Ionization Rate Coefficients of different ionic species in Copper Vapor Laser as a function electron temperature

[1]Dr Keshatti S N,[2]Dr Chawhan A G ,
[1,2]Associate Professor,
[1] Department of Physics, Shri Shivaji College, Parbhani
[2] Department of Physics, LBS College,Dharmabad Dist.Nanded

Abstract : In the present work Ionization rate Coefficients of different ionic species like helium, neon and copper have been obtained by using widely used formulae proposed by Lotz as a function of electron temperature. The knowledge of ionization potential of different ionic species is necessary for a given laser discharge. The discharge is generally characterized by the values of electron temperature, electron density, ion temperature, ion density and the types of particles which are ionized.

***Key Words* - collision, ionization, Ionization rate Coefficient, charge transfer, electron temperature**

I. INTRODUCTION

The CVL discharge consists of electrons, ions of helium (neon) and copper having different densities depending upon the electron temperature. These atoms, ions and electron undergo collision among themselves and with walls of the discharge tube. The collision between these elements results in increase or decrease of their charge unity. When the ions of charge z are produce from the ions of charge z-1, the process is called as Ionization. When ions of charge z are produced from ions of charge z+1, the process is called as recombination. Many times collision between these particles changes the energy of the colliding particles. Such type of collision might causes excitation of the particles. At the operating conditions, the total density of inert gas atoms or ions is of the order of $10^{17}/cm^3$ [1, 2]. The electron density is of the order of $10^{13}/cm^3$ [3] and the density of copper is of the order of $10^{13}/cm^3$. Among all gas lasers the collision frequency [4] between the heavy particles is high in CVL as the operating temperature is about 1400 ^{0}C much more than other laser discharge.

Ionization processes

In CVL discharge tube the inert gas particles are ionized by electron impact ionization or by collision with metastable state and singly ionized helium or neon. The ionization may take place by the process of autoionization and photoionization. All these ionization process are discussed as below.

The ionization process of Helium

Electron Impact Ionization (EII)

He I + e ------He II* + e + e

He II + e -----He III* +e + e

Photo ionization

HeI + hv ------ He II + e

HeII + hv ------ He III + e

Autoionization

Since there only two electrons in the outer most orbit of helium atom and there is no electron in the inner orbit, thus autoionization process need not be considered.

The ionization process of Neon

Electron Impact Ionization

Ne I + e ------Ne II* + e + e

Ne II + e -----Ne III* + e + e

Photo ionization

NeI + hv ------ -Ne II + e

NeII + hv ------ Ne III + e

Autoionization

NeI** ------ -Ne II* + e

NeII **------ Ne III* + e

The ionization process of Copper

Electron Impact Ionization

Cu I + e ------Cu II* + e + e

Cu II + e -----Cu III* + e + e

Photo ionization

CuI + hv ------ -Cu II + e

CuII + hv ------ Cu III + e
Autoionization
CuI^{**} ------ -Cu II^{*} + e
CuII **------ Cu III^{*} + e
The EII process may produce ions either in the ground or excited state. The stars on the species indicates the number of electrons in the excited state

The Penning reaction

There is an important class of inelastic collisions between heavy atoms or ions and helium atoms in excited states where potential energy of helium atom is transferred to atom and therefore the atom may get excited to upper state or may get ionized. Such a process is made more probable if the excited helium atom is in a metastable state and has longer lifetime within which it undergoes effective collision. The process is then known as penning effect. This process of transfer of energy is called as Penning transfer.

The inert gas atoms in the triplet metastable state like in case of He-Cd^{+} laser [1,2,3,6] may transfer their energy to the copper atoms in the ground state and ionize them as follow
He I^{*} + Cu I --------- He I + Cu II^{*} + e
Ne I^{*} + Cu I --------- Ne I + Cu II^{*} + e

The Duffenduck reaction (Charge transfer)

An ion in ground state collides with another ion or atom and transfers its energy to the colliding partner. In the process of collision energy as well as the charge is transferred from one ion to another ion or atom. This process is called as Duffenduck reaction. In this process the inert gas ions transfers their energy to copper atoms and ionize them. The copper ions produced may be either in the ground or excited state.
He II + Cu I ------------ Cu II* + He I
Ne II + Cu I ------------ Cu II* + He I
The process of penning reaction and charge transfer reaction do not produce ionization of any other species of copper.

