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Abstract

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ON EQUILIBRIUM IONIZATION CREATED BY DUST PARTICLES

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As is known, ionization in carbon-containing flames in many cases is determined mainly by thermionic emission of electrons from carbon dust particles, which are usually quite uniform and are characterized by an average radius r of the order of 10^{-6} cm and a work function $\varphi_0 = 4.35$ eV (^{1}). Since the work function from charged carbon particles must differ appreciably from φ_0, at temperatures of interest multiple ionization of dust particles may play an essential role, and this must be taken into account in calculating the equilibrium concentration of electrons in such systems. Similar calculations have recently been carried out (^{1,2}) by studying infinite series that determine the electron concentration in the presence of multiple ionization of the particles. In the present note a complete mathematical solution is given of the problem of equilibrium ionization in a system formed by dust particles, with the aid of well-studied θ-functions, which make it possible to express the equilibrium electron concentration in closed form by a formula containing, as limiting cases, both the Saha formula (valid at sufficiently low temperatures) and the simple asymptotic expression found in (^{1,2}), valid at sufficiently high temperatures, and also to investigate the region of intermediate temperatures.

We shall assume at first that the particles are identical and introduce the notation: n (cm^{-3})—concentration of particles; n_e (cm^{-3})—concentration of electrons; n_m^+ (cm^{-3})—concentration of particles having positive charge $+me_0$ (e_0 —charge of the electron, $m = 1, 2, ...$); n_m^- (cm^{-3})—concentration of particles having negative charge $-me_0$; n_0 (cm^{-3})—concentration of neutral particles. The formulation of the problem set forth below coincides completely with that adopted in (^{2}).

The conditions of quasineutrality of the system and conservation of the total number of particles make it possible to write the relations (^{2}):

$$n_e = \sum_{m=1}^{\infty} mn_m^+ - \sum_{m=1}^{\infty} mn_m^-, \qquad n = n_0 + \sum_{m=1}^{\infty} n_m^+ + \sum_{m=1}^{\infty} n_m^-. \tag{1}$$

(The summation over m in (1) is extended, as in (^{1,2}), to infinity, since the charge of particles, positive or negative, can in principle be very large.)

The equilibrium constant K_m^+ for the process of single ionization of a particle with charge $+(m-1)e_0$ can be determined from the relation $n_m^+ = K_m^+/n_e \cdot n_{m-1}^+$, where (1,3)

$$K_m = 2\left(\frac{m_e kT}{2\pi h^2}\right)^{3/2} \exp[-\varphi/kT] = K\exp[-(m-1)/2\sigma^2], \quad \varphi = \varphi_0 + \frac{(m-1)e_0^2}{r},$$

$$K = 2\left(\frac{m_e kT}{2\pi h^2}\right)^{3/2} \exp[-\varphi_0/kT], \quad \sigma^2 = \frac{rkT}{e_0^2}$$

(T—absolute temperature, m_e—electron mass). The ionization potential of a particle with charge $(m-1)e_0$ is written, as in (1), in the form

$$\varphi = \varphi_0 + \frac{(m-1)e_0^2}{r},$$

which, apparently, is valid for spherical and sufficiently well-conducting particles;

ratio of the statistical weights for the initial and final states of the particle, as in (1), is taken equal to unity.

From this we easily find the relation of n_m^+ to the concentration of neutral particles

$$n_m^+ = r_0 \prod_{i=1}^{m} K_i^+/n_e = n_0 a^m \exp\left[-\frac{(m-1)m}{2\sigma^2}\right], \quad a = K/n_e.$$

Similarly, introducing the equilibrium constant for the process of single ionization of a particle with negative charge $-me_0$, $K_m^- = 1/Ke^{-m/2\sigma^2}$, we find the relation between n_m^- and n_0:

$$n_m^- = n_0 \prod_{i=1}^{m} K_i^- n_e = n_0 a^{-m} \exp\left[-m(m+1)/2\sigma^2\right].$$

