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# THE TRANSPORT COEFFICIENTS OF NOBLE GASES AND THE IONIZATION BY PRESSURE

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Various thermophysical properties of noble gases have obtained much attention during last several tens years (see, for example, [1] for references). The electronic transport coefficients (electrical conductivity *S*, thermal conductivity *K*, thermal power $S_t$) are especially interesting because the experiments have shown that under high pressures they can rise in several orders with respect to their ordinary value and can reach almost metallic state [2-4]. This effect is analogous to the phenomena observed in metals in the vicinity of the critical point, which is known as dielectric-metal transition. This transition occurs because of the pressure ionization in both cases. It gives rise to a steep increase in the free electron density, which in turn results in a large increase in the electrical conductivity and other thermoelectrical coefficients.

There are many experimental and theoretical works studying these coefficients. Nevertheless some questions concerning theoretical description and interpretation of the measurements data are still open. Recently, new experimental data have appeared [2,3] where partial ionization of Ar and Xe gases was reached by shock compression. In [3] two numerical codes were applied to describe the results of the measurements (correspondingly SAHA IV [4] and COMPTRA04 [5]). Both codes are based on so-called generalized chemical models (GCM) and have been successfully tested for many other substances. But calculated and measured conductivity for the experiments in hand can differ in two times [3]. This discrepancy can be explained by considerable errors of measurements. Besides, the densities and temperatures achieved in measurements [2, 3] belongs to region of rarefied plasma (T ~ 6-20 kK, density <0.1 g/cm$^3$ for Ar and density <0.46 g/cm$^3$ for Xe in [2,3], while the critical densities for Ar is 0.5 g/cm$^3$ and for Xe is 1.1 g/cm$^3$). The transport properties of noble gases are studied very well in this region. But at higher densities the information about these properties is less (we have here only the measurements [6]). So below we will consider two sets of measurements ([3] for rarefied plasma, and [6] for dense liquid).

Before proceed with the transport coefficients themselves, we should note that they are strongly dependent on the ionic composition of a substance under study. The simplest way to calculate them is to use relaxation time approximation [7]:

$$\sigma = -\frac{2|e|^2\sqrt{2m_e}}{3\pi^2\hbar^3} I_{3/2}, \quad S_t = \frac{1}{|e|T}\left(\mu - \frac{I_{5/2}}{I_{3/2}}\right), \kappa = \frac{2\sqrt{2m_e}}{3\pi^2\hbar^3 T}\left(-I_{7/2} + \frac{\left(I_{5/2}\right)^2}{I_{3/2}}\right),$$

$$I_n = \int_0^\infty \varepsilon\tau(\varepsilon)\frac{\partial f_0}{\partial\varepsilon}d\varepsilon, \quad f_0 = \frac{1}{\exp\left(\frac{\varepsilon-\mu}{k_B T}\right)+1}, \quad \tau = \sum_{i,a} n_i A_{tr}(\varepsilon)\sqrt{\frac{2\varepsilon}{m_e}} \qquad (1)$$

In (1) $A_{tr}(\varepsilon)$ is the momentum cross section of electrons, $\varepsilon$ is their energy, $f_0$ is the Fermi – Dirac distribution function, $T$ is the temperature, $n_i$ is the number density of heavy particles (ions and atoms), $m_e$, $e$, $\hbar$, $k_B$ are the fundamental constants, $\tau$ is the relaxation time. The momentum cross sections of the electrons on ions and atoms are presented in [3]. One can see from (1) that mow we need the ionic composition to apply expressions (1). So below we will consider how to calculate the composition using one of variant of GSM model.

GSM models are based on the following regulations [1-5]. A noble gas consists of neutral atoms, electrons and several sorts of positive ions. The ion charge for noble gases is usually no more the 2, because of high ionization potential of atoms and ions. Nevertheless, the 3fold charged ions are also considered in our study as far as we will consider the case of big densities. The free energy of the mixture under study is presented as sum of different contributions:

$$F(N_0, N_1, N_2,\ldots, N_e,V,T)=F_{id}+F_{N\text{-}N}+F_{Ch\text{-}Ch}+F_{N\text{-}Ch} \qquad (2)$$

Here $F_{id}$ – is the free energy of ideal gas of non-interacting ions, atoms and electrons, which is well known values [1]. It is better to consider the electrons as degenerated system, as far as we intend to study the liquid region. The ideal part of free energy usually includes internal partition functions of atoms and ions. Here we used Plank-Larkin convention for these values like in [1, 5]. Others terms in (2) are the following. $F_{N\text{-}N}$ –is the contribution due to the atom-atom (neutral-neutral) interactions. $F_{Ch\text{-}Ch}$- is the contribution due to the interaction of charged species (charge-charge). $F_{N\text{-}Ch}$- is the contribution due to the interaction of atoms with charged particles. $N_s$ –is the particle number ($s$=0 – atoms, $s$=1,2,… - $s$-charged ion, $e$ – electrons). The minimization of (2) with respect to different $N_i$ gives rise to the equations of the mass action law, solution of which allows to obtain the number densities, i. e. ionic composition.

