy transferred in elastic collisions. C_{in} is rate coefficient of inelastic collisions. E_j is energy of the jth state excited by elastic collision. C_{dex} is de-excitation rate coefficient. E_i is energy of excited particles which transfers its energy to the electrons.

The sum runs over all possible energy states of the plasma particles.

All the processes which can populate or depopulate the states of plasma particles are explained below.

2. ELECTRON IMPACT EXCITATION (EIE)

In electron impact excitation, the energy from the high energy electrons is transferred to the colliding atoms or ions in the plasma. When an electron having energy more than the excitation energy of an electron rotating around nucleus of an atom / ion collides with the atom / ion may transfer its energy to the system and this may result in excitation of the rotating electron to a higher orbit. The probability of excitation depends upon energy of exciting electron and cross section of excitation at that particular energy. The excitation rate depends upon the excitation cross section and the number of effective collisions made by the electron. The number of effective collisions is function of electron velocity, which intern is a function of electron temperature (T_e).

As we know that the plasmas consists of atoms, ions and electrons, there can be two types of electron impact excitation processes depending upon whether the colliding particles are atoms in ground

state or ion in ground state. And accordingly these electron impact excitation (EIE) rate coefficients are defined as direct excitation and stepwise excitation respectively. The EIE rate coefficient is expressed in terms of excitation cross section σ and electron velocity V_e as $< \sigma V_e >$. Now for the two types of electron impact excitations we can write,

$$R = < \sigma_s V_e > \quad (2)$$

and

$$D = < \sigma_d V_e > \quad (3)$$

where,

R is EIE rate coefficient due to stepwise excitation.

D is EIE rate coefficient due to direct excitation.

σ_s is EIE cross section for states from ground state of ions.

σ_d is EIE cross section for the states from ground state of neutral atom.

The velocity of an electron is function of its energy and related to its energy E by the relation,

$$V_e = 5.9 \times 10^7 (E)^{1/2} \quad (4)$$

The number dN of the electrons having energy between E and E+dE is given for Maxwellian distribution by equation,

$$dN = N \times (2/KT_e) \times [E/(\pi KT_e)]^{1/2} \times EXP(-E/KT_e)dE \quad (5)$$

Thus the rate of excitation of energy levels by stepwise and direct excitation are respectively expressed as,

$$dR = N \times (2/KT_e) \times [E/(\pi KT_e)]^{1/2} \times (\sigma_s V_e) \times EXP(-E/KT_e)\, dE \quad (6)$$

and

$$dD = N \times (2/KT_e) \times [E/(\pi KT_e)]^{1/2} \times (\sigma_d V_e) \times EXP(-E/KT_e)\, dE \quad (7)$$

The total excitation rate coefficient can be obtained by integrating above equation within the limits from 0 to ∞.

As the excitation process does not occur if the energy of incident electron is

less than the threshold energy E_s, the excitation cross section is zero for energy less than E_s. Therefore the lower limit of integration is taken as E_s instead of zero. Further it is convenient to express the electron temperature and electron energy in eV. If T_e, E and dE are all in eV and cross section values are in cm^2, the equation (6) and equation (7) be written as,

$$R = \frac{6.7 \times 10^7}{(T_e)^{3/2}} \int_{E_s}^{\infty} \sigma_s E \, EXP(-E/KT_e) dE \quad cm^3 \sec^{-1} \quad (8)$$

and

$$D = \frac{6.7 \times 10^7}{(T_e)^{3/2}} \int_{E_s}^{\infty} \sigma_d E \, EXP(-E/KT_e) dE \quad cm^3 \sec^{-1} \quad (9)$$

respectively.

These equations clearly show that if the values of the excitation cross section are known at different values of the electron energy, the excitation rate coefficients may be obtained at different electron temperatures.

3. PENNING EXCITATION

Excitation energy can be exchanged between neutral atoms. In particular, an excited atom can get ionized by virtue of its excitation energy, if the later is larger than the required ionization energy. Such a process is made more probable if the excited atom is in metastable state and has thus longer lifetime in which the particle may undergo an effective collision. When one of the colliding atoms is in metastable state and the other one is in ground state, there is a probability of ionizing second atom and getting excited to the excited state depending upon the energy of the metastable atom. Such a process is referred to as penning excitation.

4. DUFFENDUCK EXCITATION

The process in which an ion having charge z in a ground state, when collide with the other ion having charge z' in ground state, transfers its energy to the colliding partner and the other ion gets ionized. This process of ionization and excitation of one ion and recombination of other ion is known as Duffenduck excitation or charge transfer.

