BACHELOR PROJECT

Modeling the ionization and recombination of oxygen in supernova remnants and applying this to tin droplets in nanometer laboratory setting

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Contents

1 Introduction

With the rise of computers, microchips became an important part of our lives. Our mobile phones would not be possible without the advances in the production of every smaller microchips. One of the biggest companys in this industry is ASML, a company that makes the machines that used in the production of microchips. The newest machine uses extreme ultraviolet light to make imprints on silicon plagues, which are called wafers. ASML Extreme Ultraviolet (EUV) machines are on the forefront of development in the microchip making industry. In this machine, tin is used to create a very short wavelength and energetic UV light of $13.5nm$. In order to achieve this, the tin is hit by two laser pulses. The first low energetic pulse causes the tin to form a disk-like target. Secondly, this disk is hit by a more powerful pulse $(\lambda = 10.6\mu m)$ that causes the tin to become a plasma. This plasma sends out the extreme UV light while the tin ionizes and recombines. This specific wavelength of tin can be attributed to specific ions of tin, the $Sn^{11+} - Sn^{15+}$ [1] tin, which are between 11 and 15 times ionized tin. An ion is an atom that lost at least one of its electrons, this tin lost between 11 and 15 of its initial electrons to produce this light.
After the tin produced the extreme UV, the tin needs to be captured because excess tin can collect on the first mirror, otherwise the power of the machine will gradually reduce. Currently, this is done by pumping hydrogen gas through the reaction chamber, however by understanding the charge-state characteristics a new method can be researched.
In laboratory setting at ARCNL this process is reproduced with an instrument that can measure what kind of tin charge-state after the laser pulses. Ions are charged because of the lost electrons. A specific ion could also be called charge-state.The measured charge-state can be seen in figure1.

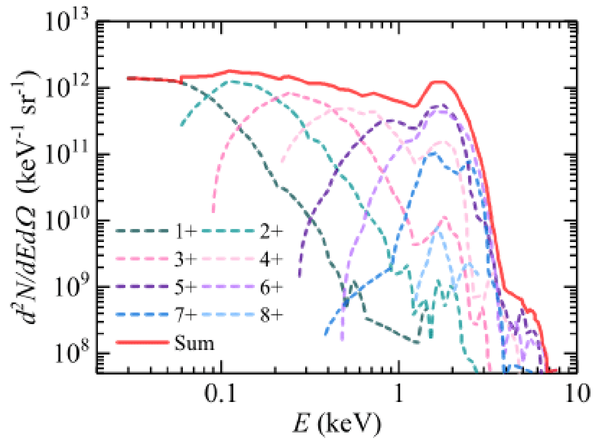

Figure 1: Experimental measurements of the tin charge-state distribution of the number of ions over the kinetic energy at the detector is shown. The total energy distribution is the sum of all the individual charge-states, which is shown in red. The individual charge-state resolved ion with kinetic energy distribution are the dashed lines. These charge states are shown for $Sn^{1+} - Sn^{8+}$.Figure taken from[1]

This figure shows that the majority of the measured charge-state is $Sn^{5+} - Sn^{6+}$. The difference in charge density between the moment after the laser pulse and collection of the tin puzzles many researchers because the charge state density is lower than calculation of the recombination might suggest. In this pilot research, an astrophysics approach will be taken to this problem. In particular, plasma physics of supernova remnants will be studied to look for a possible link.

After a star with a mass at least 8 times the mass of our own sun has undergone the last stage of its life, it implodes under its own gravity, after which it explodes. This process leaves the outer envelope in space, after which it will get heated by multiple shockwaves. This is known as a supernova remnant. This influx of energy causes the remnant to ionize and recombine over a very long timescale. Supernova remnants are almost always out of ionization equilibrium. This means that inside the remnant, ionization and recombination processes are going on. Recombination is a process in which the ion captures an electron, by which it goes down in charge-state. This stage we call non-equilibrium ionization (NEI) because the remnant is not in equilibrium. After enough time has passed, the su-

pernova remnant enters a new stage, the stage of Collisional equilibrium ionization (CEI). This happens when the remnant has reached equilibrium in ionization and recombination. In this stage, the ion densities do not change with time.
In this research, a model is made for the NEI and CEI for oxygen, after which a relation will be studied for tin. Tin is a lot bigger with an atomic number of $Z = 50$ than oxygen with atomic number, $Z = 8$ thus a study in the Z dependence of the ionization and recombination will also be studied.

