Reflectivity of Shock Compressed Xenon Plasma

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Abstract

Experimental results [1] for the reflection coefficient of shock-compressed dense Xenon plasmas at pressures of 1.6 – 17 GPa and temperatures around 30 000 K using a laser beam with $\lambda = 1.06 \ \mu m$ are compared with calculations based on different theoretical approaches to the dynamical collision frequency. It is found that a reasonable description can be given assuming a spatial electron density profile corresponding to a finite width of the shock wave front of about $2 \cdot 10^{-6} \ m$.

1 Reflectivity measurements

Experiments with an explosively driven generator of shock waves to produce dense nonideal Xenon plasmas were reported in [1]. The reflectivity was measured using a laser system with the wave length $\lambda_l = 1.06 \ \mu m$. The results of the experiments are shown in Tab. 1. The thermodynamic parameters of the plasma were determined from the measured shock wave velocity. The plasma composition was calculated within a chemical picture [2]. Working with a grand canonical ensemble [3] virial corrections have been taken into account due to charge-charge interactions (Debye approximation). Short range repulsion of atoms and ions (including multiply charged positive ions) was considered via second and third virial coefficients within a virial expansions. In the parameter range of the shock wave experiments, derivations of up to 20 % for the composition have been obtained depending on the approximations for the equation of state. This is within the accuracy of the experimental values of the reflectivity.

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Tab. 1: Experimental results for the reflectivity $R$ of Xenon plasmas at given parameter values: pressure $P$, temperature $T$, mass density $\rho$, free electron number density $n_e$ and density of neutral atoms $n_a$. 

It was suggested that the measurement of reflectivity allows to determine the concentration of free electrons in the plasma. However, investigating these data [1], it was not possible to find a direct relationship between the values of free electron density \( n_e \) and the reflectivity \( R \). The reflection coefficient increases smoothly with the free electron density. It approaches only slowly values characteristic for metals, although the critical density for metallic behaviour \( n_e^c = 1.02 \times 10^{21} \text{cm}^{-3} \), where the plasma frequency, \( \omega_{pl} = \sqrt{n_e e^2/(\varepsilon_0 m_e)} \) with \( m_e \) the electron mass, coincides with the frequency \( \omega_l \) of the probing laser pulse, is exceeded even at the lowest density. However, this critical density is taken from the RPA approximation for the dielectric function in the long–wavelength limit \( \epsilon = 1 - \omega_{pl}^2/\omega_l^2 \) where total reflection occurs due to a vanishing dielectric function. Taking collisions into account this will be smoothed out. On the other hand, a sharp boundary between plasma and undisturbed gas in front of shock wave is assumed.

In [1], the spatial structure of the ionizing shock wave was discussed, showing three characteristic zones, which may influence the electromagnetic wave propagation. In a precursor zone, the gas is heated, but the influence on the wave propagation is small. In the region of the shock wave front a steep increase of the free electron density is expected. The width of the wave front is determined by relaxation processes in the plasma. It was estimated to be of the order \( d \approx 10^{-7} \text{m} \) [1], which is one order of magnitude less than the laser wave length. Under this condition \( d/\lambda \ll 1 \), the laser beam reflection was assumed to be determined by the electron properties of the plasma behind the shock wave front. An expression derived from the Fresnel formula in the long–wavelength limit

\[
R(\omega) = \frac{\sqrt{\epsilon(\omega)} - 1}{\sqrt{\epsilon(\omega)} + 1}^2
\]  

(1)

was applied where the frequency \( \omega \) has to be taken at the laser frequency \( \omega_l = 1.8 \cdot 10^{15} \text{Hz} \). The complex frequency–dependent dielectric permittivity

\[
\epsilon(\omega) = 1 + \frac{i}{\epsilon_0 \omega} \sigma(\omega) = 1 - \frac{\omega_{pl}^2}{\omega \omega + i\nu(\omega)}
\]  

