Model and Transport Properties of Metals at High Energy Density

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Abstract – A model of the strongly coupled plasma generated by intense beams of charged particles and the electrical explosion of conductors is proposed and discussed. Expressions for the transport coefficients of locally equilibrium plasmas have been obtained that provide correct asymptotes for plasmas under normal conditions and for super dense and rarefied plasmas and are in good agreement with the results of experiments performed by DeSilva and Kunze [12].

1. Introduction

When a solid body is exposed to intense flows of charged particles or laser radiation or interacted with a high magnetic field, a strongly coupled, generally nonequilibrium, plasma is formed. The plasma characteristics, such as density ρ, hydrodynamic velocity $\mathbf{u}$, temperature T, electron concentration n_e, vary over wide range (from the condensed to the plasma state). Knowledge of the characteristics of strongly coupled plasmas at high energy density is of importance not only in the study of the physics of the interaction of charged particle and laser beams with matter, but also in technological applications of such beams.

Therefore, the main aim of this work is the development and investigation of a wideband model of plasma-like fluids that would allow one to determine the electronic thermodynamic functions, such as pressure $P_e(\rho,T)$ and internal energy $\varepsilon_e(\rho,T)$ or entropy $s_e(\rho,T)$, and the kinetic coefficients such as electric conductivity $\sigma(\rho,T)$, heat conductivity $\kappa_e(\rho,T)$, and thermoelectric coefficient $\alpha(\rho,T)$. Notwithstanding the advances in the theory of disordered media [1], this theory, unfortunately, gives no way of describing adequately the variations of the matter parameters over wide limits inherent in the interaction of intense energy flows with matter. This is why semi-empirical models [2] are used, as a rule, in constructing wideband models of matter. Obviously, the smaller the number of free (fitting) parameters determined by experiment, the more preferable the model.

Below we propose and investigate a physical model of a plasma-like medium, which involves a minimum number of free parameters. To determine these parameters, information about the properties of the medium under normal conditions and model notions about the structure of the disordered state and about the behavior of quasiparticle excitations (conduction electrons and phonons) is used. In terms of this model, called below a plasma model of metals, the metal is considered as plasma [3] in which the conduction electrons are one-particle excitations of a many-particle system.

2. Thermodynamic functions of the electronic component

Define the excitation energy for the electrons of outer atomic levels in the long-wave approximation by the expression [3]

$$E_g(\delta)=\begin{cases}0 & \text{for} \quad \delta \ge \delta_* \\ I_1/\varepsilon_r(\delta) & \text{for} \quad \delta \le \delta_*\end{cases}, \qquad (1)$$

where $\delta=\rho/\rho_0$ is the relative density; ρ_* and ρ_0 are, respectively, the metallization density of the material and its normal density; I_1 is the first ionization potential, and $\varepsilon_r(\delta)=1+3\delta/(\delta_*-\delta)$ is the relative permeability of the material.

Define the excitation energy for the electrons from inner atomic levels in the mean ion approximation, taking into account that the oscillation corrections are reduced due to the micro fields of free charged particles, by the following expression:

$$E_g=I^*(\tilde{z})+\delta I(\tilde{z})/\varepsilon_r(\tilde{z},V,T), \qquad (2)$$

where $\tilde{z}$ is the mean ion charge; $I^*(\tilde{z})$ and $\delta I(\tilde{z})=I(\tilde{z})-I^*(\tilde{z})$ are the mean ionization potential and the oscillation corrections to this potential; $I(\tilde{z})$ is the actual ionization potential;

$$\varepsilon_r(\tilde{z},V,T)=1+k_D^2\hbar^2/(2m_*\langle\varepsilon_e\rangle) \qquad (3)$$

is the relative permeability of the "gas" of free electrons; $k_D^2=\min\{k_s^2,k_{ei}^2\}, k_{ei}^2=k_{De}^2+(k_{Di}^4+k_s^4)/k_{Di}^2$; $r_s=k_s^{-1}=(3/(4\pi n))^{1/3}$; $k_{De}^2=6\pi e^2\tilde{z}n/\langle\varepsilon_e\rangle$ and $k_{Di}^2=4\pi e^2\tilde{z}^2n/(k_BT)$ are the squared Debye number for electrons and ions, respectively; $\langle\varepsilon_e\rangle$ is the mean energy of an electron; $m_*(\delta)$ is the effective mass of an electron in crystal, and k_B is Boltzmann constant. The equilibrium distribution function for the conduction electrons is the Fermi-Dirac distribution