2 Theory

In this part, the important ionization and recombination processes are explained to understand the inner workings of the plasma in supernova remnants and the tin plasma. The different equilibrium will also be expanded further.

2.1 Supernovas

There are two main types of supernovas: core collapse and thermonuclear. In a thermonuclear supernova, a white dwarf accumulates enough matter from accretion of a stellar companion. This accretion raises its core temperature, which if hot enough, can start the fusion of carbon. This carbon fusion causes the white dwarf to undergo a runaway nuclear fusion. This reaction causes the white dwarf to explode.
The other type of supernova is the core collapse. This happens to stars on the main sequence with masses around 8 times of our sun. If the star has burned most of the available fuel, the pressure of the fusion reaction cannot support the gravity of the outer envelopes. This causes gravitational collapse of the star, after which a large explosion follows. This blast pushes the outer envelopes to speeds of $300kms^{-1}$. This is the remnant of the supernova.

2.2 Plasma

Plasma is a state of matter in which the matter is ionized, which means that at least one electron has been removed from the outer shell of the element.

There are different mechanics that can ionize elements: collisional ionization and autoionization excitation are considered in this research which will be explained in the next part. The ions in the plasma can recombine, in which an electron is captured, and the element becomes less ionized. In this research, only radiative recombination and dielectric recombination is considered, which will also be explained in later parts.

2.2.1 Collisional ionization

Collisional ionization or electron impact ionization can occur when a free electron passes the ion with sufficient energy, by which an electron from the ion will transition to a free state. This happens because of the coulomb interaction between the two electrons. It is possible to calculate the time in which the coulomb force interacts with the atom with:

$$\Delta t = \frac{2b}{v} \tag{1}$$

in which v is the speed of the free electron and b the impact parameter of the collision. In astrophysics, the rate of collisional ionization occurs in a plasma is derived from the Lotz formula for the cross-section for direct impact ionization from the ground state, which is given by

$$\sigma_{CI} = \pi a_o^2 \sum_{k=m}^{N} C_k \xi_k W(U_k) \left(\frac{E_H}{\chi_k}\right)^2 \frac{ln(U_k)}{U_k} \tag{2}$$

in which a_o is the radius of the element, the summation is over all the subshells of the element of the initial ion. C_k is a constant, ξ_m is the number of equivalent electrons in the shell. The function, $W(U) = 1 - b_m exp\left[-c_m(U-1)\right]$ which is only significant for low charge state or low temperature ions and is 1 for multiple ionised atoms, in this case $C_k = 2.76$. U_m is given by ionization energy of the ion with $U_m = E/\chi_m$. Formula 2 is then simplified to the collisional ionization equation found in[2] which is fitted to empirical data and then extrapolated. The coëfficient per ion state are tabulated in1. This equation is given by

$$S_{CI} = A_{col} T^{1/2} (1 + a_i \frac{T}{T_{col}})^{-1} exp(\frac{-T_{col}}{T}) \tag{3}$$

where

$$A_{col} = (1.3 * 10^{-8}) F \xi I_{ev}^{-2} \tag{4}$$

$kT_{col} = I$ is the ionization energy, F is the focusing factor which is of 1, ξ is the ionization energy and $a_i = 0.1$ in most cases.

2.2.2 Autoionization

In this process, the initial state is a double-excited ion, which most likely be the product of dielectronic recombination. This state can also be produced by two successive excitations. If the energy of both electron is above the ionization energy, one of the electrons can spontaneously ionize and become a free electron. Autoionization is important in ions with a large number of electrons in the first inner subshell in comparison with the upper shell. The autoionization rate from[2] is given by

$$S_{au} = A_{au} T^{-1/2} exp(\frac{-T_{au}}{T}) \tag{5}$$

with A_{au} and T_{au} the coëfficients for a specific ion state and T the temperature.
These factors are not tabulated in [2] because these are highly uncertain. Autoionization does not have a large effect on the total ionization if the temperature is near the temperature of maximum equilibrium abundance.** But non-equilibrium models would be effected if $kT > I$ with I being the ionization energy.