For computation of excitation rate coefficients, we have used the formula proposed by Breton [1] which is useful for computation of excitation rate coefficient of heavy atoms like iron as a function of electron temperature. The formula proposed by Breton is based on the Bethe-Born approximation for optically allowed transitions [2] which is given below.

$$Q = 1.6 \times 10^{-5} e^{-\beta} \times \frac{f \, \overline{g}(\beta)(\beta)^{1/2}}{(\Delta E)^{3/2}} \quad (10)$$

where Q is in $cm^3 \sec^{-1}$, T_e is in eV, ΔE is the excitation energy in eV.
$B = (\Delta E / T_e)$
where,
f is the absorption oscillator strength.
$\overline{g}(\beta)$ is the average effective Ground factor.

The expression for $\overline{g}(\beta)$ which is proposed by Mewe [3] is given below.

$$\overline{g}(\beta) = A + (B\beta - C\beta^2 + D)e^{\beta} \, E_1(\beta) + C\beta. \quad (11)$$

where A, B, C and D are adjustable parameters. This formula may also include optically forbidden monopole or quadrapole transitions (for example H - like ions, the 1s → ns or 1s → nd transitions respectively) and spin exchange transitions (for example singlet-triplet transitions in He like ions). In these cases, f in equation (1) assumes the f values of the allowed transitions to the level with the same principle quantum number. For example, the transition

1s → ns and 1s → nd in the H - like sequence the f value of 1s → np is chosen: for 1s2 ^{1}S → 1s 2s^{3}S in the He like sequence, that of 1s2 ^{1}S → 1s 2p ^{1}P is used.

The iron transition included in excitation rate coefficient computations together with wavelengths λ, the

excitation energies ∆E and f values, we used values in C. Breton et al [1]. For the parameters A, B, C and D we the used values in Mewe [3] who gives these values for several transition in H, He, Li and Ne sequences by fitting the function $\overline{g}(\beta)$ to the available theoretical and experimental data. For other ion sequences, with an accuracy to within a factor of three, he proposes A = 0.15 (∆n ≠ 0) or A = 0.6 (∆n = 0), B = C = 0, D = 0.28 for allowed transitions, A = 0.15, B = C = D = 0 for forbidden monopole or quadrupole transitions and A = B = D = 0, C = 0.1 for spin-exchange transitions.

The excitation rate of an energy level of an ion is given by,

$$\frac{dN_u}{dt} = N_e N_z R_{zu} \qquad (12)$$

where,

N_e is the electron density.

N_z is the fractional density of the ion of charge z

R_{zu} is the electron impact excitation rate coefficient of the state of ion of charge z.

The excited states in the plasma are dexcited by radiative transitions. Therefore we may write,

$$\frac{dN_u}{dt} = \frac{-N_u}{\tau} \qquad (13)$$

where τ is the radiative life time of the state.

When the plasma is in steady state the excitation rate of a state would be equal to dexcitation rate. Therefore, Rate of excitation is equal to Rate of dexcitation. The energy states of the ions dexcite only because of the radiative decay and therefore, Rate of excitation is equal to Rate of dexcitation by radiative decay.

In other words, we can write, Rate of excitation is directly proportional to Rate of photon emission. Also, Rate of excitation is directly proportional to Intensity of radiation.

Thus, Intensity of radiation is directly proportional to Rate of photon emission and Rate of excitation of the energy states.

5. THE EXCITATION RATE COEFFICIENTS

Excitation Rate Coefficients are useful in computing the contribution functions of various spectral lines. In present work, to study the excitation rate coefficient, we have computed excitation rate coefficient of Fe XVI using Bretons formula [1] as a function of electron temperature and presented graphically in figures (1).
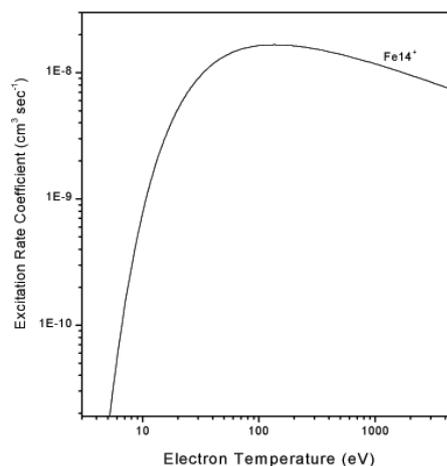

Fig. 1 *Excitation Rate Coefficient Of Iron Ions As A Function Of Electron Temperature.*

From above graph it observes that, the excitation rate coefficient (ERC) is very sensitive function of the electron temperature before it reaches its peak value but the variation of the function becomes very slow varying function of electron temperature near its saturation value.

