Semiempirical wide-range conductivity model with exploding wire verification

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Based on well-established physical relationships, a semiempirical set of equations dictating the electrical conductivity of dense, strongly coupled, partially ionized copper is presented. With the empirical coefficients, the model is tuned to experimental conductivity data obtained from exploding wire experiments [A. W. DeSilva and J. D. Katsouros, Phys. Rev. E **57**, 5945 (1998)]. The result is a wide-range conductivity model, with demonstrated accuracy from room temperature-density conditions to 0.01 g/cm^3 and 30 kK. Using magnetohydrodynamic simulation the ability to utilize the conductivity model for predictive simulations is demonstrated. A complete electrical conductivity dataset for copper has been made available to the public.

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I. INTRODUCTION

Development of accurate conductivity models for plasma has been a topic of study for several decades [1,2]. Moreover, the development of conductivity models for dense metal plasmas with non-negligible Coulomb interaction (i.e., strongly coupled plasma or nonideal plasma) has proved to be particularly challenging [3–5]. Most often the plasma ideality parameter Γ is defined as the ratio of potential energy to kinetic energy given as $\Gamma = e^2/(k_B T r_D)$, where e is the elementary charge, k_B is Boltzmann's constant, T is the temperature, and r_D is the Debye radius. A plasma is said to be nonideal when the ideality parameter is on the order of or above unity. Often, conductivity models relevant here are derived from theoretically rigorous methodologies, with limited validity ranges. As an example, the well-known Spitzer conductivity has been shown to be accurate for higher temperatures and lower density [1,3–5], whereas the Ziman formula has been shown to be accurate in the high-density regime [3–6]. However, few models show promise for maintaining accuracy through a wide temperature-density span.

With a semiempirical approach, Lee and More developed a means of calculating transport properties through a very wide parameter range with several approximations made within each range of interest [7]. Though rigorously theoretically justified, the Lee-More model uses semiempirical estimates for parameters that remain *a priori* unknown. In more recent efforts Redmer utilized a chemical potential and linear response model to predict transport properties of dense plasmas [8]. Further development of this model by Kuhlbrodt *et al.* [9,10] produced COMPTRA, a publicly available software package for the calculation of composition and transport properties of dense plasma. For the Lee-More-Desjarlais (LMD) model, using the calculations of Redmer [8], experimental conductivity of DeSilva [11], and quantum molecular dynamics (QMD) data [12], Desjarlais refined the Lee-More model to more accurately address the performance in the metal-nonmetal (MNM) transition regime [13]. Here the data referred to as QLMD indicate a tuned version of the LMD model to quantum molecular dynamic results, compiled by Cochrane and Desjarlais of Sandia National Laboratories.

Nonetheless the availability of accurate conductivity data over a wide parameter range remains limited. For instance in 1976, Bakulin, Kuropatenko, and Luchinskii (BKL) presented an empirical equation of state and transport model, which even today demonstrates reasonable accuracy [14]. Much of the exploding wire community continues to use the BKL model or other obsolete models, often owing to the lack of availability of an alternative [15–21].

It is the aim of the presented work to utilize theoretical formulations to develop a platform for a practical, semiempirical model, from which an arbitrary phase conductivity dataset is generated. This model is shown to be consistent with various other models [10,13,22], QMD simulations [23], and experimental conductivity data [11]. The results of these calculations have been made available to the public [24] and are also available from the Supplemental Material included with this publication [25].

In a previous publication a one-dimensional magnetohydrodynamic (MHD) model was benchmarked against experimental exploding wire (EW) data to assess the accuracy of the QLMD data as well as the Knoepfel model in the sub-eV regime and densities from solid density (8.94 g/cm^3) to 0.05 g/cm^3 [26]. This technique is again applied here to demonstrate the accuracy of the semiempirical model.