2.2.3 Radiative recombination

Radiative recombination occurs when a free electron with energy E gets captured by an ion. In this process, a photon is emitted. The emitted photon has absorbed energy of the ionization energy of the final configuration:

$$h\nu = \chi_n + E_e \tag{6}$$

This process is the inverse of the photoionization, in which a photon ionizes the atom. The connection between the two processes is the Milne relation. This relation expresses the capture cross-section between the two processes. The Milne relation is given by:

$$\frac{\sigma_{PI}}{\sigma_{RR}} = \frac{2mc^2 E_e}{h^2 \omega^2} \frac{w_{z+1}}{w_z} \tag{7}$$

where $E_e = h\omega - |E_{initial}|$ is the energy of the outgoing electron from photoionization and $\frac{w_{z+1}}{w_z}$ is the statistical weights of two equations. This relation is used to calculate recombination rates from photoionization data. The radiative recombination rate is obtained by integrating 7 over the velocity distribution. This gives the recombination rate for hydrogen-like ions by

$$\alpha_r = 5.197 \cdot 10^{-14} Z \lambda^{1/2} \left[0.4288 + 0.5 ln(\lambda) + 0.469 \lambda^{-1/3}\right] \tag{8}$$

with

$$\lambda = 157890 Z^2/T \tag{9}$$

This case is only applicable to hydrogen like neon with $z = 9$. To make it applicable to non-hydrogen ions [2] calculates the coëfficient for each ion state and the z dependence and tabulate them for all the charge states which gives

$$\alpha_r(T) = A_{rad}(\frac{T}{10^4 K})^{-\chi_{rad}} \tag{10}$$

with A_{rad} and χ_{rad} being coëfficients tabulated in 1

2.2.4 Dielectronic recombination

Dielectronic recombination is similar to autonization in the way that in both processes two electrons are needed, but dielectronic recombination needs one bound and one free electron. In dielectronic recombination, a free electron is captured by the ion and the excess energy from the free electron excites a bound electron. This is a resonance process because the electron orbits are discrete, which means that the incoming free electron will need a specific energy to excite the bound electron. This excited electron then radiative recombines, or it will autoionize. In the last case, the ion will not recombine. The dielectronic recombination rate thus depends on the ratio between the radiative recombination and the auto-ionization rates.

A Maxwellian electron distribution is a probability distribution of the energy of electrons. The dieletronic recombination rate, for a Maxwellian electron distribution, is given by

$$\alpha_{DR} \approx 6.55 \times 10^{-27} \left(\frac{T}{10^7 K}\right)^{-3/2} \sum_s B_s exp^{\frac{-E_s}{kT}} \tag{11}$$

with

$$B_s \equiv = \frac{w_s A_s^a A_s^r}{w_l(A_s^a + \sum A_s^r)} \tag{12}$$

in which the index s refers to the possible excitation states and with $w_s = 2l(l+1)$ is the statistical weight of the excited state.

The equation for dielectronic recombination11 is simplefied in[2] in which the coëfficients for each ion state are tabulated in 1. This equation is given by:

$$\alpha_{DR}(T) = A_{di}T^{-3/2}exp(-T_0/T) \times [1 + B_{di}exp(-T_1/T)] \tag{13}$$

2.3 Three body recombination

In hot and dense plasma three body recombination, or electron impact recombination, can occur. In this process, two free electrons enter the ion volume at the same time. One of the electrons is captured by the ion, while the other electron carries away the excess energy. This process is the inverse of the electron impact ionization or collisional ionization.

Fitting coëfficients

	ACOL	TCOL	ARAD	XRAD	ADI	BDI	T0	T1
O1	1.09E-10	158000	3.1E-13	0.678	0.00111	0.0925	175000	145000
O2	3.96E-11	407000	2E-12	0.646	0.00507	0.181	198000	335000
O3	1.67E-11	637000	5.1E-12	0.66	0.0148	0.305	241000	283000
O4	7.6E-12	898000	9.6E-12	0.67	0.0184	0.1	212000	283000
O5	3.33E-12	1320000	1.2E-11	0.779	0.00413	0.162	125000	227000
O6	1.15E-12	1600000	2.3E-11	0.802	0.106	0.34	6250000	1120000
O7	7.9E-14	8570000	4.1E-11	0.742	0.0623	0.304	7010000	1470000
O8	2.89E-14	10100000	2.62E-11	0.726	0	0	0	0