6. FRACTIONAL ABUNDANCE

Plasma consists of the electrons and the ions with different charges. The collision between the atoms, ions of different charges and electrons results in ionization. At the same time the ions may capture the electrons and results in formation of ions of lower charge. The ionization and Recombination processes compete each other so that the ionization rate and recombination rate reach, each to

a certain value and equilibrium is attained. As long as the electron temperature is not changed the equilibrium remains in a particular state. A change in electron temperature results in changing the densities of ions and electrons. Thus densities of ions and electrons are completely dictated by the electron temperature. The plasma emission depends upon the fraction of total density of species remaining in a particular ionized state, the electron density and the electron temperature.

The amount of the fraction of the total density of species remaining in a particular ionized state is called as fractional abundance of that ion.

Equation for the time rate of change of population density of ion of charge z can be written as,

$$\frac{dN_z}{dt} = n_e \left\{ -N_z S_z + N_{z-1} S_{z-1} - N_z\ \alpha_z + N_{z+1}\ \alpha_{z+1} \right\} \quad (14)$$

where z takes all values between 0 and maximum charge on the ion.

The ionization state of each element of atomic number z is controlled by electron impact ionization (including autoionization) from state $z \rightarrow z+1$ with total rate coefficient $S_{z,z}$ ($cm^3\ sec^{-1}$) and radiative plus dielectronic recombination $z+1 \rightarrow z$ with rate coefficient $\alpha_{z,z+1}$ ($cm^3\ sec^{-1}$)

In steady state, the time rate of change of population density of ion of charge z will be zero.

In steady state condition, where the time rate change of population density of ion of charge z will be zero, the equation (14) reduces to,

$$N_z\ \alpha_z = N_{z+1}\ \alpha_{z+1} \quad (15)$$

The population density ratio ($N_{z,z+1}/N_{z,z}$) of two adjacent ion stages $Z^{+(z+1)}$ and Z^{+z} can be derived by using steady state equation (15).

$$\frac{N_{z+1}}{N_z} = \frac{S_z}{\alpha_{z+1}} \quad (16)$$

where $S_{(z)}$ is ionization rate coefficient of ion of charge z. α_{z+1} is recombination rate coefficient of ion of charge z+1. N_z and N_{z+1} are densities of ion with charge z and z+1 respectively.

6.1 EXPRESSION FOR FRACTIONAL ABUNDANCE

Thus, population density ratio ($N_{z,z+1} / N_{z,z}$) can be evaluated in terms of S_z and α_{z+1}. As the values of S_z and α_{z+1} are fully determined by the electron temperature. Therefore the fractional abundance and population density of any ion in the plasma depends only on the electron temperature. The fractional abundance of a Fe XV species in the tokamak plasma is evaluated by using equation (16) and the procedure followed by [4] is considered to get formula for Fractional abundance.

The fractional abundance of an ion of charge z can be written as,

$$F_z = \frac{N_z}{\sum_{z'} N_{z'}} \quad (17)$$

Where F_z, the fractional abundance of ion of charge z. N_z, the density of ion with charge z. The sum runs over all possible ionized states.

To study the behavior of Fractional abundance of Fe XV, using equation (17) as a function of electron temperature is computed and presented graphically in figure (2) as a function of electron temperature.

At lower electron temperature, the fractional abundance curves are non-linear. As a electron temperature increases, the fractional abundance

increases quite linearly. But as we reach towards the peak, the rise in fractional abundance becomes slightly non-linear. The fractional abundance decreases non-linearly near the peak of the curve and further if electron temperature increases the fractional abundance decreases almost linearly up to certain electron temperature. As electron temperature increases further, the fall in fractional abundance becomes non-linear and approaches to zero.
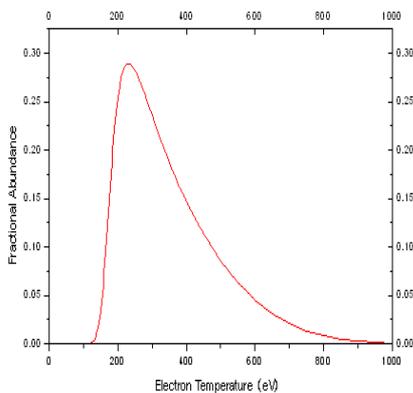

Fig. 2 *Fractional Abundance of Fe XV as function of electron temperature*

7. THE CONTRIBUTION FUNCTION

The contribution function is an electron temperature dependent part of the flux emitted by a spectral line and it is a measure of spectral line intensity because, spectral line intensity is proportional to their contribution function. The contribution function can be defined as the product of fractional ion abundance and the excitation rate coefficient of the upper state of the transition emitting the spectral line in consideration. The equation for contribution function can be written as,

$$C(z) = N_z \ R_{zu} \qquad (18)$$

Where N_z is the fractional density of the ion of charge z and R_{zu} is the electron impact excitation rate coefficient of the state u of ion of charge z

8. RESULTS AND DISCUSSION

We have computed contribution function C(z) by taking product of

fractional abundance N_z of ion of charge z and electron impact excitation rate coefficient R_{zu} of the state u of ion of charge z for few spectral line ($\lambda = 340$ A^o) for Fe XVI.

