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Determination of Thermal Conductivities and Gas Temperature Distribution for Gas Discharges in Ne and He mixtures with Hydrogen, Copper and Bromine

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Abstract. Thermal conductivities of binary gas systems are calculated on the base of 12-6 Lenard-Jones and rigid sphere inter-atomic interaction approximations for the case of gas discharges in Ne and He with small admixtures of hydrogen, copper and bromine. Assuming that the gas temperature varies only in the radial direction and using the calculated thermal conductivities, analytical solution of the steady-state heat conduction equation is found for two cases of uniform and non-uniform power input, respectively. For both cases the average gas temperature is found.

One of the main problems in plasma physics is to determine the characteristic constants for basic plasma processes, such as asymmetric charge transfer, Penning ionization, diffusion, heat conduction etc., which are fundamentally important and widely used in gaseous discharges, laser physics, plasma technologies, gas-discharge mass spectroscopy, absorption and emission spectroscopy, and plasma in general. It is well known that characteristic constants for the heavy particle interaction, including the above mentioned, depend on the gas temperature. In particular, in the metal vapour or metal halide lasers the thermal mode, i.e. the radial temperature distribution, are of great importance for the stability of the laser operation and for the achievement of high output laser parameters as well, because it controls not only laser level kinetics, but also the active particles concentration, i.e. particles on whose transition laser oscillation is obtained. Experimental technique for the gas temperature measurement, using spectral lines broadening, is definitely imprecise.

In order to obtain gas temperature distribution, the following steady-state heat conduction equation is solved:

$$\boldsymbol{div}.\left(\boldsymbol{k}\ \boldsymbol{gradT_g}\right)+\boldsymbol{q_v}=0 \qquad (1)$$

where $\boldsymbol{k}$ is the thermal conductivity, $\boldsymbol{T_g}$ is the gas temperature, and $\boldsymbol{q_v}$ is the power deposited into the discharge per unit volume. For our deep ultraviolet (DUV) Cu^+ laser the optimal value of $\boldsymbol{q_v}$ is 20 $W.cm^{-3}$. Assuming that the gas temperature varies only in the radial direction, equation (1) assumes the following form:

$$\frac{1}{\boldsymbol{r}}\frac{\boldsymbol{d}}{\boldsymbol{dr}}\left(\boldsymbol{rk}\frac{\boldsymbol{dT_g}}{\boldsymbol{dr}}\right)+\boldsymbol{q_v}=0 \qquad (2)$$

The dependence of thermal conductivity $\boldsymbol{k}$ of gases and gas mixtures on gas temperature is given, as in [1], by:

$$\boldsymbol{k}=\boldsymbol{B}\cdot\boldsymbol{T_g}^{\boldsymbol{a}} \qquad (3)$$

where $\boldsymbol{B}$ and $\boldsymbol{a}$ are constants (within a certain temperature range), which are specific for each gas or gas mixture. The constants $\boldsymbol{B}$ and $\boldsymbol{a}$ could be obtained through fitting the existing experimental data taken from [2]. Unfortunately, except for rare gases, data for the thermal conductivities of chemical elements of our interest are either very scarce in the literature or are within a narrow temperature range, which is not of interest. That is why, it is necessary to calculate thermal conductivities, in order to obtain gas temperature distribution via solving steady-state heat conduction equation. There are two widely used theoretical approaches for thermal conductivity determination – rigid, i.e. hard, sphere and 12-6 Lenard-Jones approximations, which consider different interaction between the particles. Following [3] the thermal $\boldsymbol{k_1}$ and $\boldsymbol{k_2}$ for the rigid sphere and 12-6 Lenard-Jones approximations are expressed as follow:

$$\boldsymbol{k}_1=0.083264\frac{\boldsymbol{T_g}^{\frac{1}{2}}}{\mu^{\frac{1}{2}}.\boldsymbol{d}^2} \qquad \boldsymbol{k}_2=0.083264\frac{\boldsymbol{T_g}^{\frac{1}{2}}}{\mu^{\frac{1}{2}}\cdot\sigma^2\cdot\Omega_{\boldsymbol{V}}\left(\frac{\boldsymbol{k_bT_g}}{\varepsilon_0}\right)} \qquad (4)$$