II. BACKGROUND THEORY

As stated the goal is to develop a model to calculate electrical conductivity in the arbitrary phase approximation as a function of temperature T and mass density ρ. For high density, the electrical conductivity is known to be inversely proportional to the temperature [27]. Further, from evaluating QMD simulation results it was observed that for densities above the critical point the conductivity exhibits $\sim\rho^{7/3}$ dependence [12]. These relationships are well represented by a modified form of the conductivity equation given by Knoepfel [28];

$$\sigma_1 = \frac{\sigma_0}{1+\beta(T-T_0)}\left(\frac{\rho}{\rho_0}\right)^{\alpha(T)}. \tag{1}$$

It was found that

$$\alpha(T) = \begin{cases} 5 - 2.5\frac{T}{5\text{ kK}} & \text{for } 300\text{ K} \leqslant T \leqslant 5\text{ kK} \\ 2.5 - 1.5\frac{T}{30\text{ kK}} & \text{for } 5\text{ kK} < T \leqslant 30\text{ kK} \end{cases} \tag{2}$$

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produced the best fit with experimental data available in the open literature. Here σ_1 is the conductivity at high density, and σ_0 is the conductivity at room temperature T_0 and density ρ_0. The parameters α and β are empirical coefficients where α is defined by Eq. (2), and β is taken to be a constant 5×10^{-4} K^{-1}.

Equation (1) provides a reasonable approximation for electrical conductivity for densities in the vicinity of liquid-solid densities approaching ρ_0. Approximation of the conductivity in the vapor (ionized) regime requires a more involved approach. For this region, the Saha equation can be used to approximate the electron density, n_e.

$$K = 2\frac{\Sigma^+}{\Sigma}\frac{1}{\Lambda_e^3}\exp\left\{-\frac{W_{iz}}{k_B T}\left[1-\left(\frac{1.5e^2}{W_{iz}R_{ws}}\right)^{1.5}\right]\right\}, \quad (3)$$

and

$$n_e = \tfrac{1}{2}(\sqrt{K^2 - 4n_T K} - K). \quad (4)$$

Note that for the higher densities of interest here, the Saha equation invokes the density modification factor in the exponential proposed by Desjarlais [13]. This behavior is well documented in literature and most commonly referred to as a reduction of the ionization potential due to inter-Coulomb interaction between charged particles [3]. Here n_T is the total density of heavy particles, both neutrals and ions. The partition functions of the atom and ion are given as Σ and Σ^+, respectively. The ionization potential is W_{iz}, and $R_{ws} = (3/4\pi n_T)^{1/3}$ is the Wigner-Seitz radius. The electron thermal wavelength is denoted as $\Lambda_e = (h^2/2\pi m_e k_B T)^{1/2}$, where h is the Planck constant and m_e is the electron mass. With this the electrical conductivity in the region relative to the modified Saha equation σ_2 can be estimated using the generic electrical conductivity equation,

$$\sigma_2 = \frac{n_e e^2 \tau_e}{m_e}. \quad (5)$$

The average time between electron momentum transfer collisions τ_e is calculated using an empirical modification to the hard-sphere approximation.

$$\tau_e = \frac{1}{n_T \sigma_{\mathrm{HS}} v_{th}}\left(\frac{\rho}{\rho_0}\right)^{0.15+0.15\frac{T}{30kK}}. \quad (6)$$

Here σ_{HS} indicates the characteristic hard-sphere cross section assumed to be constant and equal for both ions and neutrals. A momentum transfer cross section of 3×10^{-15} cm^2 was found to provide the best result which is reasonably consistent with the hard-sphere cross section given by Desjarlais [13]. The average electron thermal velocity is given as $v_{th} = (3k_B T/m_e)^{1/2}$.