(2)

has been related to the dynamical conductivity \( \sigma(\omega) \) or the dynamical collision frequency \( \nu(\omega) \). The Drude formula

\[
\sigma(\omega) = \frac{\epsilon_0 \omega_{pl}^2}{\nu(0) - i\omega}
\]  

(3)

follows if the collision frequency is taken in the static limit \( \nu(0) = \epsilon_0 \omega_{pl}^2/\sigma(0) \) relating it to the static conductivity \( \sigma(0) \). Different expressions for \( \sigma(0) \) have been considered in [1], but no satisfying explanation of the experimental results has been given there. As will be seen in the following discussion, the Drude model is not an appropriate approximation under the experimental conditions considered. In the present work, improvements in the calculation of the dielectric function as well as considerations concerning the shape of the wave front will be discussed to find a consistent theoretical approach to the measured reflectivities.
2 Reflection by a step-like plasma front

In this section, we investigate the reflection coefficient at a shock wave front where its width \( d \) shall be neglected. According to the Fresnel formula, the reflection coefficient at a step-like plasma front \[4\]

\[
R(\omega) = \left| \frac{1 - Z(\omega)}{1 + Z(\omega)} \right|^2 ,
\]

is related to the surface impedance \( Z \) (normal incidence). The surface impedance can be related to the transverse dielectric function via

\[
Z(\omega) = -\frac{i\omega}{\pi c} \int_{-\infty}^{\infty} dk \frac{1}{k^2 - \omega^2 \epsilon_t(k, \omega)/c^2} . \tag{5}
\]

This is a more general expression than (1) for the reflectivity. Assuming that the transverse dielectric function \( \epsilon_t(k, \omega) \) is independent of the wave vector \( k \), the integral (5) can be evaluated leading to the expression (1) given above.

In general, the dielectric function is related to a dynamical, nonlocal collision frequency \( \nu(k, \omega) \),

\[
\epsilon_t(k, \omega) = 1 - \frac{\omega_{\text{pl}}^2}{\omega[\omega + iv_t(k, \omega)]} , \tag{6}
\]

which is defined by extending the above definition (2) to finite values of the wave vector \( k \). In recent papers \[5, 6\], an approach to the dielectric function within a linear response theory was developed. Different approximations have been investigated with respect to their consistency. Having this in mind, we are able to give a more precise description of the dielectric function at the plasma parameters considered here.

2.1 Born approximation

Before considering the nonlocal dielectric function below, we discuss the long–wavelength limit \( k \to 0 \), replacing \( \epsilon_t(k, \omega) \) by \( \epsilon_t(0, \omega) \) in Eq. (5). In this case, the transverse and longitudinal dielectric function are identical. The dynamical collision frequency can be evaluated in Born approximation with respect to the statically screened potential (Debye potential), see \[5\], as (the non-degenerate case is considered)

\[
\nu^{\text{Born}}(\omega) = -ig n_e \int_0^\infty dy \frac{y^4}{(\bar{n} + y^2)^2} \int_{-\infty}^{\infty} dx e^{-2(x-y)^2} \frac{1 - e^{-4xy}}{xy(xy - \bar{\omega} - i\eta)} , \tag{7}
\]

where

\[
\bar{n} = \frac{\hbar^2 n_e e^2}{8\epsilon_0 m_e (k_B T)^2} ,
\]

\[
g = \frac{e^4 \beta^{3/2}}{24\sqrt{2}\pi^{5/2} \epsilon_0^3 m_e^{1/2}} ,
\]

and \( \bar{\omega} = \hbar \omega /(4 k_B T) \). The second integral in (7) is a complex quantity,

\[
\int_{-\infty}^{\infty} dx e^{-2(x-y)^2} P \frac{1 - e^{-4xy}}{xy(xy - \bar{\omega})} + i \pi e^{-(\bar{\omega}/y-y)^2} \frac{1 - e^{-4\bar{\omega}}}{y \bar{\omega}} .
\]
Evaluating the collision frequency in the static limit ($\omega = 0$), the result is the Ziman formula [7] applied to a Debye potential in the case of non-degeneracy,

\[ \nu_{\text{Born}}(0) = 4\pi g n_e \int_0^{\infty} dy \frac{y^3}{(\bar{n} + y^2)^2} e^{-y^2}. \]  