$f_0 = 1/(\exp((\varepsilon - \mu_1)/k_B T) + 1)$, where the chemical potential $\mu_1 = \mu_{eff} - E_g$ (with μ_{eff} being the effective chemical potential) and the electron energy ε are functionals of the average number of conduction electrons $\tilde{z}$ in an atomic cell of volume $V = 1/n = MA/\rho$ (with M and A being, respectively, the unit atomic mass and the atomic weight of the material).

The average number of electrons per atomic cell, $\tilde{z}$, is related to f_0 by the normalization condition

$$\tilde{z}(V,T) = \frac{2^{1/2}(m_* k_B T)^{3/2}}{\pi^2 \hbar^3} F_{1/2}\left(\frac{\mu_{eff} - E_g}{k_B T}\right), \qquad (4)$$

and the thermodynamic functions of electronic component: electron energy

$$\varepsilon_e(V,T) = \varepsilon_{Te}(V,T) + \varepsilon_{ion}(V,T) \qquad (5)$$

with

$$\varepsilon_{Te}(V,T) = \begin{cases} \tilde{z} k_B T \dfrac{F_{3/2}(x)}{F_{1/2}(x)} - \dfrac{3}{5}\mu_0 \bar{z} & \text{for } \rho \geq \rho_* \\ \tilde{z} k_B T \dfrac{F_{3/2}(x)}{F_{1/2}(x)} & \text{for } \rho_* \geq \rho \end{cases}, \qquad (6)$$

$$x = \frac{\mu_{eff} - E_g}{k_B T};$$

$$\varepsilon_{ion} = \begin{cases} \int_0^{\tilde{z}} E_g(z)dz - \int_0^{\bar{z}} \bar{E}_g(z)dz, & \rho \geq \rho_* \\ \int_0^{\tilde{z}} E_g(z)dz & \rho \leq \rho_* \end{cases}, \qquad (7)$$

$\mu_0 = \mu_{eff}(V, T=0)$; $\bar{z}_c = \tilde{z}(V, T=0)$ is the average ion charge without considering oscillation corrections to mean ionization potential; the electronic pressure

$$P_e(V,T0 = g_e \varepsilon_{Te}(V,T)/V, g_e = \frac{2}{3} - \frac{d\ln\beta}{d\ln\delta}, \beta = \frac{m_*}{m}; \qquad (8)$$

the entropy

$$s_e(V,T) = k_B \tilde{z}\left(\frac{5}{3}\frac{F_{3/2}(x)}{F_{1/2}(x)} - x\right). \qquad (8)$$

In (4)-(8) $F_\nu(x)$ $(\nu > -1)$ is the Fermi-Dirac function:

$$F_\nu(x) = \int_0^\infty \frac{y^\nu dy}{\exp(y-x)+1}. \qquad (9)$$

To ensure a correct asymptote in the low temperature range and $\rho < \rho_*$, we write the effective chemical potential in the form

$$\mu_{eff}(V,T) = \mu_{TFC}(V,T) + \frac{E_g(V)}{2} + \delta\mu^{(1)}(V), \qquad (10)$$

where $\mu_{TFC}(V,T)$ is the chemical potential in the statistical Tomas-Fermi model with quantum and exchange corrections (TFC) [4]. However, the TFC model is inapplicable for normal conditions and for low temperatures and densities below normal densities. Since in the definition of the thermodynamic functions the chemical potential is under the integral sign, we may introduce additional corrections to the chemical potential of the TFC model with $T = 0$ to ensure the required asymptotes of thermodynamic functions. With this purpose we have introduced into (10) an additional correction $\delta\mu^{(1)}(V)$:

$$\delta\mu^{(1)}(V) = \begin{cases} \varepsilon_{F0} - \mu_{TFC}(V_0), & V \leq V_0 \\ \dfrac{\hbar^2}{2m_{*0}}\left(\dfrac{3\pi^2 z_0}{V}\exp\left(-\alpha\dfrac{1-\delta^{1/3}}{\left(\delta/\delta_*\right)^{1/3}-1}\right)\right)^{\frac{2}{3}} - & \\ -\mu_{TFC}(V), & V_0 \leq V \leq V_* \\ -\mu_{TFC}(V), & V_* \leq V \end{cases},$$

$$\alpha = \frac{3\left(1-\delta_*^{1/3}\right)}{\delta_*^{1/3} z_0}\left.\frac{d\tilde{z}}{d\delta}\right|_{\delta=1}, z_0 = \tilde{z}(\delta = 1), \qquad (11)$$

$$m_{*0} = m_*(\delta = 1).$$

In (11) ε_{F0} is the Fermi energy for $V = V_0$ and $T = 0$.

Thus the corrections to the chemical potential introduced by expression (11) allow us to calculate the equilibrium ionic composition of plasma over wide ranges of ρ and T with any degree of degeneracy of the plasma electronic component.

Value of the metallization density ρ_* is found from the universal equation of a condition of metals at $T = 0$, offered in [5]. Let's assume that is equal to value of density on spinodal of the stretched crystal. In result it is received: for Al $\delta_* = 0.663105$, Cu $\delta_* = 0.681989$ and W $\delta_* = 0.698817$. Note that these values are close to value for phase transition metal - insulator in mercury, which satisfies to the inequality $0.612 < \delta_* < 0.763$ [6].

3. Electronic transport coefficients

In finding the electronic transport coefficients for plasma-like media, we may ignore the collective interaction of conduction electrons, i.e. restrict ourselves to the consideration of the ideal gas of quasi-particle excitations. Since in this work we restrict ourselves to the approximation of a quasistationary electromagnetic field which is valid under condition $\omega_f \ll \omega_{pi} \sim \omega_m \ll \omega_{pe} \sim 10^{16}\,\text{s}^{-1}$ (with ω_f being the frequency of the electromagnetic field; ω_{pi}, ω_{pe} the ionic and electronic plasma frequencies, and ω_m the Debye frequency of the lattice vibrations), we here consider the transport coefficients for the case of weak electromagnetic fields. Solving the kinetic equation for conduction electrons in form presented by Shabansky [7] with the above restrictions and using the known definitions of the electric current density and the heat flux, we obtain the following expressions for

generalized Ohm's and Fourier's laws for plasma-like media:

$$\mathbf{E}+\frac{1}{c}\nabla\mu_1=\frac{\mathbf{j}}{\sigma}+\alpha\nabla T,\quad \mu_1=\mu_{eff}-E_g;$$
$$\mathbf{q}'=\mathbf{q}-\left(\varphi-\frac{\mu_1}{e}\right)\mathbf{j}=\frac{\mu_1K_{00}-eK_{01}}{\mu_1M_{00}-eM_{01}}\alpha T\mathbf{j}-\kappa_e\nabla T, \tag{12}$$

where the conductivity

$$\sigma=M_{00}; \tag{13}$$

the thermoelectric coefficient

$$\alpha=\frac{1}{eT}\left(\mu_1-\frac{eM_{01}}{M_{00}}\right); \tag{14}$$

the electronic heat conductivity

$$\kappa_e=\frac{K_{00}}{eT}\left(\frac{M_{01}}{M_{00}}\left(\mu_1-\frac{eK_{01}}{K_{00}}\right)-\frac{K_{01}}{K_{00}}\left(\mu_1-\frac{eK_{02}}{K_{01}}\right)\right); \tag{15}$$