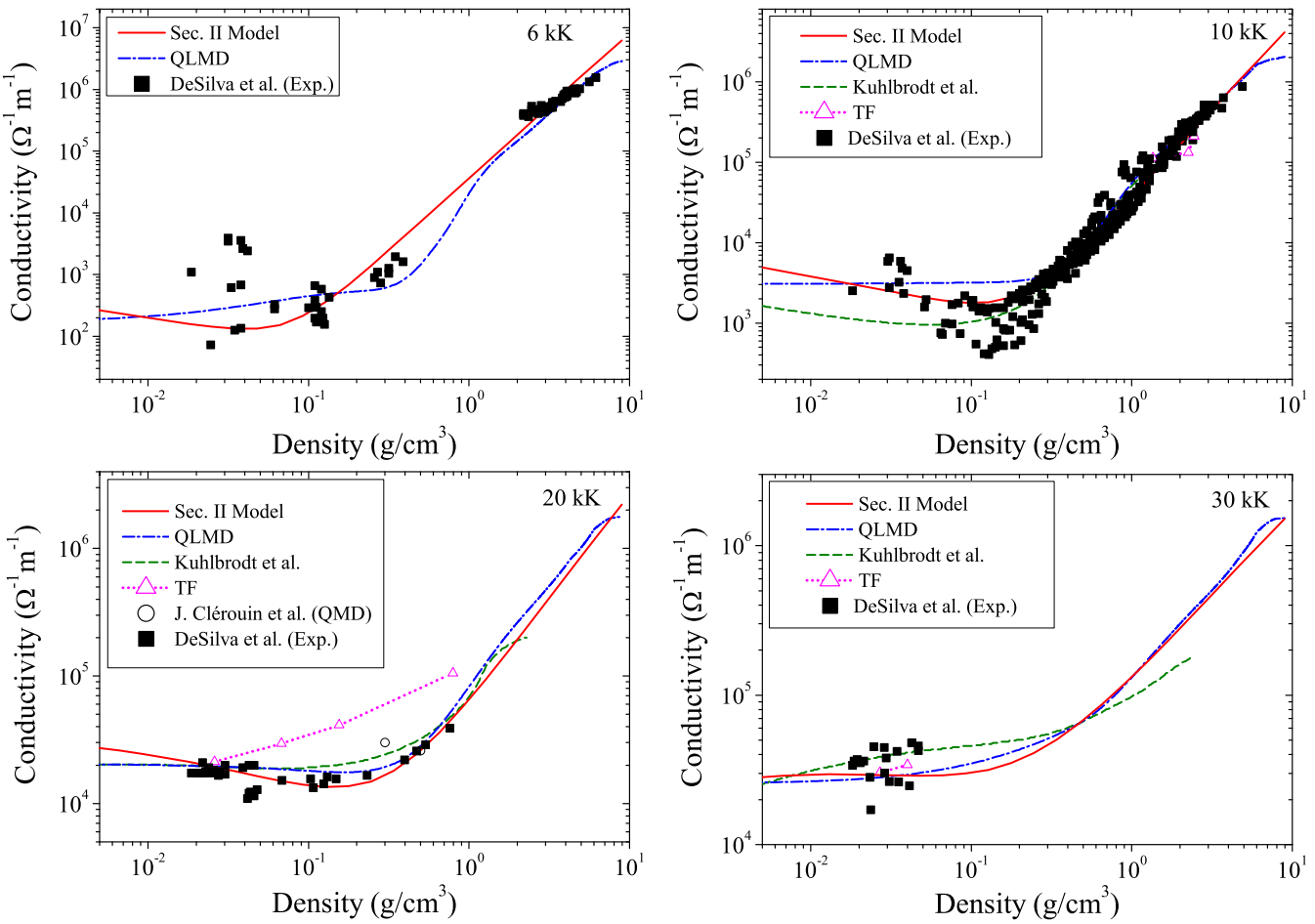

FIG. 1. (Color online) Empirically calculated conductivity isotherms versus mass density with comparison to QLMD [12], Kuhlbrodt and Redmer [9], Tkachenko and Fernández de Córdoba (TF) [22], Clérouin (QMD) [23], DeSilva (experimental) [11].

Equation (1) provides a decent approximation to conductivity for liquid-solid densities, while Eq. (5) is more appropriate for the modified Saha regime. By comparison with available conductivity data both theoretical and experimental, the following equation was found to provide a smooth transition between σ_1 and σ_2.

$$\sigma = \sigma_1 \left(\frac{\rho}{\rho_0}\right)^{\gamma} + \sigma_2 \left(1 - \frac{\rho}{\rho_0}\right)^{\gamma}, \tag{7}$$

where γ is an empirical factor taken to be 0.15. The final conductivity σ provides an accurate means of approximation to the electrical conductivity from room temperature and density, up to 30 kK and densities as low as 0.01 g/cm^3.

