Lowering of the Ionization Potential in Dense Aluminum Plasmas[1]

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From the hypervelocity impact of microparticles on a massive target, the high concentration of energy in the material at the impact region produces a dense plasma. As the energy content and the per cent of ionization of a dense plasma increases, the interaction between the electric microfields from the ions and electrons results in a decrease in the ionization potential of the atoms and ions in the plasma. The effective ionization potential, I_i^*, for each ionic species, i, is given in Fig. 1 by equation 1, where ΔI_i is the reduction in the ionization potential for the i^{th} species of the atom and I_i is the ionization potential of the isolated ionic species. The reduction in the ionization potential was found by experiment and was reported (Elenbaas, 1951) and it has been recognized in several theoretical studies (Ecker *et al.*, 1956; Margenau *et al.*, 1959). The microfields result in the disappearance of the upper energy levels of the atoms and ions as they merge into the continuum.

The purpose of this study is to ascertain the most accurate value for the density of ionization from an application of the corrected Saha equation, Equation 2 in Fig. 1, to dense plasmas. Solutions are obtained with a computer by a cyclic calculation of the convergence on the electron density. The results in this paper indicate that the amount of ionization for dense plasmas at low temperatures is substantially higher than previously predicted. As a consequence, the effective temperature is much lower than was expected from earlier studies.

Low Density Plasmas

There are essentially two methods for determining the reduction in ionization potential, ΔI_i. One becomes a direct calculation of ΔI_i, such as on the basis of thermodynamics (Ecker *et al.*, 1956), or on the broadening of bound energy levels (Margenau *et al.*, 1959). The second is a calculation of the maximum quantum number, g_i^*, which is used to obtain ΔI_i and is illustrated by the Rouse paper which is considered below. The simplest way to estimate ΔI_i from the maximum quantum number is to assume that no bound state may have a radius greater than the Debye radius.

In one form or another, the preceding calculations usually employ the Debye radius. This quantity is an effective radius for the action of the electric field from an ion. Beyond this radius, the electric field from an ion is assumed to decrease abruptly from the Coulomb value to zero. This assumption was postulated during early work on electrolytes (Debye *et al.*, 1923; Fowler *et al.*, 1939). The density range for an accurate application of the Debye equation was established by Kirkwood and Poirier (Kirkwood *et al.*, 1954) and will be compared with the results which will be given later in this paper. According to Equation 4, Fig. 1, the numerical value of the Debye radius, D, varies as the square root of the temperature, or the square root of the effective kinetic energy of the atoms and ions, and inversely as the square root of the maximum ionic charges in the plasma. The term, Z_i, in this equation is the dimensionless charge parameter expressed in number of electron charges.

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1. Effective Ionization Potential (I_i^*): $I_i^* = I_i - \Delta I_i$

I_i = Isolated Atom's (or Ion's) Ionization Potential

ΔI_i = Reduction of Ionization Potential

2. Saha Equation: $\frac{n_{i+1}\, n_e}{n_i} = \frac{2(2\pi m_e kT)^{3/2} Q_{i+1} e^{-I_i^*/kT}}{h^3 Q_i}$

n_i = Number Density of i^{th} Species

n_e = Number Density of Electrons

Q_i = Electronic Partition Functions

3. Electronic Partition Function (Q_i): $Q_i = \sum_{g=1}^{g^*} W_{ig} e^{-E_{ig}/kT}$

W_{ig} = Degeneracy of g^{th} Level

g^* = Maximum Principal Quantum Number

4. Debye Radius (D): $D = \frac{2.36 \times 10^9 \left(\frac{kT}{e}\right)^{\frac{1}{2}}}{\left(n_e + \sum_i n_i Z_i^2\right)^{\frac{1}{2}}}$

T = Temperature in Electron Volts

Z_i = Ionic Core Charge Parameter (Number of Electron Charges)

5. Kelley's Equation: $g_i^{*2} = \frac{.804\, Z_i D}{a_o}$

g_i^* = Maximum Principal Quantum Number for i^{th} Species

a_o = Radius of 1^{st} Bohr Orbit

6. ΔI_i Equation-Rouse: $\Delta I_i = I_i \left[\frac{1}{(g^* + 1)^2}\right]$

I_i = Isolated Atom's (or Ion's) Ionization Potential

7. Limit of Debye Theory: $n_{cr} = \left(\frac{3}{4\pi}\right)\left[\frac{kT}{(e_{i\,max})^2}\right]^3$

n_{cr} = Total Particle Density

$e_{i\,max}$ = Maximum Ionic Charge (in e.s.u.) in the Pla

Fig. 1. Equations used in article (see text).