Penning ionization rate and rate coefficient

The rate of production of CuII ions by penning process depends upon the density of neutral copper, density of helium metastable states and penning transfer coefficient P. The ionization rate by penning process can be expressed as

$$\frac{dN_{CuII}}{dt} = N_{CuI} * N_{He} * P$$

where Penning reaction rate coefficient is dictated by gas temperature, gas density and reaction cross section. The gas temperature governs the effective number of collisions between helium and copper atoms. The velocity of helium may be treated as an effective velocity. The rate coefficient P, the reaction cross section σ_p and the thermal velocity vHe are related as
P = < vHe σ_p >

The ionization rate coefficient can be expressed in terms of energy of helium atoms, the gas temperature θ in eV and the reaction cross section σ_p as

$$P= \frac{6.7*10^7}{86(\theta)^{3/2}} \int_0^\infty \sigma_p \; E \exp(-E/\theta)\, dE \ cm^3/sec$$

where E is the energy helium atom expressed in eV.
The penning excitation cross section σ_p is independent of the velocity colliding helium atoms [5]. And thus can be taken out of integration and we write

$$P = \frac{7.79 * 10^5}{\theta^{3/2}} \; \sigma_p \int_0^\infty E exp(-{}^{E}/_{\theta}) dE \; {}^{cm^3}/_{sec}$$

The above integral is a standard integral and substituting its value from standard integral table [14], the above equation reduces to

$$P = \frac{7.79*10^5}{\theta^{3/2}} \sigma_p \frac{1!}{(\frac{1}{\theta})^2}$$

$$P = 7.79 * 10^5 \sigma_p \, \theta^{1/2} cm^3 sec^{-1}$$

In the above equation gas temperature is expressed in eV. If it is to be expressed in degree Kelvin, then above equation becomes

$$P = 7.23 * 10^3 \sigma_p \, \theta^{1/2} cm^3 sec^{-1}$$

The Penning reaction cross section is assumed to be independent of velocity of helium atoms

Duffenduck ionization rate and rate coefficient

The rate of production of copper ions (CuII) by Duffenduck reaction depends upon the density of copper atoms, helium ion density and rate coefficient T of Duffenduck process. Rate of ionization of Duffenduck process is expressed as

$$\frac{dN_{CuII}}{dt} = N_{HeII} N_{CuI} T$$

The rate coefficient of Duffenduck reaction is expressed as
T = < vHe σ_T >
where vHe is thermal velocity of helium atoms relative to copper atoms and σ_T is charge transfer cross section.
The Duffenduck ionization rate coefficient can be expressed in terms of energy of helium atoms, the gas temperature θ in eV and the reaction cross section σ_T as

T= $\frac{6.7*10^7}{86(\theta)^{3/2}}\int_0^\infty \sigma_T\ E$ exp(-E/θ) dE cm³/sec

Charge transfer cross section also does not depend upon the velocity of colliding particles. Thus the Duffenduck reaction rate coefficient has the same form as the Penning reaction rate coefficient.

$T = 7.23 * 10^3 \sigma_T\, \theta^{1/2} cm^3 sec^{-1}$

Where θ is temperature in degree Kelvin.

Electron Impact Ionization

An astrophysist Seaton [12, 13] developed theory for obtaining fractional abundance of ions in order to study the spectral emission of solar corona. He proposed the equation for ionizations and recombination rate coefficients and hence the fractional abundances of ionic species. The equation proposed by him for obtaining ionizations rate coefficient depends upon ionization potential I and the electron temperature T is written as

$$S = 2.0 * 10^{-8}\left(J/_{I^2}\right) T^{1/2} 10^{-5040(\frac{I}{T})cm^3 sec^{-1}}$$

where J is the number of electrons in the outer most shell from where ionization takes place, I is ionization potential in eV and T is the electron temperature in degrees Kelvin.

But it is believed that this formula gives spurious results and hence mat not be considered for calculations of ionizations rate coefficient.

The electron impact ionization rate coefficient S_z is a function of electron velocity distribution, electron energies and electron impact ionization cross section σ_z. Mathematically it is expressed as

$S_z = < v_e\, \sigma_z >$

It is clear that S_z can be computed if ionization cross-section σ_z and velocity distribution of the discharge electron v_e is known

Wilson and White proposed [8] an empirical equation for the calculation of ionization rate coefficient, which is expressed as

$$S = J\,\frac{0.9 * 10^{-5}}{X^{\frac{3}{2}}} * \frac{\left(kTe^{1/2}/_{\chi^{1/2}}\right)}{\left(4.88 + \frac{kT_e}{\chi}\right)} \exp\left(\frac{-\chi}{kT_e}\right) cm^3/sec$$

Where χ is ionization potential in eV, T_e is electron temperature in degree Kelvin and J is the number of electron in the outer most orbits with same quantum number.