Various expressions for different contributions of (2) are possible. At low densities, when our substance is a weakly coupled medium, the contributions $F_{N\text{-}N}$ are usually disregarded. Moreover, in this case different models give rise to the similar results (see [3], for example). $F_{N\text{-}Ch}$ contribution is usually described in the 2nd virial coefficient approximation [1-5]. I. e.

$$VF_{N-Ch} = 2k_B T \sum_i N_a N_i B_{ia}(T)\,, \tag{3}$$

where $B(T)$ is the second virial coefficient, which is unambigously defined by the polarization potential. Here we used the same polarization potential as in [1]. The interaction between charges can be described by various approximated expression. At low densities the most successful approximation was offered in [8] (it is used in SAHA IV [2]). For higher densities it is possible to use Pade approximations [1, 5]. In present calculations we use the approximation offered in [9]. At low densities above terms are sufficient to obtain sensible results. Below in Table 1 there is comparison of Ar conductivity calculated in present work ($\sigma_{Our}$) with models and measurement of [3]. One can see that the difference between the models is not great. We should remind that the accuracy of the measurements is low, so all three models give acceptable results.

Table 1. . The conductivity of Argon in the gaseous region of low densities.

| density, $g/cm^3$ | T, K | $\sigma_{measur}$, S/m | $\sigma_{Our}$, S/m | $\sigma_{SAHAIV}$, S/m | $\sigma_{Comptra}$, S/m |
|---|---|---|---|---|---|
| $2.53*10^{-02}$ | $7.85*10^{3}$ | $8.80*10^{1}$ | $1.47*10^{2}$ | 1.46e+02 | 1.33e+02 |
| $2.54*10^{-02}$ | $8.18*10^{3}$ | $1.60*10^{2}$ | $2.17*10^{2}$ | 2.11e+02 | 1.91e+02 |
| $2.56*10^{-02}$ | $9.38*10^{3}$ | $7.70*10^{2}$ | $7.21*10^{2}$ | 6.13e+02 | 5.60e+02 |
| $2.57*10^{-02}$ | $9.82*10^{3}$ | $7.20*10^{2}$ | $8.57*10^{2}$ | 8.48e+02 | 7.71e+02 |
| $2.59*10^{-02}$ | $1.05*10^{4}$ | $9.40*10^{2}$ | $1.25*10^{3}$ | $1.32*10^{3}$ | $1.20*10^{3}$ |
| $2.62*10^{-02}$ | $1.11*10^{4}$ | $1.24*10^{3}$ | $2.06*10^{3}$ | $1.84*10^{3}$ | $1.66*10^{3}$ |
| $6.09*10^{-02}$ | $1.19*10^{4}$ | $1.00*10^{3}$ | $2.43*10^{3}$ | $2.14*10^{3}$ | $2.30*10^{3}$ |
| $6.22*10^{-02}$ | $1.27*10^{4}$ | $2.20*10^{3}$ | $2.91*10^{3}$ | $3.04*10^{3}$ | $3.28*10^{3}$ |
| $6.26*10^{-02}$ | $1.30*10^{4}$ | $3.00*10^{3}$ | $3.67*10^{3}$ | $3.43*10^{3}$ | $3.56*10^{3}$ |
| $6.34*10^{-02}$ | $1.34*10^{4}$ | $3.11*10^{3}$ | $4.30*10^{3}$ | $3.99*10^{3}$ | $4.17*10^{3}$ |
| $6.67*10^{-02}$ | $1.46*10^{4}$ | $5.40*10^{3}$ | $6.08*10^{3}$ | $5.94*10^{3}$ | $6.26*10^{3}$ |
| $6.77*10^{-02}$ | $1.49*10^{4}$ | $6.03*10^{3}$ | $6.67*10^{3}$ | $6.51*10^{3}$ | $6.86*10^{3}$ |
| $6.87*10^{-02}$ | $1.52*10^{4}$ | $3.50*10^{3}$ | $7.29*10^{3}$ | $7.10*10^{3}$ | $7.51*10^{3}$ |
| $7.30*10^{-02}$ | $1.63*10^{4}$ | $1.20*10^{4}$ | $1.41*10^{4}$ | $9.18*10^{3}$ | $9.33*10^{3}$ |
| $7.43*10^{-02}$ | $1.66*10^{4}$ | $1.38*10^{4}$ | $1.49*10^{4}$ | $1.02*10^{4}$ | $1.03*10^{4}$ |

At high densities (liquid region), which were obtained in measurements [6], we need to take into account the interaction atom-atom. This interaction is regarded using the Fluid Variational Theory [10] (see also [1] for references). This theory gives the upper bound for the free energy $F_{N-N}$. More exact results (but more time-consuming) can be obtained by means of the integral equations technique, which is usual tool of liquid theory [10, 11]. Here we used the latter approach with the Exp-6 potential like in [1]. The results for Argon are presented in Table 2. Our results are in good agreement with measurements in shock waves of [6], relative error of which is also presented in 4th column of table 2.

Table 2. The conductivity of Argon in the fluid region of high densities.

| P, GPa | T, K | density, g/cm$^3$ | $\sigma_{measur}$, S/m | $\sigma_{Our}$, S/m |
|---|---|---|---|---|
| 23.2 | $7.350*10^3$ | 2.80 | 4.00±13 | 3.00 |
| 27.6 | $9.159*10^3$ | 2.90 | 47.0±13 | 40.0 |
| 32.8 | $1.135*10^4$ | 2.95 | $2.16*10^2$±48 | $1.9*10^2$ |
| 36.7 | $1.305*10^4$ | 3.00 | $7.57*10^2$±160 | $7.31*10^2$ |
| 41.4 | $1.505*10^4$ | 2.05 | $2.36*10^3$±520 | $2.16*10^3$ |
| 49.1 | $1.823*10^4$ | 3.17 | $3.70*10^4$±550 | $3.43*10^4$ |
| 67.1 | $2.410*10^4$ | 3.50 | $1.37*10^4$±2500 | $1.10*10^4$ |

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