(8)

In the following Tab. 2, the resulting values $R_{\text{dc}}^{\text{Born}}$ for the reflectivity calculated from the Drude formula (3) with the static collision frequency (8) are compared with the reflectivities $R_{\text{dynamical}}^{\text{Born}}$ resulting from the dynamical collision frequency in Born approximation (7) taken at the laser frequency $\omega_l$.

Compared with the observed reflectivities, the results obtained in Born approximation are too small. Similar values were also reported in [1]. As well known, the Born approximation (Faber-Ziman result) underestimates the value of the dc conductivity. The correct low-density value of $\sigma_{\text{dc}}$ is given by the Spitzer formula and can be obtained using a renormalization factor as discussed in [5], see also discussion in Sec. 2.3 below. The use of the dynamical conductivity increases the reflectivity by about 15%, but it also fails to produce the steep dependence of the reflectivity on the electron density as observed in the experiment, see Tab. 1.

2.2 Nonlocal conductivity

The general expression (4), (5) for the reflection coefficient contains an integral over the $k$ dependent transverse dielectric function. We will discuss the effect of the nonlocal conductivity using the Mermin approximation as given in [6, 8]. The RPA solution is extended by introducing a complex frequency argument which contains the collision frequency. The Mermin expression for the dielectric function obeys particle number conservation. For the transverse dielectric function we obtain [8]

\[ \epsilon_{\text{Mermin}}(k, \omega) = \epsilon_{\text{Mermin}}^\text{RPA}(k, \omega + i\nu(\omega)) - 1 \]

(9)

with

\[ \epsilon_{\text{Mermin}}^\text{RPA}(k, \omega) = 1 + \frac{(1 + i\nu(\omega)) \left[ \epsilon_{\text{RPA}}^\text{RPA}(k, \omega + i\nu(\omega)) - 1 \right]}{1 + i\nu(\omega) \left[ \epsilon_{\text{RPA}}^\text{RPA}(k, \omega + i\nu(\omega)) - 1 \right]}.

Tab. 2: Reflectivities from step-like density profiles, calculated at the experimental parameter values. $R_{\text{dc}}^{\text{Born}}$ - Drude formula (3) with static collision frequency (8), $R_{\text{dynamical}}^{\text{Born}}$ - dynamical collision frequency in Born approximation (7), $R_{\text{dc}}^{\text{Mermin,Born}}$ - Eq. (5) with the Mermin nonlocal dielectric function and static collision frequency in Born approximation.
\[ \mu_{\text{Mermin}}(k, \omega) = 1 + \frac{(1 + i \nu(\omega)) \left[ \mu^{\text{RPA}}(k, \omega + i \nu(\omega)) - 1 \right]}{1 + i \nu(\omega) \left[ \mu^{\text{RPA}}(k, \omega + i \nu(\omega)) - 1 \right] / \left[ \mu^{\text{RPA}}(k, 0) - 1 \right]} , \]

\[ \mu^{\text{RPA}}(k, \omega) = \frac{1}{1 - \left( \frac{\omega}{e_k} \right)^2 (\epsilon_t^{\text{RPA}}(k, \omega) - \epsilon_t^{\text{RPA}}(k, \omega))} \]

The RPA expressions for the dielectric function of a Maxwellian plasma are

\[ \epsilon_l^{\text{RPA}}(k, \omega) = 1 + \frac{\kappa^2}{k^2} \left( 2 + z_c D(z_c) + z_i D(z_i) \right) , \]

\[ \epsilon_t^{\text{RPA}}(k, \omega) = 1 + \frac{1}{\omega^2} \left( \omega^2_{pl,c} D(z_c) + \omega^2_{pl,i} D(z_i) \right) , \]

with

\[ z_c = \frac{\omega}{k} \sqrt{\frac{m_c}{2k_B T}} , \quad \omega^2_{pl,c} = \frac{n_e e^2}{\epsilon_0 m_c} , \quad c = e, i \]

and the Dawson integral

\[ D(z) = i \pi^{1/2} e^{-z^2} [1 + \text{Erf}(iz)] . \]