Lotz [9,10,11] also proposed a semi empirical formula for the calculation of ionization rate coefficient which is expressed as

$$\sigma = \sum_i a_i \chi_i \frac{(ln\, E/_{P_i})}{(Ep_i)}[1 - b_i] exp\left\{-c_i\left(E/_{P_i}\right) - 1\}\right] cm^2$$

Where E is the energy of the electron, P_i is the binding energy of the electron which is to be removed and χ_i is the number of the electrons in the i[th] sub shell. The constants a_i, b_i and c_i can be determined using experimental results. When the energy E of the colliding electron is very near to Pi, the factor E/Pi≈1. Hence

$$\sigma = \sum_i a_i \chi_i \frac{ln\left(E/_{P_i}\right)}{EP_i}[1 - bi] cm^2$$

For the electron energy very high compared to P_i, the factor E/P_i <<1 and thus above equation get modified to

$$\sigma = \sum_i a_i \chi_i \frac{ln\left(E/_{P_i}\right)}{EP_i}$$

This derivation of rate coefficient from cross section depends upon electron velocity distribution.

Kushner [3] is of the opinion that electron energy distribution in the CVL discharge is Maxwellian velocity distribution. The density of the electrons having energy range between E and E+dE which follow the Maxwellian distribution function is given by

$$\frac{dn}{n} = \left(2/_{kT}\right)\left(E^{1/2}/_{\pi k T^{1/2}}\right) exp(-E/kT) dE$$

Where n is the electron density and is the electron temperature in eV.

Assuming Maxwellian velocity distribution the electron impact ionization rate coefficient using Lotz cross section is obtained by equation

$$S_z = 6.7 * 10^7 \sum_{i=1}^{N}\left(a_i\chi_i/T_e^{3/2}\right)\left\{\frac{1}{p_i/T_e}\int_{p_i/_{T_e}}^{\chi}\frac{e^{-x}}{x}dx - \frac{b_i exp(c_i)}{\left[\frac{p_i}{T_e} + c_i\right]}\int_{\left(\frac{p_i}{T_e}+c_i\right)}^{\chi}\frac{e^{-y}}{y}\right\} cm^3 sec^{-1}$$

Where T_e is the electron temperature in eV, p_i is the ionization energy in eV of the electrons in the i[th] sub shell of the ion charge z and χ is the number of electrons in the sub shell.

The lower limit of the integration goes on changing as the electron temperature and ionization potential changes. The contribution of the second term may be neglected in comparison with the first term as the values of the constants b_i and c_i are very small. Thus the expression for the electron impact ionization can be modified to

$$S_z = 6.7 * 10^7 \sum_{i=1}^{N} \left(a_i \chi_i / T_e^{3/2}\right) \left\{ \frac{1}{p_i/T_e} \int_{p_i/_{T_e}}^{\chi} \frac{e^{-x}}{x} dx \right\} cm^3 sec^{-1}$$

II. RESULTS AND DISCUSSION

We have calculated penning ionization rate coefficient P as a function of gas temperature θ. The maximum value of θ is taken as 2000 ^{0}K as the operating temperature of the CVL is 1400 ^{0}C [7]. For the calculations of penning reaction rate coefficient the metastable density is considered as $5x10^{12}$ cm-^{3}. The equation for penning reaction rate coefficient shows that as the gas temperature is increased the penning reaction rate coefficient increases. It also increases as the density of copper atoms in the ground state increases. The behavior is as shown in fig 1.

We have calculated charge transfer rate coefficient as a function of gas temperature. The behavior is as shown in fig 2. The behavior of charge transfer rate coefficient is same as that shown in fig 1 except dividing factor 2. The electron density in the discharge is of the order of 10^{13} cm^{-3} [2] for the optimum conditions of the laser operation. Obviously the density of helium ions and copper atoms should not exceed 10^{13} cm^{-3}. The density of helium ions is less than 10^{13} cm^{-3}. This indicates that the Duffenduck rate is less than penning rate by a factor of 2.

We have calculated ionization rate coefficient for HeI and HeII as a function of electron temperature for the electron temperature ranging from 0 to 10 eV by using Lotz formula and the results are displayed in figure 3. The ionization of HeI starts from T = 1. 5 eV and goes on increasing up to T= 4 eV. Above this electron temperature the ionization rate gets saturated. The ionization of HeII starts at about T=4.5 eV and it increases as the electron temperature is increased up to 6 eV. For the electron temperature higher than 6 eV the ionization rate get saturated.