$$M_{0\beta}=\frac{2m_*e^{2-\beta}}{3\pi^2\hbar^3}\frac{\partial}{\partial\mu_1}\int_0^\infty\varepsilon^{\beta+1}l_{\mathbf{j},eff}(\varepsilon)f_0\left(\frac{\mu_1}{k_BT}\right)d\varepsilon, \tag{16}$$
$$\beta=0,1;$$

$$K_{0\gamma}=\frac{2m_*e^{2-\gamma}}{3\pi^2\hbar^3}\frac{\partial}{\partial\mu_1}\int_0^\infty\varepsilon^{\gamma+1}l_{\mathbf{q},eff}(\varepsilon)f_0\left(\frac{\mu_1}{k_BT}\right)d\varepsilon, \tag{17}$$
$$\gamma=0,1,2.$$

In (16)-(17) $l_{\mathbf{j},eff}(\varepsilon), l_{\mathbf{q},eff}(\varepsilon)$ are the mean free paths of electrons. The necessity of use of a mean free path $l_{\mathbf{q},eff}\neq l_{\mathbf{j},eff}$ in the Fourier's law is connected with the fact that heat in degenerate plasma is transferred not only by electron diffusion on the Fermi surface with relaxation time $\tau_{\mathbf{j},eff}$, but also by electron transition between their states under and over the Fermi surface [8]. At $T\ll\Theta$ (with Θ being the Debye temperature) the second process is essentially faster than the first process is. Assume that these processes are independent, we use the following expression for $l_{\mathbf{q},eff}$ [8]:

$$l_{\mathbf{q},eff}=\frac{l_{\mathbf{j},eff}}{1+3\pi^{-2}(k_Fk_D^{-1})^2(\Theta T^{-1})^2}. \tag{18}$$

The effective mean free path of conduction electrons $l_{\mathbf{j},eff}$ $l_{\mathbf{j},eff}$ is given by

$$l_{\mathbf{j},eff}(\varepsilon)=\begin{cases}r_s, & r_s>l_{\mathbf{j}}(\varepsilon)\\ l_{\mathbf{j}}(\varepsilon), & r_s<l_{\mathbf{j}}(\varepsilon)\end{cases}. \tag{19}$$

In determining $l_{\mathbf{j}}$ we use the analogy between the scattering of x-radiation in matter and the scattering of conduction electrons by density fluctuations that was first used by Frenkel [9] to explain the temperature dependence of the resistivity of metals. This analogy is in fact the essence of the so-called Ziman formula [8] for the mean free path. According to this theory, the mean free path is given by

$$l_{\mathbf{j}}^{-1}=\frac{n}{4\pi k^4}\int_0^{2k}S^2(q)\left|\left\langle\mathbf{k}+\mathbf{q}\,|\,w_i\,|\,\mathbf{k}\right\rangle\right|^2|\varepsilon(q)|^{-2}q^3dq, \tag{20}$$

where $S^2(q)$ is the static structure factor; $\left\langle\mathbf{k}+\mathbf{q}\,|\,w_i\,|\,\mathbf{q}\right\rangle$ is the form factor of the effective potential of a "bare" ion; $\varepsilon(q)=1+k_D^2/q^2$ is the static permeability of a "metallic" plasma.

For a structure factor we use an expression [8] taking into account that for $T\ll\Theta$ the wave number $q_D=\omega_m/c_s$ (with c_s being the sound velocity) serves as a truncation factor:

$$S^2(q)=S^2(0)\frac{q\Theta/(q_DT)}{\exp\left(q\Theta/(q_DT)\right)-1}=$$
$$=G^{-1}(\rho,T)\frac{q\Theta/(q_DT)}{\exp\left(q\Theta/(q_DT)\right)-1}, \tag{21}$$

where $G(\rho,T)=K_s/(nk_BT)=c_s^2/c_{Ti}^2$ (with $c_{Ti}=(k_BT/m_i)^{1/2}$ being the isothermal sound velocity at $\gamma=1$; $K_s=\delta(\partial P_s/\partial\delta)_T$ the isothermal compressibility modulus; P_s the "structural" part of the total pressure). It is $G(\rho,T)$ that determines, in the long-wave approximation, the density fluctuations.