Solutions of the Saha equation on the basis of the g_i^* method were reported in a series of papers for a plasma in ionization equilibrium. (Rouse, 1961, 1962a, 1962b, 1962c). This series of papers is chosen for special consideration because it is claimed that they are applicable to liquid metals and constitute the only group which has been found in the published literature. In the first two papers, values of the ionization were obtained by use of the uncorrected Saha equation, which is equivalent to using the perfect gas law for the equation of state. In the third paper, a correction for ΔI_i was introduced but this method was modified for the last paper. In the final paper, which was to apply to liquid metals, ΔI_i was obtained from computed values of the maximum quantum number, g_i^*, on the basis that no bound state may have a radius greater than the Debye radius. Kelley's relation, Equation 5 in Fig. 1, was used for g_i^*, in which a_o is the radius of the first Bohr orbit, D is the Debye radius and Z_i is the dimensionless core-charge parameter. A Balmer type of equation was assumed for determining the maximum effective ionization potential. For this approximation, ΔI_i is given in Fig. 1 by Equation 6. This is essentially a Debye correction of the ionization potential and it would be valid only in regions of high temperature and low density for which the Debye-Hückel theory is valid.

The preceding discussion on the Rouse papers is concerned with lowering of the ionization potential on the assumption that the energy levels of the bound states are not affected by the microfields. In addition to the reduction of the ionization potential, the microfields change the positions of the bound levels. This may be introduced into the Saha equation by means of the electronic partition function, Q_i, which is given in Fig. 1 by Equation 3. The partition function is expressed as a summation over bound states for which $w_{i,g}$ and $E_{i,g}$ are the degeneracy and the energy, respectively, of the g^{th} level. Corresponding to the lowering of the ionization potential, the atom has a highest bound excitation state with a principal quantum number g_i^*. The summation, in Equation 3, is limited by this maximum quantum number. Since the Saha equation is affected much more by the ionization potential than by this secondary consideration, the effect of the modified partition functions was neglected.

Dense Plasmas

The major difficulty in applying the Debye-Hückel theory is its limited region of validity. In addition to this, Duclos and Cambel (1962) have shown that in the density region for which the theory is valid, the resulting corrections are very small and may, in many cases, be neglected. It may be shown that the upper density limit for a valid application of the Debye-Hückel theory is given in Fig. 1 by Equation 7 (Ecker and Kröll, 1963). In this equation, the critical density, n_{cr}, is the maximum total particle density for which the Debye theory is valid. It is dependent upon the cube of the absolute temperature and inversely upon the sixth power of the maximum ionic charge in the plasma.

Recently, equations were reported that may be used for the direct calculation of the reduction of the ionization potential for plasma densities above and below the critical density; see Fig. 2 and Equation 7 (Ecker and Kröll, 1963). The upper limit of validity of these equations is reported by the authors to be the semi-classical limit which is shown in Fig. 2 by Equation 8. For this limit, the electron density is the limiting factor. A comparison of the regions of validity, in a singly ionized plasma, for the Debye theory and for the Ecker and Kröll equations is shown in Fig. 3. The lines are the upper limit of validity. The region of interest for dense plasmas lies above the Debye limit and probably below the semi-classical limit.

For dense plasmas, the reduction of the ionization potential is found with the Ecker and Kröll equations, which are Equations 9 through 13 in Fig. 2. In these equations, D is the Debye radius, e_i is the core charge in e.s.u., *epsilon*[2] is the dielectric constant (taken as unity to calculate the curves) and T is the temperature in degrees Kelvin. The summation in Equation 11 is over the distribution of ions and electrons at the critical density. The average distance between particles is r_o. This dependence has a marked effect on the calculated degree of ionization at high densities and low plasma temperatures. For particle densities, n_T, which are less than n_{cr}, the ionization potential is given on Fig. 2 by Equation 9. When n_T is greater than n_{cr}, Equation 10 must be used. The general characteristics of the new solution is illustrated by the Ecker and Kröll calculation of ΔI_i for a hydrogen plasma at various temperatures and electron densities which are shown in Fig. 4.

RESULTS

The degree of ionization at equilibrium for a dense aluminum plasma was calculated for several temperatures and densities by use of the uncorrected ionization potential and by two other methods which determine a value for ΔI_i. The first calculation used the uncorrected Saha equation and gave the lowest curve on both Figs. 5 and 6. A second computation used Rouse's correction, Equations 5 and 6, for the reduction of the ioniza-

8. Semiclassical Limit (for Electrons): $n_e < \left(\frac{2\pi m_e kT}{h^2}\right)^{3/2}$

9. ΔI_i for $n_T \leq n_{cr}$: $\Delta I_i = \frac{1}{2\epsilon D}\left[e_{i+1}^2 - e_i^2 + e^2\right]$