III. DISCUSSION

The results of the formulations given in Sec. II are depicted in Fig. 1 along with the experimental data available. As a general rule, the model was optimized to best capture the results of experimental conductivity data and QMD simulation results. Additional theoretical models were used as an attempt to demonstrate either validity or potential limitations in the empirical model.

For each of the isotherms given, it is shown that the conductivity model is capable of reasonably capturing the behavior exhibited by the experimental data of DeSilva [11]. Due to the overall scarcity of data only limited optimization was possible. The model is in fair agreement with the QLMD data, with notable departures at lower densities of ~0.1 g/cm^3 and below. Similar observations are made when the model given in Sec. II is compared with data from Kuhlbrodt *et al.* This indicates low-density limitations in the Sec. II model, a consequence of its semiempirical nature. Further comparison with the data given by Tkachenko and Fernández de Córdoba (TF) indicates merely fair agreement at 10 and 30 kK, with notable deviations at 20 kK. Given the agreement between all other theoretical formulations, QMD data, and experimental data at 20 kK, the TF data have to be considered inaccurate at 20 kK.

In a previous study a simple capacitor discharge circuit was utilized to explode a single EW in air at atmospheric pressure [26]. The system capacitance and inductance were 1.85 μF and 2.7 μH, respectively. By varying the initial voltage on the capacitor, different temperature-density trajectories were achieved in the sub-eV regime. Comparison of experimental voltage and current with MHD predicted voltage and current provided a means of verifying the conductivity models applied within the MHD simulation. It was revealed that using QLMD data yielded strong agreement between the measured voltage and current waveforms and the MHD predicted voltage and current waveforms, whereas simulations with Knoepfel conductivity demonstrated obvious limitations [26]. The MHD