To determine the form factor $\left\langle\mathbf{k}+\mathbf{q}\,|\,w_i\,|\,\mathbf{k}\right\rangle$, we use the effective potential (pseudopotential)

$$w_i(r)=\frac{e\tilde{z}}{r}-\frac{e(Z-\tilde{z})}{r}\exp\left(-\frac{r}{r_c}\right) \tag{22}$$

(With r_c being the radius of screening of skeleton electrons) for both the charged and the neutral component of plasma, that is, our model uses the average ion (atom) approximation. Below we use for r_c the approximate expression

$$r_c=\frac{Z-\tilde{z}}{Z^{2/3}}\left(\frac{\left\langle r^2\right\rangle_a}{6}\right)^{1/2} \tag{23}$$

with the values of $\left\langle r^2\right\rangle_a$ taken from [10]. Expressions (22) and (23) describe approximately the variation in the effective pair scattering potential over wide ranges of P and T.

In calculating the cross section for the electron scattering by ions, we restrict ourselves by the case of Lorentz plasmas. Calculating for this case the integral in (20), in view of (21) - (23), we obtain the following expression for the mean free path $l_{\mathbf{j}}(\varepsilon)$:

$$l_{\mathbf{j}}(\varepsilon)=\frac{\varepsilon^2G(\rho,T)}{\pi ne^4\left(\tilde{z}^2\Lambda_1-2\tilde{z}\left(Z-\tilde{z}\right)\Lambda_2+\left(Z-\tilde{z}\right)^2\Lambda_3\right)}, \tag{24}$$

where

$$\Lambda_1=b_1^4\int_0^{\frac{2k\Theta}{q_DT}}\frac{\xi^4d\xi}{\left(\exp(\xi)-1\right)\left(1+b_1^2\xi^2\right)^2}, \tag{25}$$

$$\Lambda_2=b_1^2b_2^2\int_0^{\frac{2k\Theta}{q_DT}}\frac{\xi^4d\xi}{\left(\exp(\xi)-1\right)\left(1+b_1^2\xi^2\right)\left(1+b_2^2\xi^2\right)}, \tag{26}$$

$$\Lambda_3 = b_2^4 \int_0^{\frac{2k\Theta}{q_D T}} \frac{\xi^4 d\xi}{\left(\exp(\xi)-1\right)\left(1+b_2^2\xi^2\right)^2} \qquad (27)$$

are analogs of Coulomb's logarithm; $b_1 = q_D T/(k_D\Theta)$; $b_2 = q_D r_{cd} T/\Theta$; $r_{cd} = r_c/(1+k_D r_c)$. In (24) the second bracketed term takes into account the simultaneous scattering by the nucleus and by the electrons of the ionic skeleton, while the third one involves only the scattering by the electrons of the ionic skeleton. For $T \ll \Theta$ we have $b_1\xi \ll 1, b_2\xi \ll 1$, and $\Lambda_1 = 4! b_1^4$, $\Lambda_1 = 4! b_1^2 b_2^2$, $\Lambda_2 = 4! b_2^4$. Accordingly $l_j^{-1} \sim T(T/\Theta)^4$. In this case, the electrons of the ionic skeleton also contribute to the mean free path of electrons.