Substituting the thus determined n_m^+ and n_m^- in (1), we find the formulas (2):

$$\frac{n_e}{n} = \frac{\sum\limits_{m=-\infty}^{\infty} m a^m \exp\left[-\frac{m(m-1)}{2\sigma^2}\right]}{\sum\limits_{m=-\infty}^{\infty} a^m \exp\left[-\frac{m(m-1)}{2\sigma^2}\right]}, \quad \frac{n_0}{n} = \frac{1}{\sum\limits_{m=-\infty}^{\infty} a^m \exp\left[-\frac{m(m-1)}{2\sigma^2}\right]}. \tag{2}$$

Using elementary transformations, n_e/n can be expressed by means of elliptic θ-functions. Let $\ln a = 2\pi v$. Then

$$\sum_{m=-\infty}^{\infty} a^m \exp[-m(m-1)/2\sigma^2] = \exp[\pi v + 1/8\sigma^2]\times$$

$$\times \sum_{n=-\infty}^{\infty} \exp[(2n+1)\pi v] \exp\left[-\frac{(n+\frac{1}{2})^2}{2\sigma^2}\right] = \exp[\pi v + 1/8\sigma^2]\theta_2(-iv, \rho),$$

where (4,5) $\theta_2(x, \rho)$ is an elliptic θ-function,

$$\theta_2(x, \rho) = \sum_{-\infty}^{\infty} q^{(n+\frac{1}{2})^2} \exp[(2n+1)\pi x i], \quad q = e^{-\pi\rho}$$

(i.e., here $\rho = 1/2\pi\sigma^2$). Hence we have:

$$\frac{n_e}{n} = \frac{1}{2} + \frac{1}{2\pi}\frac{d}{dv}\ln\theta_2(-iv, \rho), \quad \frac{n_0}{n} = \frac{1}{\exp[\pi v + 1/8\sigma^2]\theta_2(-iv, \rho)}.$$

Using the known transformations

$$\theta_2(iv, \rho) = \rho^{-1/2} e^{\pi v^2/\rho} \theta_0\left(-\frac{v}{\rho}, \frac{1}{\rho}\right)$$

and $\theta_0(x, \rho) = \theta_3\left(\frac{1}{2} - x, \rho\right)$ (4), we finally find

$$\frac{n_e}{n} = y + \frac{\rho}{2\pi}\frac{d}{dy}\ln\theta_3(y, \rho), \quad \frac{n_{\mp}^{\pm}}{n} = \rho^{-1/2}\exp\left[-\frac{\pi(y \mp m)^2}{\rho}\right]\cdot\frac{1}{\theta_3(y, \rho)}. \tag{3}$$

Here

$$y = \sigma^2 \ln\frac{K}{n_e} + \frac{1}{2}, \quad \rho = 2\pi\sigma^2, \quad m = 1, 2, \ldots .$$

Let us now examine some limiting cases in formulas (3). First let $\rho \gg 1$ (sufficiently high T and r). Using the known asymptotic expressions for $\theta_3(y, \rho)$, $\frac{d}{dy}\ln\theta_3(y, \rho)$, valid for $\rho \gg 1$ (4), we easily find in this case**

$$\frac{n_e}{n} = y - 2\rho e^{-\pi\rho}\sin 2\pi y, \quad \frac{n_{\mp}^{\pm}}{n} = \frac{1}{\sqrt{2\pi\sigma^2}}\exp\left[-\frac{(y \mp m)^2}{2\sigma^2}\right], \tag{4}$$

where the remainder $-2\rho e^{-\pi\rho}\sin 2\pi y$ is always small for $\rho \gg 1$.

* Written by means of infinite series,

$$\theta_3 = \sum_{m=-\infty}^{\infty} q^{n^2} e^{2\pi n y i}, \quad q = e^{-\pi\rho},$$

this formula coincides with that found in (2).