where μ is the particle mass in amu, $\boldsymbol{T_g}$ is the gas temperature in K, $\boldsymbol{d}$ is the rigid sphere diameter (sum of atomic radii of the interacting particles) in Å, σ is the inter-atomic distance in Å, at which the potential energy is zero, $\boldsymbol{\varepsilon_0}$ is potential well depth, $\boldsymbol{\Omega_V}$ is collision integral, which depends on the interaction potential. $\boldsymbol{\Omega_V}$ for rigid sphere model is unit, while for the Lenard-Jones potential the following expression is used: $\frac{1}{\Omega_{\boldsymbol{V}}}=0.697\left[1+0.323\ln\left(\frac{\boldsymbol{k_bT_g}}{\varepsilon_0}\right)\right]$.

Thermal conductivities of binary gas systems are calculated on the base of the empirical method of Brokaw [3] for the case of gas discharges in He (10 Torr) and Ne (20 Torr) with small admixtures of hydrogen (0.03 Torr), copper (0.3 Torr), and bromine (0.3 Torr), which are optimal pressures for the DUV Cu^+ laser operation.

The results for thermal conductivities are presented in table 1.

Table 1. ***B*** and ***a*** – constants, which are for ***k*** in $W.m^{-1}.K^{-1}$, determining thermal conductivity, RSph – Rigid Sphere approximation, L–J – Lenard – Jones approximation.

gas or gas mixture	***B*** (exp. fit)	***a*** (exp. fit)	***B*** (RSph)	***a*** (RSph)	***B*** (L–J)	***a*** (L–J)
Ne	$9.7x10^{-4}$	0.685	$38.3x10^{-4}$	0.500	$12.3x10^{-4}$	0.648
He	$34.9x10^{-4}$	0.670	$90.9x10^{-4}$	0.500	$46.2x10^{-4}$	0.626
H [800K, 1600K]	$4.4x10^{-4}$	1	$130x10^{-4}$	0.500	$31x10^{-4}$	0.649
H [1600K, 2600K]	$4.4x10^{-25}$	7.56				
Cu	-	-	$58.6x10^{-4}$	0.500	$0.9x10^{-4}$	0.982
Br	-	-	$3.3x10^{-4}$	0.500	$0.6x10^{-4}$	0.740
Ne-H [800K, 1600K]	$9.7x10^{-4}$	0.686	-	-	-	-
Ne-H [1600K, 2600K]	$5.9x10^{-4}$	0.753	-	-	-	-
Ne-Cu	-	-	$10.0x10^{-4}$	0.681	$9.4x10^{-4}$	0.689
Ne-Br	-	-	$9.8x10^{-4}$	0.683	$9.7x10^{-4}$	0.679
He-Cu	-	-	$35.4x10^{-4}$	0.666	$30.7x10^{-4}$	0.681
He-Br	-	-	$32.5x10^{-4}$	0.658	$29.0x10^{-4}$	0.675

One can easily draw dependence (3) of thermal conductivity $\boldsymbol{k}$ on gas temperature $\boldsymbol{T_g}$, in order to see the sufficiently fair agreement between experimental data fit and our calculations of thermal conductivity.

For a gas-discharge tube with radius $\boldsymbol{R}$ ($\boldsymbol{R}$ of 3.55 mm is optimal radius for the DUV Cu^+ laser) in a cylindrical geometry, considering the following boundary conditions $\boldsymbol{T_g}\big|_{\boldsymbol{r}=\boldsymbol{R}} = \boldsymbol{T_w}$ (experimentally measured optimal quartz tube temperature $\boldsymbol{T_w}$ is 830 K) and $\frac{d\boldsymbol{T_g}}{d\boldsymbol{r}}\big|_{\boldsymbol{r}=0} = 0$, the solution of the equation (2) is, as it is found in [1]:

$$\boldsymbol{T_g}(\boldsymbol{r}) = \left(\boldsymbol{T_w}^{1+\boldsymbol{a}} + \frac{1+\boldsymbol{a}}{4\boldsymbol{B}}\boldsymbol{q_v}\left(\boldsymbol{R}^2 - \boldsymbol{r}^2\right)\right)^{\frac{1}{1+\boldsymbol{a}}} \tag{5}$$

For calculation of characteristic constants, it is convenient to use the average gas temperature in the discharge zone, which is found by averaging (5) over the radius:

$$\langle \boldsymbol{T_g} \rangle = \frac{4\boldsymbol{B}}{(2+\boldsymbol{a})\cdot \boldsymbol{q_v}\boldsymbol{R}^2}\left(\boldsymbol{T}_0^{\,2+\boldsymbol{a}} - \boldsymbol{T_w}^{2+\boldsymbol{a}}\right) \tag{6}$$

where $\boldsymbol{T_0} = \boldsymbol{T_g}(\boldsymbol{r}=0)$.