4. Discussion

From the above consideration of the plasma model it follows that for the determination of the transport coefficients, and other characteristics of a plasma-like medium, it is necessary to know the isothermal compressibility modulus K_s which, in the long-wave approximation, determines the fluctuations of density (structure factor) and, hence, the scattering of electrons by ions. The isothermal compressibility modulus is determined by the "structural part" of the equation of state $P_s(\rho,T) = P_\pi(\rho) + P_i(\rho,T)$ (with $P_\pi(\rho)$ being the potential part of the total pressure $P(\rho,T)$, and $P_i(\rho,T)$ the lattice part of $P(\rho,T)$). Below, as in [3], we use for the calculation of the electronic coefficients the equation of state proposed by Kolgatin and Khachaturiyants [11].

Using above obtained expressions, we have calculated the mean charge of the ion and transport coefficients for copper in a wide range of ρ and T. Fig. 1a presents the results of experiments by DeSilva and Kuntze [12] taken from a review [13] together with the results of the analysis performed by authors of [12] with the use of well-known theoretical models of strongly coupled plasma (see also [13]).

For the dependence $\sigma(\Gamma)$ where $\Gamma = \tilde{z}^2 e^2 n^{1/3}/(k_B T)$ is the nonideality parameter to be represented unambiguously, it is necessary to know the law of variation of $n(T)$. Authors of [12] used in analyzing experimental data a zero-dimensional self-consistent code with well-known theoretical models employed as plasma models. In this case, the experimental estimates of temperature were accurate to within 30%. Since we do not know the law of variation of $n(T)$ in experiments of [12], we, when comparing our model with their results, took independent values of n and T in the following ranges of parameters: $1.557\cdot10^{17} \le n \le 8.55\cdot10^{22}$ cm^{-3}, $605 \le T \le 2.812\cdot10^{10}$ K and used an additional fitting parameter which shifted our results to the region of large values of the nonideality parameter, which is quite admissible in view of the great uncertainty of the information about the variations of plasma parameters in the experiment. So obtained values of $\sigma(\Gamma)$ are given in Fig. 1b. Comparison of experimental (Fig. 1a) and theoretical values of $\sigma(\Gamma)$ (Fig.1b) shows their qualitative and quantitative agreement.

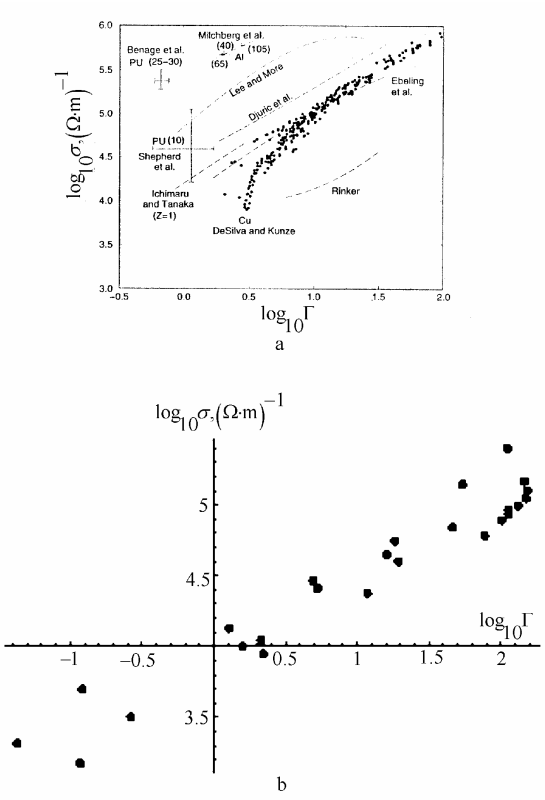

Fig.1. Conductivity of strongly coupled copper plasma after DeSilva and Kunze [12] and Redmer [13] (• - results of experiments [12]; --- - theoretical predictions) (a) and our model (b).

5. Conclusions

In this work we suggested a physical model of strongly coupled plasma and obtained the wide-band expressions for the thermodynamic functions of the electronic component of such plasma and for the electronic transport coefficients. Our results allow to conclude that the plasma model offers a qualitative and quantitative, with sufficient accuracy for applications, description of the behavior of the transport coefficients of a plasma-like medium at high energy densities over a wide range of its parameters.

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