** The formula $n_e/n = \sigma^2 \ln(K/n_e) + 1/2$ was first found by A. E. Einbinder (^{1}). The correct condition for its applicability, $2\pi\sigma^2 \gg 1$, was indicated in (2).

We note that, according to (4), for $\rho \gg 1$ the concentration of particles with charge m is characterized by the Gaussian distribution (^{2}), while y has the meaning of the positive charge corresponding to the greatest concentration.

For $q = e^{-\pi\rho} \ll 1$ (sufficiently low T and r), using the asymptotic expression for $d\ln\theta_3(y,\rho)/dy$, valid for $e^{-\pi/\rho} \ll 1$ (^{4}), from which it follows that

$$\frac{\rho}{2\pi}\frac{d\ln\theta_3}{dy} = -y + \sum_{n=1}^{\infty}(-1)^{n-1}\frac{\operatorname{sh}\dfrac{2\pi n y}{\rho}}{\operatorname{sh}\dfrac{\pi n}{\rho}} \simeq$$

$$\simeq -y + \sum_{n=1}^{\infty}(-1)^{n-1}a^n + \sum_{n=1}^{\infty}(-1)^{n-1}(a^n - a^{-n})e^{-n/2\sigma^2},$$

we obtain in this case the Saha formula

$$\frac{n_e}{n} = \frac{K/n_e}{1+K/n_e} + O(\rho) \quad \text{or} \quad \frac{n_e}{K} = -\frac{1}{2} + \sqrt{\frac{1}{4} + \frac{n}{K}} \tag{5}$$

with a correction $O(\rho)$ of order $n_e/Ke^{1/2\sigma^2}$ for $K/n_e \ll 1$.

Finally, note that, independently of the magnitude of σ^2, as $n \to \infty$, n_e is determined from the condition $y \to 0$. Indeed, as $n \to \infty$, n_e must remain finite, and therefore y as $n \to \infty$ is determined by the equation

$$y + \frac{\rho}{2\pi} d\ln\theta_3/dy = 0,$$

which, as is easy to show, has the unique solution $y = 0$. Thus, as $n \to \infty$, $n_e \to n_e^0 = Ke^{1/2\sigma^2}$, i.e., for $\sigma^2 \gg 1$, $n_e^0 = K$, where K is nothing other than the equilibrium ionization above the surface of a substance characterized by the work function φ_0.

Using tables of θ-functions (^{5}), one can find the values of n_e/n also for intermediate values of the parameters, for which formulas (4), (5) are not valid. In Fig.

1 are given graphs found in this way of the dependence of $\lg n_e/K$ on $\lg n/K$ for various values of the parameter σ^2, covering the entire range of variation of r and T of interest. From these graphs it is seen that the Eyring formula

$$\frac{n_e}{n} = \sigma^2 \ln \frac{n_e}{K} + \frac{1}{2}$$

is satisfied with good accuracy throughout the whole range of variation of n/K already for $\sigma^2 \gtrsim 0.2$.

In conclusion, let us note that the formulas found are easily generalized to the case in which dust particles of different sorts (having different r and φ_0) are present in the system. If we introduce the quantities $n^+_{m_i}$, $n^-_{m_i}$, $n_0^{(i)}$, and $n^{(i)}$, where $n^\pm_{m_i}$ is the number of particles of the i-th sort with charge $\pm m_i$; $n_0^{(i)}$ is the number of neutral particles; $n^{(i)}$ is the total number of particles of the i-th sort; n is the total number of particles, then, using the expressions for the constants $K^\pm_{m_i}$ and the relations

$$n_e = \sum_i \left(\sum_{m_i=1}^{\infty} (m_i n^+_{m_i} - m_i n^-_{m_i}) \right), \qquad n^{(i)} = n_0^{(i)} + \sum_{m_i=1}^{\infty} n^+_{m_i} + \sum_{m_i=1}^{\infty} n^-_{m_i},$$

