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Theoretical study on some plasma parameters and thermophysical properties of various gas mixtures in gas-discharge lasers

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Abstract. Using the well-known Wassiljewa equation and a new simple method, the thermal conductivities of various 2- and 3-component gas mixtures were calculated and compared under gas-discharge conditions optimal for two prospective lasers excited in a nanosecond pulsed longitudinal discharge. By solving the non-stationary heat-conduction equation for electrons, a 2D numerical model was also developed for determination of the radial and temporal dependences of the electron temperature $T_e(r, t)$.

1. Introduction

Determination of basic plasma parameters, such as gas temperature, electron temperature, electron concentration, etc. is one of the main and relevant problems in the physics of gas discharges, gas-discharge lasers, laser-induced breakdown spectroscopy, gas-discharge mass-spectroscopy, plasma technologies and plasma in general. The characteristic constants of the heavy-particle interaction depend on the gas temperature, while the electron temperature and electron density determine the characteristic constants of elastic and inelastic electron-heavy particle collisions. For gas-discharge lasers in particular, the abovementioned plasma parameters influence the development of population inversion, and hence the output laser parameters. The gas temperature distribution, i.e., the thermal mode, is also important for the stability of the laser operation and the active particles density.

The experimental techniques for determining the gas temperature that make use of the Doppler broadening of spectral lines or the focal distance of thermal lens are definitely imprecise. Recently, the theoretical determination of the gas temperature spatial distribution by solving analytically or numerically the steady-state heat conduction equation was proved to be a quite simple and efficient technique [1]. The thermophysical properties of gases and gas mixtures are important parameters in solving the corresponding partial differential equation. For example, the heat conductivity influences the gas temperature distribution, as found by solving the steady-state heat conduction equation. Both research and industrial plasma devices, gas-discharge lasers inclusive, often comprise multicomponent gas mixtures rather than pure gases. The theory for calculating the heat conductivity of

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multicomponent gas mixtures was developed around the beginning of the last century. Since then, various methods have been proposed. Most of them are empirical and reduce to some form of the original Wassiljewa equation [2, 3]. Due to the far-too-complex character of the Wassiljewa equation and its approximations, a new simple method based on iterative application of Brokaw's empirical equation for binary gas systems was proposed and applied to determining the thermal conductivity of multicomponent gas mixtures of our interest [4].

In this paper, using Wassiljewa equation and the new simple method quoted, the heat conductivities of various 2- and 3-component gas mixtures are calculated and compared under gas-discharge conditions optimal for two prospective lasers, namely deep-ultraviolet $\text{Cu}^+ \text{Ne-H}_2\text{-CuBr}$ and middle-infrared $\text{Sr atom He-(Ne-)SrBr}_2$ lasers, which are excited in a nanosecond pulsed longitudinal discharge (NPLD).

The widely applied techniques for experimental determination of the electron temperature, such as Langmuir probes, laser Thomson scattering and the spectral-line-ratio method, are not suitable and, hence, are inapplicable to high-voltage, high-current and high-power NPLDs due to the unavoidable excessive noise. Unlike the gas temperature calculation, theoretical determination of the electron temperature requires years-consuming development of complex kinetic models, which include tens of energy levels per particle, and solving the corresponding ordinary or partial differential kinetic equations of dubious validity.

In this paper, the radial and temporal dependences of the electron temperature $T_e(r, t)$ are determined through numerically solving the nonstationary heat conduction equation for electrons.

2. Theory

Following [3], the heat conductivity of a gas mixture k_m is expressed by Wassiljewa empirical relation as follows:

$$k_m = \sum_{i=1}^N \frac{y_i k_i}{\sum_{j=1}^N y_j A_{ij}}, \quad (1)$$

where k_m is the heat conductivity of the gas mixture in $\text{W m}^{-1} \text{K}^{-1}$, k_i is the heat conductivity of the pure i component in $\text{W m}^{-1} \text{K}^{-1}$, y_i and y_j are the mole fractions of components i and j , and A_{ij} is a function, which for $i = j$ is unit ($A_{ii} = 1$), while for $i \neq j$ remains to be obtained. Several methods have been proposed with varying complexity and accuracy for determination of A_{ij} [3, 5-8]. The simplest approach is to use the following expression [3, 5]:

$$A_{ij} = \frac{\left[1 + \left(\frac{k_i}{k_j} \right)^{\frac{1}{2}} \left(\frac{\mu_i}{\mu_j} \right)^{\frac{1}{4}} \right]^2}{\left[8 \left(1 + \frac{\mu_i}{\mu_j} \right) \right]^{\frac{1}{2}}}, \quad (2)$$

where μ_i and μ_j are the masses of particles i and j in amu, k_i and k_j are the heat conductivities of pure components i and j in $\text{W m}^{-1} \text{K}^{-1}$.