Using the static collision frequency (8), the nonlocal dielectric function was calculated. The results \( R_{\text{Mermin,Born}}^{\text{dc}} \) are also given in Tab. 2. There is no essential modification if the \( k \)-dependence of the dielectric function is taken into account. This can be explained by the fact that, at the conditions given, the main contributions to the integral over \( k \) come from the region of \( k \approx 0.0001a_B^{-1} \). A comparison of the mean free path and the much larger skin depth also shows, that nonlocal effects are not relevant here. We conclude that neither the account of the dynamical properties of the collision frequency nor the account of the \( k \) dependence in the dielectric function will essentially modify the calculated reflectivity. In particular, the discrepancy between the calculated and measured reflectivity as a function of the electron density, see Tab. 1, cannot be cured.

### 2.3 Strong collisions and renormalization

The Born approximation can and should be improved considering strong collisions and renormalization as described, e.g., in [5]. Restricting ourselves to the static case, we discuss different approximations for \( \sigma_{\text{dc}}^{\text{Born}} \). We introduce dimensionless parameters \( \Gamma, \Theta \) characterizing the non–ideality and degeneracy, respectively, of the plasma:

\[ \Gamma = \frac{e^2}{4\pi \epsilon_0 k_B T} \left( \frac{4\pi n_e}{3} \right)^{1/3} , \quad \Theta = \frac{2m_e k_B T}{\hbar^2} (3\pi^2 n_e)^{-2/3} . \]

The dc conductivity for the statically screened Coulomb potential in Born approximation \( \sigma_{\text{dc}}^{\text{Born}} \) was already given in Sec. 2.1 via (8). In the low-density limit, the dc-conductivity reads

\[ \sigma_{\text{dc}}^{\text{Born}} = 0.299 \frac{(4\pi \epsilon_0)^2 (k_B T)^{3/2}}{e^2 m_l^{1/2}} \left[ \frac{1}{2} \ln \frac{\Theta}{\Gamma} \right]^{-1} . \]

(13)
However, the correct expression for the dc conductivity in this limit is given by the Spitzer formula

$$\sigma_{dc}^{\text{Spitzer}} = 0.591 \frac{(4\pi e_0)^2 (k_BT)^{3/2}}{e^2 m^{1/2}} \left[ -\frac{3}{2} \ln \Gamma \right]^{-1}.$$  \hspace{1cm} (14)

It is obtained by taking into account strong collisions which modify the Coulomb logarithm in (13). The prefactor also changes from taking into account higher moments of the distribution function.

Recently, an interpolation formula for the dc conductivity of a fully ionized Coulomb plasma was derived [9],

$$\sigma_{dc}^{\text{ERR}} = a_0 T^{3/2} \left( 1 + \frac{b_1}{\Theta^{3/2}} \right) \left( D \ln(1 + A + B) - C - \frac{b_2}{b_2 + \Gamma \Theta} \right)^{-1} \hspace{1cm} (15)$$

where \( T \) in K, \( \sigma \) in (\( \Omega m \))\(^{-1} \), and with the functions

\[
A = \Gamma^{-3} \frac{1 + a_4/\Gamma^2 \Theta}{1 + a_2/\Gamma^2 \Theta + a_3/\Gamma^4 \Theta^2} \left[ a_1 + c_1 \ln(c_2 \Gamma^{3/2} + 1) \right]^2,
\]

\[
B = b_3 (1 + c_3 \Theta)/\Gamma \Theta / (1 + c_3 \Theta^{4/5}),
\]

\[
C = c_4/(\ln(1 + \Gamma^{-1}) + c_5 \Gamma^2 \Theta),
\]

\[
D = \left( \Gamma^3 + a_5 (1 + a_6 \Gamma^{3/2}) \right)/(\Gamma^3 + a_5).
\]