10. ΔI_i for $n_T > n_{cr}$: $\Delta I_i = \frac{C}{2\epsilon r_o}\left[e_{i+1}^2 - e_i^2 + e^2\right]$

11. Constant "C" in 10: $C = 2.2\left[\sum_\beta (n_{cr})_\beta (e_\beta)^2\right]^{1/2} \Big/ \left[k^{1/2} T^{1/2} n_{cr}^{1/3}\right]$

$\sum_\beta n_{\beta_{cr}}$ = Sum Over Distribution at Critical Density

12. Constant "r_o" in 10: $r_o = \left(\frac{3}{4\pi n_T}\right)^{1/3}$

13. Total Particle Density (n_T): $n_T = n_e + \sum_i n_i$

ϵ = Dielectric Constant

D = Debye Radius (Equation 4)

e_i = Core Charge of the i^{th} Species (in e.s.u.)

T = Temperature (in ^oK)

e_β = Charge of β Species (in e.s.u.)

$(n_{cr})_\beta$ = Number Density of β Species at Critical Density

Fig. 2. Equations used in article (see text).

[2]Greek letters used in the figures are spelled out in the text.

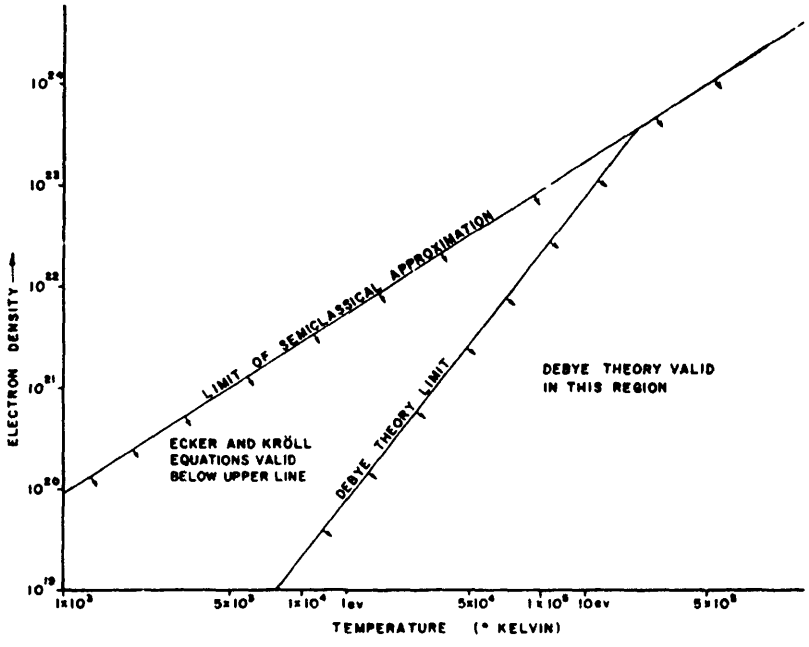

Fig. 3. Regions in which Debye theory and Ecker and Kröll's equations are valid in a singly ionized plasma.

tion potential and this calculation gave the curve which is just above the lowest in both Figs. 5 and 6. The third calculation used Equations 9 through 13, the Ecker and Kröll method, to determine ΔI_1. A much higher degree of ionization is found at high densities according to the curves in Fig. 5 and at low temperatures according to the curves in Fig. 6. As the energy per particle, or the effective temperature, is increased and as the density of the plasma is reduced, the results from the three methods converge to an identical degree of ionization. These results are to be expected. All corrections reduce to zero as the temperature increases, or the density decreases. When the corrections become zero, the uncorrected perfect gas law is an accurate equation of state.