we easily find the formula for n_e, which is a simple generalization of (3):

$$\frac{n_e}{n} = \sum_i \frac{n^{(i)}}{n} \left(y_i + \frac{\rho_i}{2\pi} \frac{d \ln \theta_3(y_i, \rho_i)}{dy_i} \right), \tag{6}$$

where the quantities y_i, ρ_i refer to particles of the i-th sort,

$$\rho_i = 2\pi\sigma_i^2, \qquad \sigma_i^2 = \frac{r_i kT}{e_0^2}, \qquad y_i = \sigma^2 \ln \frac{K_i}{n_e} + \frac{1}{2}.$$

Formula (6) makes it possible to find n_e/n easily also in the case when dust particles of several sorts with strongly differing-

properties. Suppose, in particular, that the dust grains differ only in their radii, and that their density as a function of the radius varies continuously according to a Gaussian law, i.e.

$$dn/n = n^{(i)}/n = \frac{1}{\sqrt{2\pi x^2}} \times \exp\left[-\frac{(r-R)^2}{2x^2} \right] dr$$

(it is assumed that $R^2/2x^2 \gg 1$). If

Fig. 1

Figure 1: Fig. 1

$$\rho_0 = 2\pi \frac{kTR}{e_0^2} \gg 1,$$

Fig. 1

it is natural to use the formula derived earlier

$$y + \frac{\rho}{2\pi}\frac{d}{dy}\ln\vartheta_3(y,\rho) \simeq y - 2\rho e^{-\pi\rho}\sin 2\pi y,$$

and then the electron concentration is

$$\frac{n_e}{n} = \frac{1}{\sqrt{2\pi x^2}}\int_0^\infty \exp\left[-\frac{(r-R)^2}{2x^2}\right]\left(y - 2\rho e^{-\pi\rho}\sin 2\pi y\right)\, dr \simeq$$

$$\simeq \sigma_0^2 \ln\frac{K}{n_e} + \frac{1}{2} - \frac{2}{\sqrt{2\pi x^2}}\int_0^\infty \rho \sin 2\pi y \exp\left[-\pi\rho - \frac{(r-R)^2}{2x^2}\right] dr,$$

$$\sigma_0^2 = RkT/e_0^2, \qquad \rho_0 = 2\pi\sigma_0^2, \qquad \rho = 2\pi\sigma^2.$$

Since in the integral written above the exponent has a minimum equal to

$$-\left(\pi\rho_0 - \frac{\pi^2}{2}\rho_0^2\frac{x^2}{R^2}\right),$$

then, for

$$\pi\rho_0 - \frac{\pi^2}{2}\rho_0^2\frac{x^2}{R^2} \gg 1,$$

it can be evaluated by the saddle-point method. Thus we find:

$$\frac{n_e}{n} = \sigma_0^2\ln\frac{K}{n_e} + \frac{1}{2} - 2\rho_m \sin 2\pi y_m \exp\left[-\pi\rho_0\left(1 - \frac{\pi}{2}\rho_0\frac{x^2}{R^2}\right)\right], \qquad (7)$$

$$\rho_m = 2\pi\sigma_m^2 = \rho_0 - \pi\rho_0^2\frac{x^2}{R^2}, \qquad y_m = \sigma_m^2\ln\frac{K}{n_e} + \frac{1}{2}.$$

It follows from (7) that Einbinder' s formula also holds in the case when the radii of the dust grains are not constant but are distributed according to a Gaussian law, provided that the dispersion x of this distribution is sufficiently small, namely that it satisfies the condition

$$\pi\rho_0 - \frac{\pi^2}{2}\rho_0^2\frac{x^2}{R^2} \gg 1, \qquad 2x^2/R^2 \ll 1.$$

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Note: Figure translations are in progress. See original paper for figures.

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