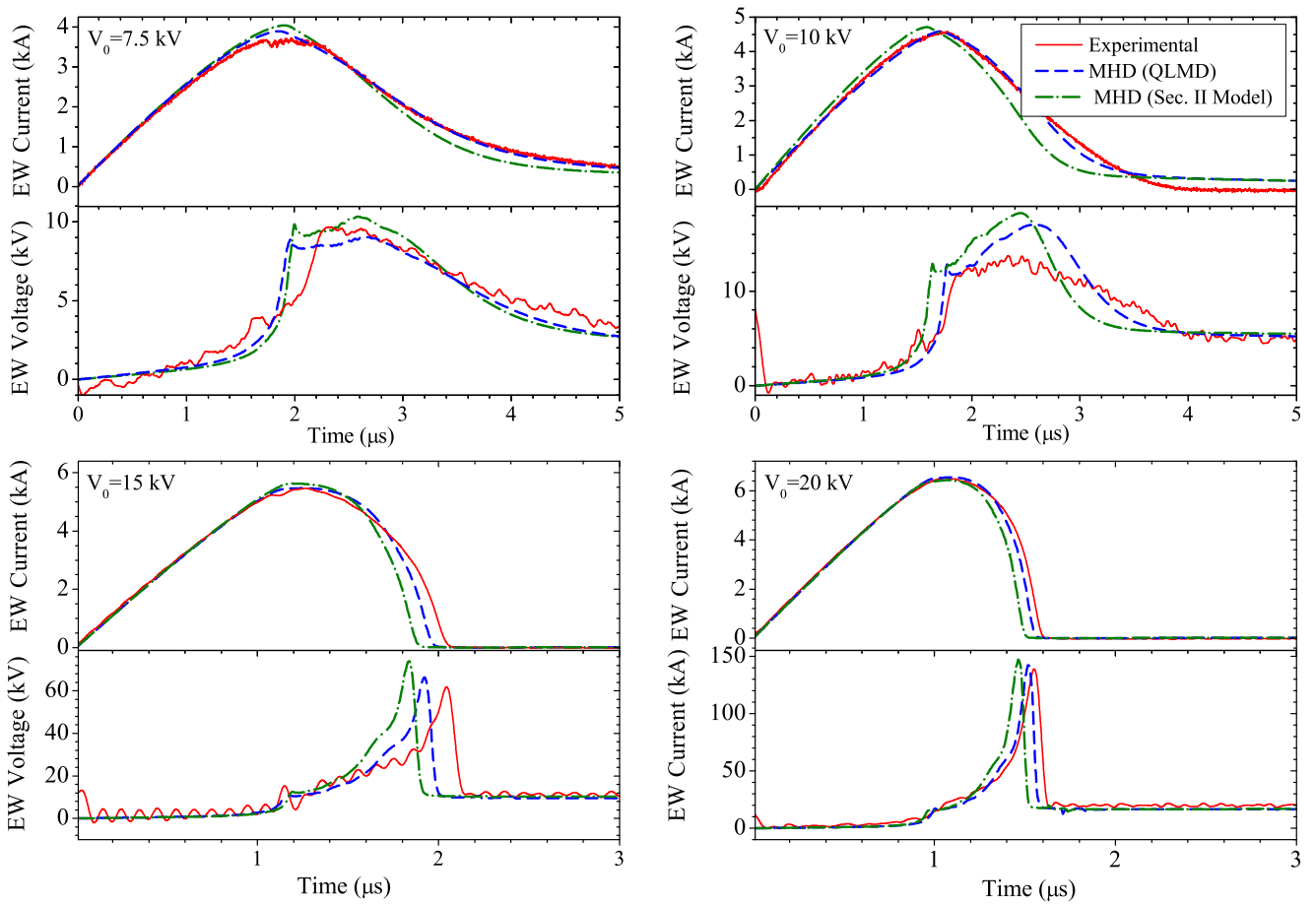

FIG. 2. (Color online) Experimental and MHD predicted voltage and current waveforms from capacitor discharge EW experiments with a 127-μm-diameter 18-cm-long copper wire in air at various initial capacitor voltages.