The contribution function of ion in consideration rises almost linearly up to its peak value as electron temperature rises. As the electron temperature increases above the electron temperature where contribution function becomes maximum, the contribution function decreases linearly up to the electron temperature at which contribution function is about 60% of its peak value. For further increase in electron temperature the contribution function decreases non-linearly and non-linearity in curves increases as electron temperature rises for higher values.

As we know that, contribution function depends upon fractional ion abundance, excitation rate coefficient and electron temperature. Fractional ion abundance and excitation rate coefficient is a function of electron temperature. We have studied, the variation in fractional ion abundance, excitation rate coefficient and contribution function of spectral line ($\lambda = 340$ A^o) of Fe XVI ion as a function of electron temperature and the results are displayed in figure (3).
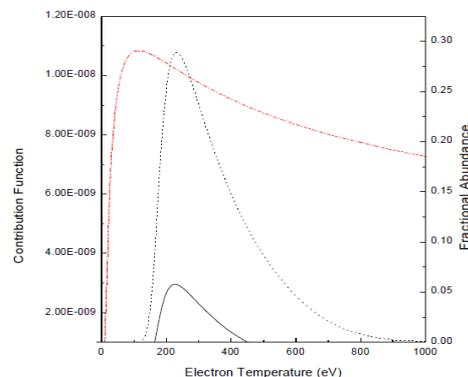

Fig. 3 *Fractional Abundance (dotted curve), Excitation Rate Coefficient (dash dot curve) And Contribution Function (solid curve) of Spectral Line ($\lambda = 340$ A^o) For Fe XVI Ion.*

The nature of curve shows that, while excitation rate coefficient is approaching to its peak value, the fractional ion abundance start showing its existence. The excitation rate coefficient reaches a saturation and changes very slowly with electron temperature. It means that the fractional ion abundance is a very slowly varying function of electron temperature until the excitation rate coefficient reaches to its peak value. During this range of temperature where fractional ion abundance is slowly varying function of electron temperature, the fractional ion abundance is very small, so contribution function is also very small. While the excitation rate coefficient starts to fall after reaching its peak, it becomes very slow varying function of electron temperature in the electron temperature range 125 eV to 1000 eV. During this range of electron temperature fractional ion abundance is very sensitive to changes in electron temperature. In the range of electron temperature 125 eV to 1000 eV the ERC is a very slow varying function of electron temperature where fractional ion abundance is very sensitive function of electron temperature. So, the contribution function is very less dependent on excitation rate coefficient and fully dependent on fractional ion abundance. Thus, the fractional ion abundance only dictates the shape of the contribution function curve.

To compare the contribution function curve with fractional ion abundance, we have plotted the dotted curve by multiplying fractional ion abundance of Fe XVI by 3.6 and compared with contribution function curve (solid curve) of same ion in figure (4). From figure we may see that the dotted curve and solid curve have almost same nature.
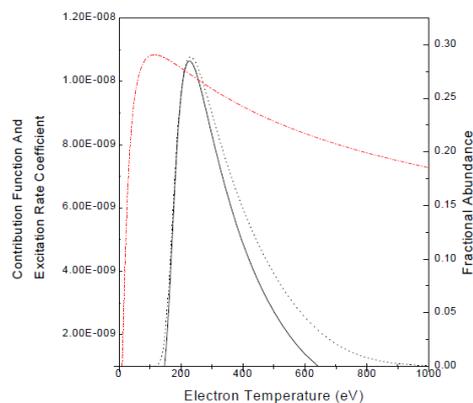

Fig. 4 *Fractional Abundance (dotted curve) is compared with contribution function multiplied by 3.6 (solid curve) of spectral line (λ =340 Ao) for Fe XVI Ion. Dash dot curve represents the Excitation Rate Coefficient of Fe XVI ion.*

9. CONCLUSION

The contribution function is very less dependent on excitation rate coefficient and fully dependent on fractional ion abundance. Thus, the fractional ion abundance only dictates the shape of the contribution function curve.

10. REFERENCES

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