The ionization rate coefficient for CuI, CuII and CuIII are obtained using Lotz formula as a function of electron temperature. The results are displayed in figure 4. In computations of ionization of CuI, CuII and CuIII the removal of 3d electron is also considered in addition to the removal of 4s electron. The contribution of removal of 3p electron is not considered as they are tightly bounded and the probability of their removal is also very small. The ionization of CuI starts from electron temperature 0.5 eV and increases up to 2.5 eV. When the temperature is increased above 2.5 eV the increase in the rate of ionization decreases. The ionization of CuII starts at about 1.5 eV and go on increasing up to 5 eV. Above this temperature rate of increase of this coefficient becomes less and starts saturating for higher temperatures. The ionization of CuIII starts at about T= 3 eV and increases as electron temperature is increased. The rate coefficient gets saturated at temperatures more than 9 eV.

We have calculated ionization rate coefficient for NeI and NeII as a function of electron temperature and the results are displayed in figure 5. The behavior of rate coefficient as analogous to the behavior of He and Cu.

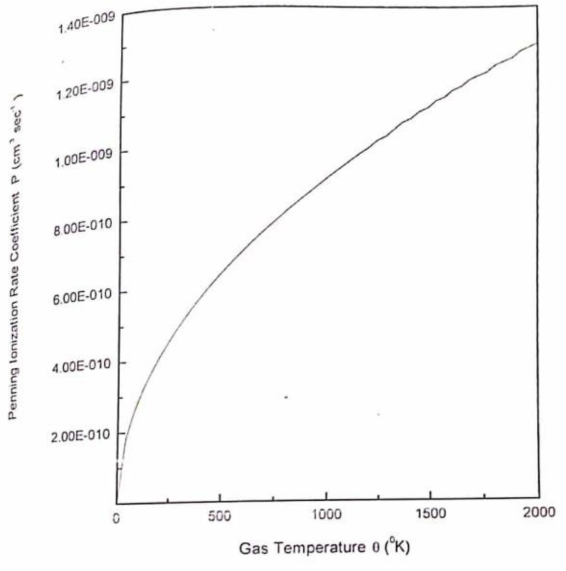

Fig.1 Penning Ionization rate coefficient P
As a function of gas temperature Ɵ

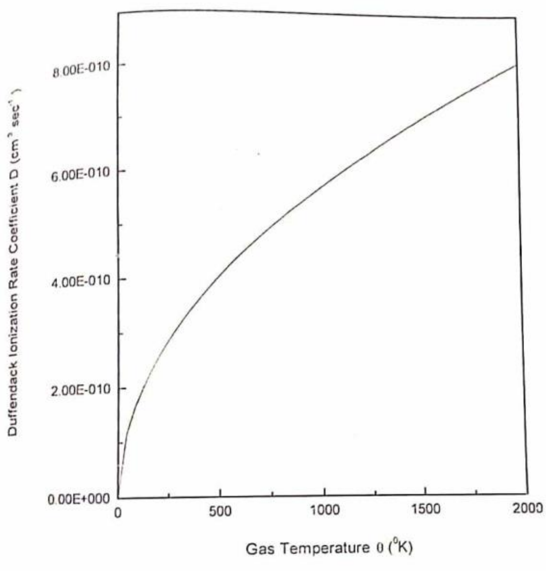

Fig2.Duffendack Ionization Rate Coefficient D
As a function of gas temperature Ɵ

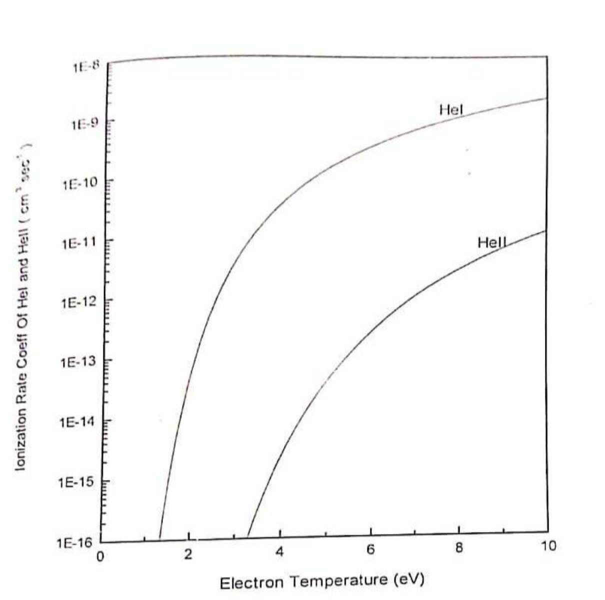

Fig.3.Electron Impact Ionization rate Coff of He I And He II as a function of electron temperature