For binary gas mixtures, Brokaw's empirical equation [3, 9] is widely used. The thermal conductivity k_m of the gas mixture is calculated as follows:

$$\begin{aligned} k_m &= q k_{m_i} + (1 - q) k_{m_R}, \\ k_{m_i} &= y_1 k_1 + y_2 k_2, \\ \frac{1}{k_{m_R}} &= \frac{y_1}{k_1} + \frac{y_2}{k_2}, \end{aligned} \quad (3)$$

where k_1 and k_2 are the heat conductivities of pure components 1 and 2 in $\text{W m}^{-1} \text{K}^{-1}$, y_1 and y_2 are the mole fractions of components 1 and 2, q is a function of the mole fraction of the lighter component given in [3]. The new simple method proposed in [4] is based on an iterative application of Brokaw's equation.

To determine the radial-time-resolved electron temperature, the following nonstationary heat conduction equation is numerically solved for the electron gas:

$$\eta C_e \frac{\partial T_e}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left(r k_e(T_e) \frac{\partial T_e}{\partial r} \right) + q_v(t) \quad , \quad (4)$$

where C_e and $k_e(T_e)$ are the heat capacity and heat conductivity of the electron gas, R is the discharge zone radius equal to 3.55 mm, T is the period between the excitation pulses equal to 50 μs at the pulse repetition frequency of 20 kHz, $q_v(t)$ is the electric power density deposited into the NPLD for electron heating, η is a coefficient specifying the discrepancy between the real heat capacity of the electron gas and the one predicted by the classical statistical mechanics, i.e. $C_e = \frac{3}{2} k_B N_e(t)$, where $N_e(t)$ is the time-dependent electron density and k_B is the Boltzmann constant.

3. Results and discussion

Figure 1 shows the heat conductivities as a function of gas temperature are for various 2-component gas mixtures. The heat conductivities calculated by equation (1) and (3) are plotted with solid and dash-dot lines, respectively. The discrepancy is less than 6 %, with the exception of the Ne-H₂ mixture, where using the Wassiljewa equation obviously does not account for the hydrogen molecule dissociation above 1600 K.

Figure 2 presents the heat conductivities as a function of the gas temperature for various 3-component gas mixtures. The heat conductivities calculated by equation (1) and (3) are plotted with solid and dash-dot lines, respectively. The discrepancy is less than 7 %, with the exception of the Ne-H₂-Cu mixture.

In our previous study [10] we determined the electronic heat conductivity from the

Wiedemann-Franz law $\frac{k_e}{\sigma} = c T_e$ used

in plasma physics, where σ is the specific electrical conductivity, $c = \frac{\pi^2}{3} \left(\frac{k_B}{e} \right)^2$ is a constant, k_B is

Boltzmann constant, and e is the electron charge, assuming that σ is independent of the spatial coordinates and has a value of $\bar{\sigma}$. Our preliminary results showed that the electronic heat conductivity $k(T_e) = T_e$ derived from the Wiedemann-Franz law does not reflect the physical reality for the nonstationary electron temperature [10]. This is why we undertook a power index scanning for the electronic heat conductivity in an algometric form, i.e. $k_e = B T_e^a$, as widely used for solving analytically and numerically the stationary heat conduction equation to determine the gas temperature.

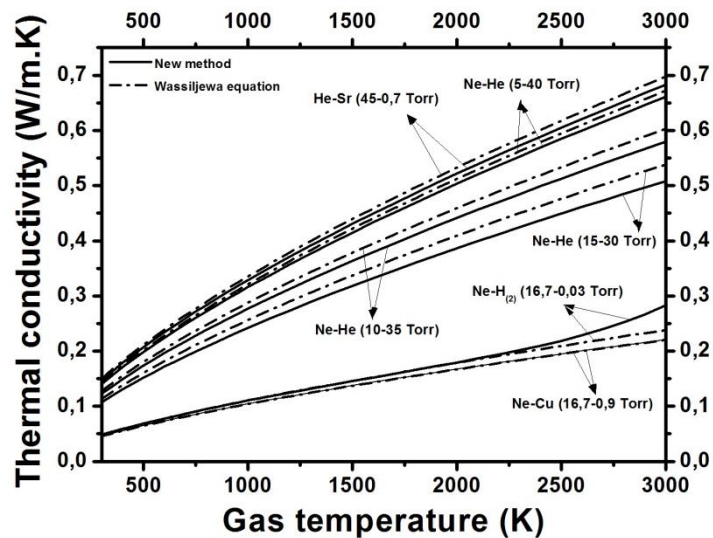


Figure 1. Thermal conductivities as a function of the gas temperature for various 2-component gas mixtures.