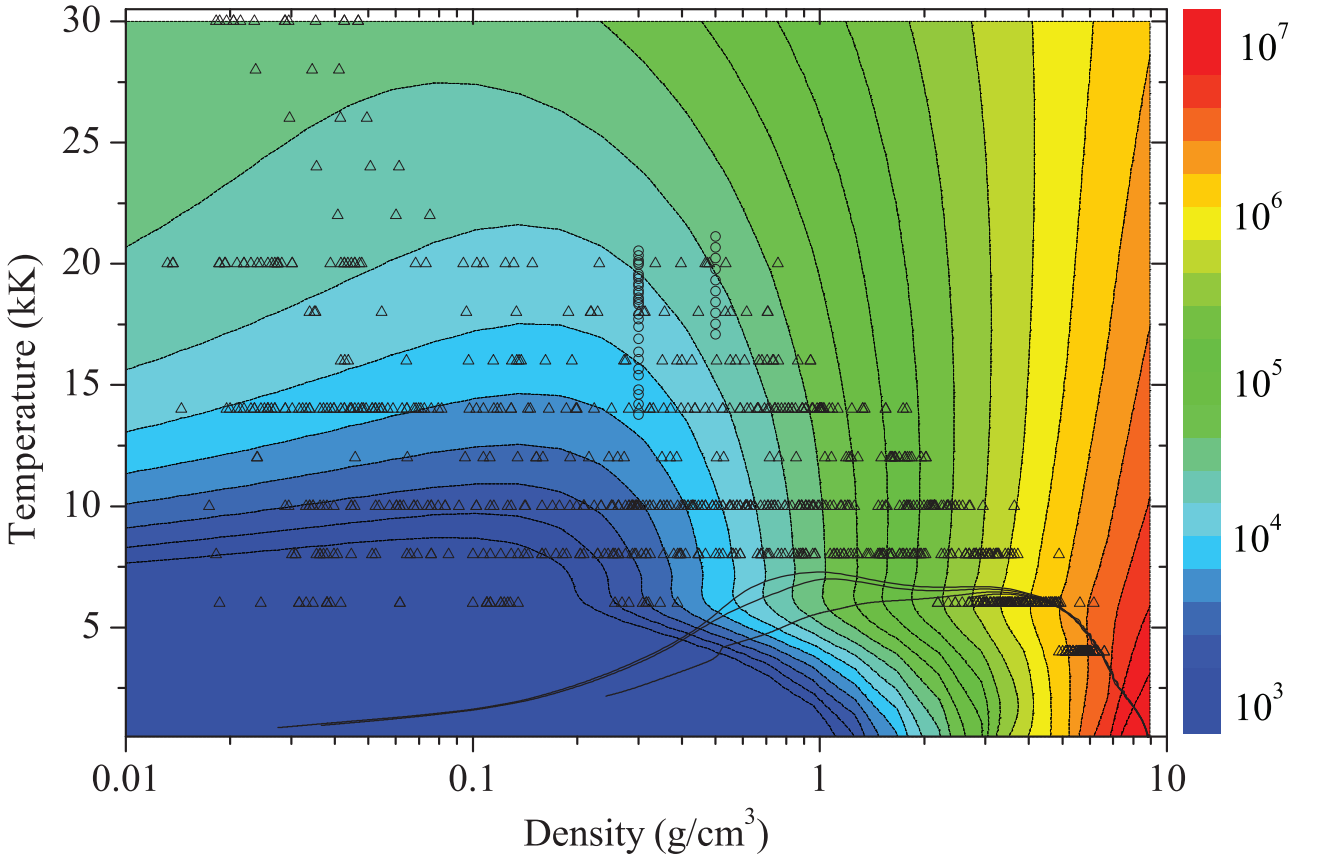

FIG. 3. (Color online) Conductivity contour plot ($\Omega^{-1}\,m^{-1}$) with temperature-density trajectories from EW experiments in Fig. 2 (solid lines), experimental conductivity data (triangles) [11], and QMD simulated data (circles) [23].

simulation waveforms using the QLMD data are included Fig. 2, along with additional waveforms demonstrating the performance of the MHD model with the Sec. II conductivity model.

Using MHD with the empirical model, each of the experimental waveforms is replicated within a reasonable degree of accuracy. For the lower initial capacitor voltages $V_0 =$ 7.5 kV and 10 kV, negligible error is observed, with QLMD based simulations holding no significant advantage over the empirical conductivity based simulations. At the higher initial capacitor voltages $V_0 = 15$ kV and 20 kV, the voltage and current are better represented by the QLMD based simulations. Nonetheless, the empirical conductivity model based MHD simulations were still able to capture the voltage and current behavior to a moderate degree of accuracy.

Figure 3 depicts the empirical conductivity versus both temperature and density, including the temperature-density trajectories from the EW experiments shown in Fig. 2, the experimental conductivity data points from DeSilva *et al.* [11], and the QMD simulation points from J. Clérouin *et al.* [23]. Ultimately, the experimental and QMD data along with the temperature-density trajectories indicate the regions at which the presented model has demonstrated reasonable accuracy.

As stated previously, few models exhibit the ability to transition from high-density degenerate regimes to low-density regimes largely owing to the starkly different conduction mechanisms in action. As a more advanced approach, QMD presents the ability to treat electrons without discriminating between bound and free states; thus all conduction mechanisms are captured. Otherwise, no theoretical model has demonstrated the ability to transition across the regimes of interest while maintaining a high degree of accuracy. Even in the QLMD derivations empirical blending is used to transition from the Thomas-Fermi regime to the modified Saha regime. This work provides a simplistic approach to calculating the electrical conductivity over a wide temperature-density span. It is expected that this model will exhibit limitations in the high-density and high-temperature extreme due to a limited validity of Eq. (1). This could be addressed with the application of a more appropriate model. However, this region is highly atypical, for instance, in most exploding wire experiments.

Obviously, the developed semiempirical model has limitations in its accuracy as discussed; however, this is expected given its basic foundation. The ultimate goal was to derive a straightforward conductivity model, capable of covering a broad temperature-density span with practical accuracy. The developed model, wholly defined within a few basic equations, was shown to be in reasonable agreement with data from numerous conductivity resources through a wide temperature-density span. Moreover, the calculated conductivity demonstrated predictive capabilities via MHD simulation of an exploding wire. Though further verification of this model is necessary, in its present state, the model is suitable for a broad range of applications requiring accurate conductivity data in the range of 300 K–30 kK, 0.01–8.94 g/cm^3, and possibly beyond.

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