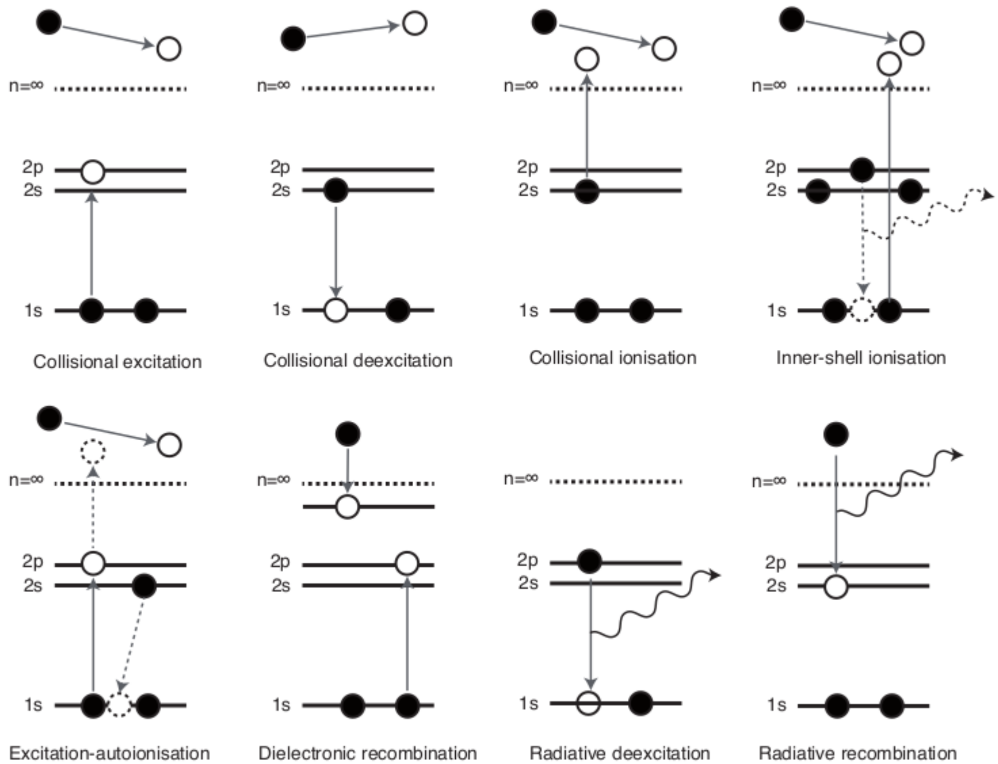

Figure 2: Schematics of some of the electron-ion recombination en ionization processes. The open circle is the state in which the electron ends up in most processes, except inner-shell ionization and excitation-autoionization. The last step in these processes is indicated by a dashed circle. Figure taken from Vink(2020)[3]

2.4 Collisional ionization equilibrium (CIE)

Very low density and optically thin plasmas are frequently in a steady state. Examples of steady state plasmas are supernova remnants and the plasmas found in the Tokamaks in a fusion reactor. One of the simplest forms of a steady state plasma is one in collisional ionization equilibrium. This means that the plasma is optically thin for its own radiation and that there is no external radiation that affect the balance of the ions. In this case, the recombination of one ion means that another ion ionizes. The first term in 15 is equal to zero and the population density of two adjoining ion states can then be formulated as

$$\frac{N_{z+1}}{N_z} = \frac{n_e S_z(T)}{n_e \alpha_{z+1}} = \frac{S_z(T)}{\alpha z + 1} \tag{14}$$

in which the S_z is the ionization rate of ion z and α_{z+1} is the recombination rate of ion $z + 1$.

2.5 Non-equilibrium ionization (NEI)

Supernova remnant plasma are almost always out of ionization equilibrium, which are also known as NEI. The plasmas are not in equilibrium because not enough time has passed since the supernova remnant was shocked. Besides, only a few ionizing collisions have occurred per ion. Plasmas of other objects like galaxies and cool stars are indicated as collisional ionization equilibrium or for short CIE. Different ion species are denoted as $n_{i,z}$ with z the ionization state and i an index to indicate a specific atom.

The differential equation which governs the ionization stages for a given electron temperature is given by

$$\frac{dn_{i,z}}{dt} = n_e \left\{\alpha_{i,z+1}\left(T_e\right) n_{i,z+1} + S_{i,z-1}(T_e) n_{i,z-1} - n_{i,z}\left[\alpha_{i,z}(T_e) + S_{i,z}\right]\right\} \tag{15}$$

with S_z and α_z being the ionization and recombination rate coefficients. The first two terms on the right-hand side are the gains to the ion density. The last term is the decrease in ion density due to recombination and ionization, making the adjacent ion densities higher. This system is a differential equation, since there are $Z + 1$ states it is a system of $Z + 1$ differential equations. The evolution of these equations are governed by the combination of time and the electron density, $n_e t$ instead of just t. This is because all the rates are proportional to the electron density. For this reason, $n_e t$ is taken as a singular parameter, which is also known as the ionization timescale or the ionization age.