Following [4], from $\boldsymbol{q_V} = \boldsymbol{j}.\boldsymbol{E}$ and $\boldsymbol{E}(\boldsymbol{r}) = \boldsymbol{E}_0.\boldsymbol{J}_0\left(\frac{2.4}{\boldsymbol{R}}\boldsymbol{r}\right)$, where $\boldsymbol{J}_0\left(\frac{2.4}{\boldsymbol{R}}\boldsymbol{r}\right)$ is the Bessel function of the first kind of zero order, one can obtain $\boldsymbol{q_V}(\boldsymbol{R}) = \boldsymbol{Q}_0.\left[\boldsymbol{J}_0\left(\frac{2.4}{\boldsymbol{R}}\boldsymbol{r}\right)\right]^2$, where the constant Q_0

remained to be obtained. In order to obtain analytical solution, a polynomial fit of the third degree is used instead of $[J_0(x)]^2$, i.e. $[J_0(x)]^2 \approx b + c.x + d.x^2 + e.x^3$, where $x = (2.4.r)/R$. Through fitting, the following values of ***a***, ***b***, ***c***, and ***d*** are obtained:

b = 1.005, c = -0.016, d = -0.5702, and e = 0.1687.

In this way, the following expression for $q_V(r) = Q_0 \cdot \left[b + c\frac{2.4}{R}r + d\left(\frac{2.4}{R}\right)^2 r^2 + e\left(\frac{2.4}{R}\right)^3 r^3 \right]$ is obtained. Comparing the areas, bounded between the functions $q_0 = constant$ and $q_V = q_V(r)$ and the variable axis r, the following expression for Q_0 is obtained:

$$Q_0 = \frac{q_0}{R\left(\frac{b}{2} + \frac{c}{3}2.4 + \frac{d}{4}2.4^2 + \frac{e}{5}2.4^3\right)} = 2.086 q_0 \tag{7}$$

For this case of non-uniform power deposition and taking into account the boundary conditions, the solution of (2) has the following form:

$$T_g = \left\{ T_w^{a+1} + \frac{(a+1)Q_0}{B}\left[\frac{b}{4}\left(R^2 - r^2\right) + \frac{2.4c}{9R}\left(R^3 - r^3\right) + \frac{2.4^2 d}{16R^2}\left(R^4 - r^4\right) + \frac{2.4^3 e}{25R^3}\left(R^5 - r^5\right) \right] \right\}^{\frac{1}{a+1}} \tag{8}$$

In this case the average gas temperature is found by comparing the area bounded between the gas temperature profiles for $q_0 = constant$ and $q_V = q_V(r)$ and the variable axis r. The gas temperature distributions (5) and (8) for uniform and non-uniform power input, respectively, could be effortlessly figured, because both they are analytical solutions. The equation (5) and (8) are obviously different, but the attention must be drawn to the result that average gas temperatures in both definitely different cases are almost equal. The discrepancy varies from 0.2 % to 1 % - the averaged value is about 0.6 %.

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References

[1] D. N. Astadjov, N. K. Vuchkov and N. V. Sabotinov, IEEE J. Quantum Electron. 24(9), 1927 (1988)

[2] Handbook 1991 ***Tables of physical constants***, ed I S Grigoryev and E Z Meylihov (Moscow: Energoatomizdat) pp 340-4

[3] R. C. Reid and T. K. Sherwood 1966 ***The properties of gases and liquids*** (New York: McGraw-Hill Book Company)

[4] P. Blau 1996 ***Pulsed Metal Vapour Lasers,*** ed C E Little and N V Sabotinov (Dordrecht: Kluwer Academic Publishers) pp 215-20