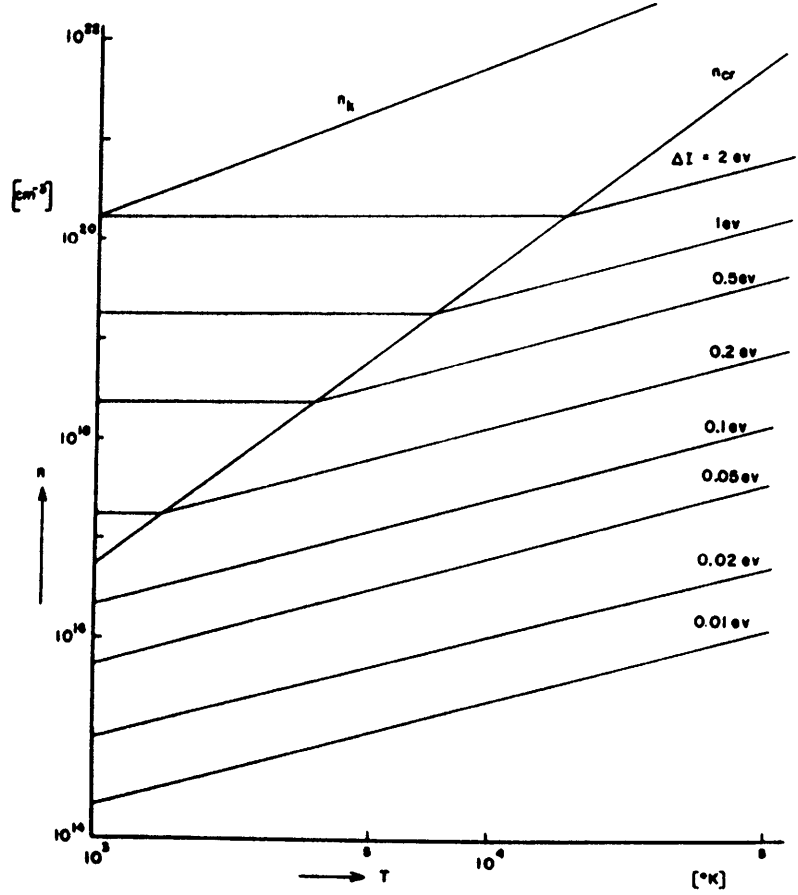

Fig. 4. Lowering of the ionization potential (ΔI) as a function of the charge carrier density n and temperature T. n_{cr} is the critical density; n_k gives the limit for the classical description of the electrons (Ecker and Kröll, 1963).

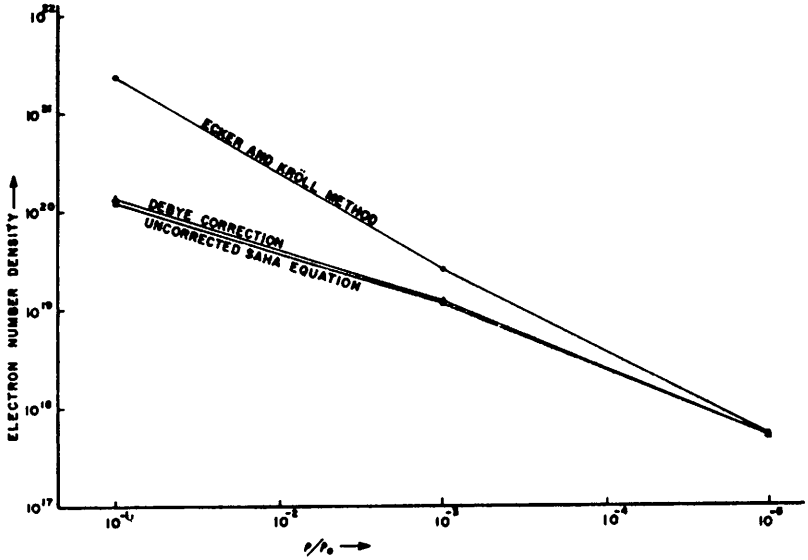

Fig. 5. Comparison of ionization electron density calculated for several densities of an aluminum plasma. The three curves are solutions of the three methods for determining ionization. *Rho* is the solid density of aluminum.

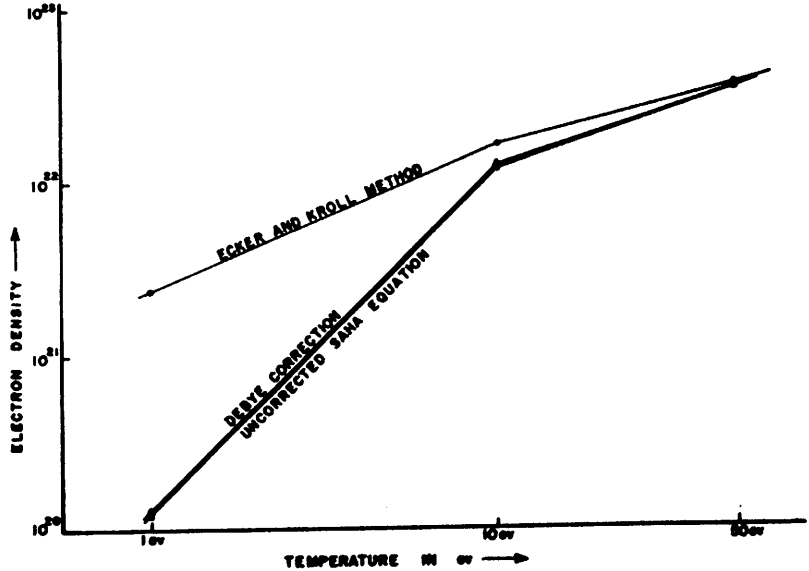

Fig. 6. Comparison of the calculated electron densities in an aluminum plasma with a heavy particle density of $6.02 \times 10^{22}/cm^3$. The three curves represent solutions obtained using the indicated method to correct the ionization potential.

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