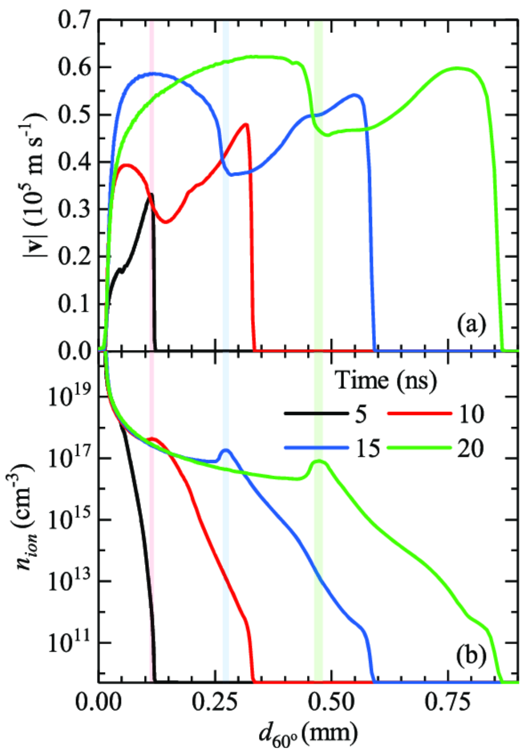

Figure 3: One dimensional outline of the speed (a) of the plasma during the laser pulse and subsequently during the plasma expansion in the instrument and the ion number density in (b) of the ions, at different laser pulse durations. Figure taken from [1]

2.6 Dimension analysis

If supernova remnants calculations and laboratory nanometer scale experiments have overlap, a dimension analysis needs to be made. In supernova remnants, the timescales of the plasma are usually given as $n_e t$ which is called the ionization age of the plasma. The electron density times the time, $n_e t$, in supernova remnants is in the range of $10^9 - 10^{13} cm^{-3} s$ [3].
To calculate the $n_e t$ of the tin plasma, the electron density and timescale is required. In figure 3 is shown how the ion density evolves over time during and after the main laser pulse. To calculate the electron density of the plasma this equation

$$n_e = z \times n_i on \tag{16}$$

was used, in which the z is equal to the median charge-state of the plasma which is estimated to be Sn^{13+} which is equal to a $z = 13$. In figure 3 it is shown that the n_{ion} is around $10^{17} - 10^{20}$ which makes the electron density $13 \times 10^{17} - 10^{20}$. The time over which the plasma evolves is around a few nanoseconds, this makes the $n_e t$ of the tin plasma around $1.3 \times 10^9 - 10^{12}$.

2.7 Isoelectronic sequencing

One approach to the lack of recombination and ionization coëfficients is to try an isoelectronic sequencing approach. Isoelectronic atoms are two atoms or ions that have the same electronic structure and the same number of electrons in their other electron shell. These atoms or ions typically have similar chemical properties. An isoelectronic sequence is a set of spectra that are produced by different elements, which are ionized in such a way that they have the same electronic buildup.

3 Methods

3.1 Approach

In order to produce 4 a Python script was programmed. The dielectronic 13 and radiative 10 rates are summed to one recombination rate per oxygen ion state.

3.2 Euler method

To solve the $z + 1$ coupled differential equation from15, the Euler method was chosen because it is a simple but accurate procedure. The Euler method is the simplest equation from the Runge-Kutta method, which is a numerical way to approximate exact solutions. For a given initial value problem,

$$\frac{dy}{dt} = f(t, y), y(t_0) = y_0 \tag{17}$$

where $f(t, y)$ is a well known function with known initial conditions, the next value for y_n is

$$y_{n+1} = y_n + hf(t_n, y_n) \tag{18}$$

with h the step size. The $f(t,y)$ is equal to the left-hand side of equation 15. To get the best approximation of the exact solution, h needs to be as small as possible. The error per step of the Euler method is proportional to the square of the step size.