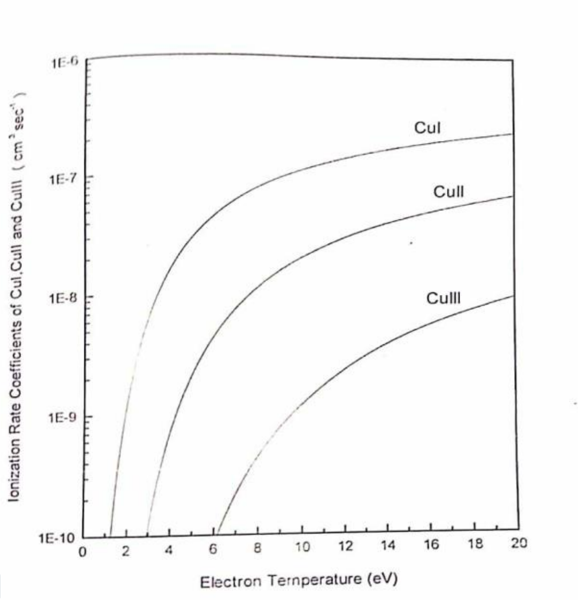

Fig.4. Electron Impact Ionization rate Coefficient of Cu I, Cu II And Cu III as function of Electron temperature

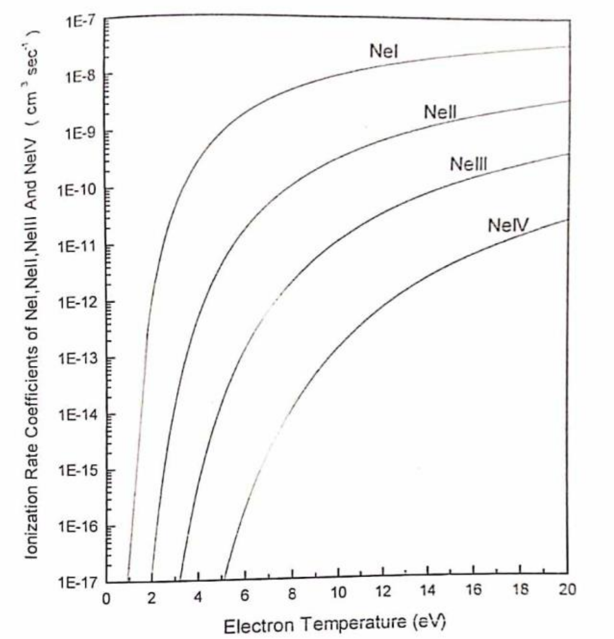

Fig.5 Electron Impact ionization Rate Cofficient of Ne I, Ne II , Ne III and Ne Iv as function of electron temperature

REFERENCES

[1] P G Browne and M H Dunn J Phys B : At mol phys, Vol 6, pp 1103-17 (1973)
[2] T Goto, Y Shimizu, S Hatttoti and T Sakurai J phys D: Appl phys, Vol 16 pp 261-68 (1983)
[3] M J Kushnar J Quantumm Electronics, Vol QE-17, No 8, pp 1555-65 (1983)
[4] W T Silfvast Appl Phys. Lett 15, pp 23, (1979)
[5] P Gill and C E Webb J Phys D: Appl Phys, Vol II, pp 245-55 (1978)
[6] A L Mckenzie J phys B : Atom and Mol phys, Vol 10, No 10 pp 2023-33
[7] T W Alger and W L Bennet Rev Sci Instrum, vol 53, pp762 (1982)
[8] Wilson and WhiteUnpublished
[9] W Lotz J Optical society of America, Vol 57, pp 873 (1967)
[10] W Lotz J Optical society of America, Vol 58, pp 915 (1968)
[11] W Lotz Z Physik, Vol 216, pp 241 (1968)
[12] M J Seaton Planet Space Sci, Vol 12, pp 55 (1964)
[13] M J Seaton Mon Not R Astro Soci, Vol 119 pp 81, (1959)
[14] B O Pierce: Revised by Ronald M FosterA short table on Integrals, fourth edition (1986)