Equation (2) is numerically solved under the initial condition:

$$T_e(r,0) = T_e^0(r) = \left[T_e(R,0)^{1+a} + \frac{1+a}{4B} q_v(0)(R^2 - r^2) \right]^{\frac{1}{1+a}},$$

and the boundary conditions:

$$\lim_{r \rightarrow 0} r k_e(T_e) \frac{\partial T_e}{\partial r} = 0 \text{ and } T_e(R, t) = 880 \text{ K.}$$

(5)

The time-dependent electric power and electron concentration was experimentally determined in [11] by time-resolved measurement of electrical discharge parameters, such as tube voltage and discharge current. The $q_v(t)$ pulse is derived from the electric power pulse, taking into account that only 1 % of this power is deposited into heating of electrons [10], and is fitted by a Gaussian-type function:

$$q_v(t) = q_v^0 + \frac{A}{w \sqrt{\frac{\pi}{2}}} e^{-2 \left(\frac{t-t_0}{w} \right)^2} \quad (6)$$

while the electron density $N_e(t)$ is fitted by an exponential function:

$$N_e(t) = N_e^0 + A e^{\frac{t-t_0}{w}} \quad (7)$$

The fitting parameters for both functions are given in table 1.

Table 1. Fitting parameters for the electric power density $q_v(t)$ and electron concentration $N_e(t)$.

Function	q_v^0 or N_e^0	A	w	t_0
$q_v(t)$	$1,61588 \cdot 10^8$	1210,21118	$3,60545 \cdot 10^{-8}$	$9,48298 \cdot 10^{-8}$
$N_e(t)$	$-3,52795 \cdot 10^{18}$	$1,06363 \cdot 10^{19}$	$2,97375 \cdot 10^{-8}$	$2,07038 \cdot 10^{-8}$

Figure 3 illustrates the time-resolved electron temperature in an NPLD used for excitation of deep ultraviolet $\text{Cu}^+ \text{Ne-H}_2\text{-CuBr}$ laser for different radial distances and $k_e(T_e) = T_e^{0,02}$.

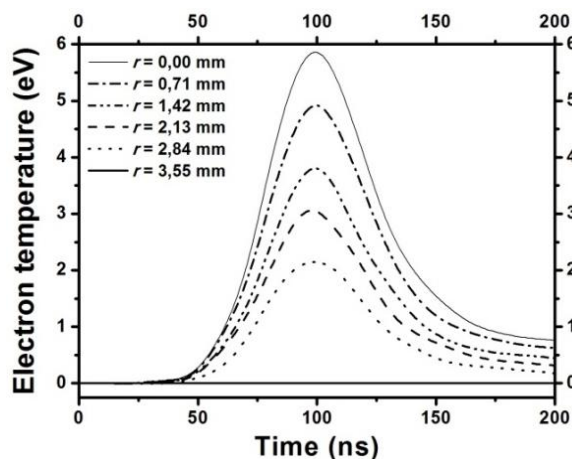


Figure 3. Temporal dependence for different radial distances of the electron temperature in an NPLD used for excitation of a deep ultraviolet $\text{Cu}^+ \text{Ne-H}_2\text{-CuBr}$ laser.

4. Conclusions

In this paper, using Wassiljewa equation and a new simple method, the thermal conductivities of various 2- and 3-component gas mixtures are calculated and compared under gas-discharge conditions optimal for two prospective lasers excited in an NPLD. Using the new method for heat conductivity calculation is preferable when dissociation of molecules occurs in a gas discharge.

A 2D numerical model is also developed for determination of the radial and temporal dependences of the electron temperature $T_e(r, t)$ by solving numerically the nonstationary heat conduction equation for electrons. The result is in fair agreement with the time-dependent electron temperature obtained by the time-resolved measurement of electrical discharge parameters [11] and with the existing self-consistent models developed for Ne-Cu and Ne-CuBr lasers excited in an NPLD [12, 13].

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