3.3 Python model

3.3.1 CEI

3.3.2 NEI

4 Results

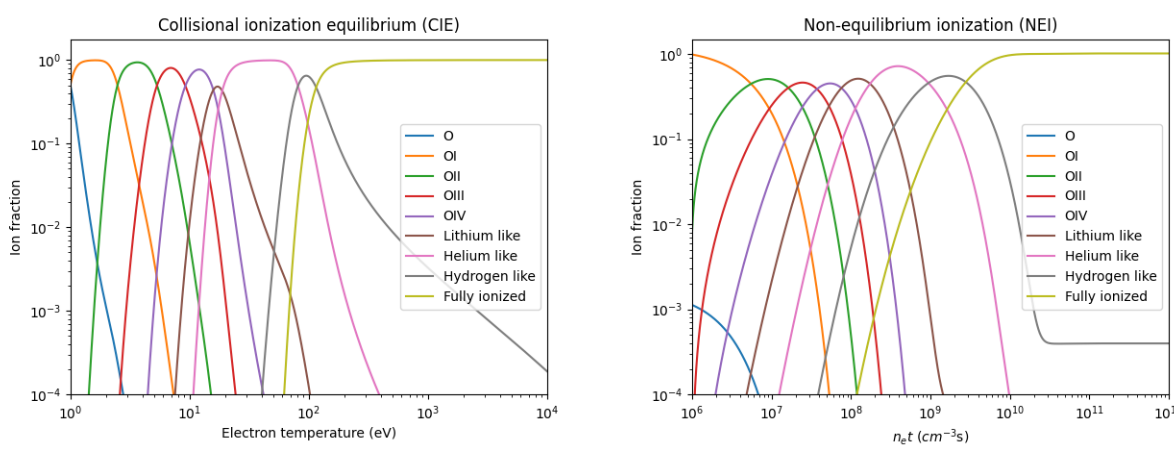

Figure 4: The effects of Collisional ionization equilibrium (CIE) and Non-equilibrium ionization (NEI) on oxygen. The left shows the fraction of each oxygen ion as a function of electron temperature for collisional ionization equilibrium. The right panel shows the ion fraction as function of ionization age, $n_e t$, for a fixed temperature of $kT_e = 1keV$, with initial conditions of $kT_e = 2eV$. The fractions were calculated using Python and the Non-equilibrium ionization is approximated with Euler method.

The first result is shown in figure 4 which is tthe result from the Python model for Collisional ionization equilibrium and the non-equilibrium ionization.

The ionization and recombination rates of different atoms were studied. One of the results is shown in 5. In this graph, neon and iron are considered because from the available data on atoms this was the set with the biggest Z difference. Iron seems to have a higher ionization and recombination rate than neon.

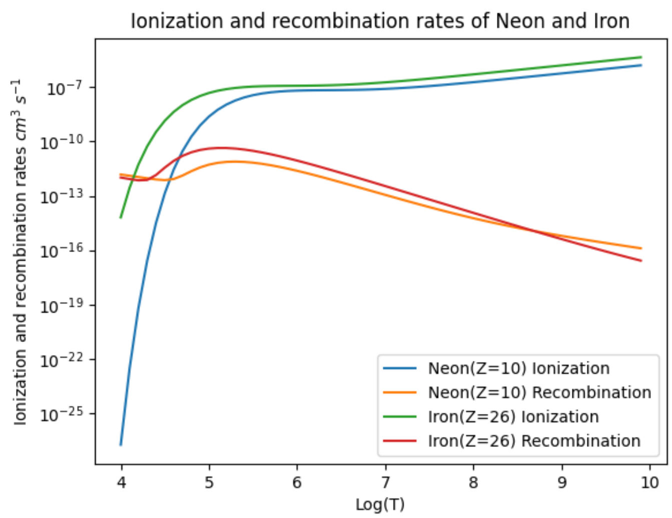

Figure 5: In this graph, the ionization and recombination rates are shown for neon and iron at specific temperatures, measured in $log(T)$

5 Discussion

There is a difference between the NEI 4 graph and the graph of NEI in [3]. It seems that the result ionizes quicker. This can be explained by several factors. In [3] SPEX was used, this is software made for calculations applied to supernova remnants, which is more up to date with the latest models on all the ionization and recombination processes.
The CEI plot seems to overlap better with the plot from [3]. The autoionization is left out in the tabulated data from [2] because these coëfficients would be too inaccurate. This probably does have an effect on the result. It is expected that without autoionization the NEI would have taken longer to become totally ionized, but the results in comparison with [3] would suggest otherwise.

The extrapolation to tin with the model is problematic. No source was found for tin recombination and ionization coëfficient which could be used in this model. Another method of getting these coëfficient was studied: isoelectronic sequencing. However, no sufficient material was found. One of the main concerns with this method would be the inaccuracy with the ionization. This because if iron (Z=26) and tin are compared (Z=50) the collisional ionization would be a lot lower for tin because the free electron need to be a lot more energetic to overcome the larger coulomb force of tin.

In figure 5 the ionization and recombination rate of neon and iron are plotted. It is shown that the iron has a higher ionization and recombination rate. But at, $log(T) = 8.7$ neon has a higher recombination rate. This figure is not enough to make a prediction if the recombination and ionization rate is dependent on the Z of the atom.

In follow-up research, a more detailed study in isoelectronic sequency which could potentially hold the recombination and ionization rates of tin.

6 Conclusion

As explained in section2.6, the dimension analysis suggest that the timescales and densities of supernova remnants and the that of tin in a laboratory setting are comparable. A model for collisional ionization equilibrium and non-equilibrium was made for oxygen, not for tin. This is mainly due to the lack of ionization and recombination rate coëfficients for tin.
No clear Z dependence of the ionization and recombination rates could be found in the data from [2]. This research did successfully produce a model made in Python for the collisional ionization equilibrium and the non-equilibrium ionization.

7 Acknowledgements

I want to thank Jacco Vink and John Sheil for coming up with an interesting and challenging project which combines two of my interest in physics, astrophysics and nano-lithography. I also want to thank Emanuele Greco and again John Sheil for daily supervising my project and being readily available for my questions and making suggestion on which way to go with this research.

8 References

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9 Appendix

9.1 Further results

Log(T)	O1	O2	O3	O4	O5	O6	O7	O8	O9
4	0.00	3.129	0	0	0	0	0	0	0
4.1	0.011	1.614	0	0	0	0	0	0	0
4.2	0.154	0.525	0	0	0	0	0	0	0
4.3	0.703	0.096	4.616	0	0	0	0	0	0
4.4	1.321	0.022	2.896	0	0	0	0	0	0
4.5	1.699	0.017	1.727	0	0	0	0	0	0
4.6	1.951	0.067	0.88	0	0	0	0	0	0
4.7	2.297	0.265	0.345	3.269	0	0	0	0	0
4.8	2.823	0.652	0.116	2.043	0	0	0	0	0
4.9	3.447	1.13	0.067	1.168	4.274	0	0	0	0
5	4.142	1.674	0.154	0.561	2.727	0	0	0	0
5.1	4.962	2.337	0.414	0.232	1.616	4.999	0	0	0
5.2	0	3.114	0.833	0.145	0.87	3.269	0	0	0
5.3	0	3.982	1.378	0.249	0.415	1.994	4.206	0	0
5.4	0	4.945	2.045	0.529	0.213	1.1	2.46	0	0
5.5	0	0	2.854	0.993	0.256	0.555	1.198	0	0
5.6	0	0	3.904	1.73	0.621	0.414	0.449	0	0
5.7	0	0	0	2.725	1.282	0.633	0.147	0	0
5.8	0	0	0	3.775	2.03	0.991	0.051	4.08	0
5.9	0	0	0	4.769	2.745	1.359	0.021	2.738	0
6	0	0	0	0	3.41	1.708	0.017	1.749	4.827
6.1	0	0	0	0	4.04	2.051	0.042	1.087	3.186
6.2	0	0	0	0	4.664	2.41	0.111	0.673	2.025
6.3	0	0	0	0	0	2.809	0.245	0.432	1.221
6.4	0	0	0	0	0	3.279	0.471	0.34	0.691
6.5	0	0	0	0	0	3.832	0.796	0.38	0.373
6.6	0	0	0	0	0	4.442	1.194	0.517	0.2
6.7	0	0	0	0	0	0	1.626	0.704	0.109
6.8	0	0	0	0	0	0	2.066	0.911	0.061
6.9	0	0	0	0	0	0	2.501	1.123	0.036
7	0	0	0	0	0	0	2.925	1.333	0.021

Table 2: This table shows the fraction of a specific charge-state at a specifc $log(T)$, the fraction is in the form $-log(N_i/N_{tot})$. These fractions are calculated from equations and tabulated coëfficients from[2] for oxygen.