The set of parameters is given by \( a_0 = 0.03064, a_1 = 1.1590, a_2 = 0.698, a_3 = 0.4876, a_4 = 0.1748, a_5 = 0.1, a_6 = 0.258, b_1 = 1.95, b_2 = 2.88, b_3 = 3.6, c_1 = 1.5, c_2 = 6.2, c_3 = 0.3, c_4 = 0.35, c_5 = 0.1 \). They are fixed by the low-density expansion of the dc conductivity (14), the strong degenerate limit and numerical data in for the dc conductivity in the intermediate parameter region.

Using the Drude formula (3) with the conductivities \( \sigma_{dc}^{\text{ERR}} \) we obtain the reflectivities \( R_{dc}^{\text{ERR}} \), see Tab. 3. For comparison, experimental values for the dc conductivity [10] are given. The fit formula seems to overestimate the conductivity. The results for the reflectivities \( R_{dc}^{\text{ERR}} \) are rather high, even exceeding the measured values. Obviously, the size of the calculated reflectivities can be shifted considerably according to the approximations made for the dc conductivity. But the strong increase of the measured values can not be explained yet.

<table>
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<th>( P )/GPa</th>
<th>( \sigma_{\text{exp}} )</th>
<th>( \sigma_{dc}^{\text{Born}} )</th>
<th>( \sigma_{dc}^{\text{ERR}} )</th>
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</table>

Tab. 3: Values of the dc conductivity in (\( \Omega m \))\(^{-1} \) for different approximations. \( \sigma_{\text{exp}} \) – experimental estimates [10], \( \sigma_{dc}^{\text{Born}} \) – static Born approximation (8), \( \sigma_{dc}^{\text{ERR}} \) – interpolation formula (15) and corresponding reflectivity \( R_{dc}^{\text{ERR}} \) calculated using Drude formula (3).
It is possible to extend the approach given here for the dc conductivity to the dynamic conductivity, as shown in [5] using the Gould-DeWitt approach. However, as already shown for the Born approximation, which is part of the Gould-DeWitt approach, we do not expect a significant modification of the density dependence of the reflection coefficient on the electron density. We also do not expect a significant modification if the nonlocal, \( k \) dependent dielectric function is considered, because only the long-wavelength limit contributes in calculating the impedance. Furthermore, within a more accurate treatment the contribution of the interaction with neutral atoms should be included as well. However, at the temperatures considered here the influence of neutrals on the conductivity is small.

In conclusion of this Section, we could show that improvements in the theory of the dielectric function lead to substantial modifications in the reflectivity. For the parameter values considered here, the theory predicts a high value of the reflectivity close to the values obtained from the interpolation formula (15). However, we are still not able to describe the strong variation of the measured reflectivity with the electron density.

### 3 Smooth density profile

Obviously, it is not possible to interpret the measured values of the reflection coefficient of dense Xenon plasmas within the assumption of a step-like density profile, i.e. \( d \approx 0 \) for width of the shock wave front. In particular, the steep increase of the reflectivity only at densities above the critical one can not be explained despite a highly sophisticated approach to the calculation of the dielectric function.

Using the interpolation formula for the dc–conductivity (15) and the Drude formula (3), effective densities necessary to reproduce the measured values for the reflection coefficient can be deduced. They have been found to lie between 0.75 and 1.6 of the critical density \( n_{cr} = 1.02 \times 10^{21} \text{ cm}^{-3} \) where the plasma frequency coincides with the frequency of the probe laser.

These effective densities can be considered as an argument that the reflection of electromagnetic radiation occurs already in the outer region where the density is low. Within a simplified picture, considering a profile with increasing electron density, the radiation penetrates the low-density region of the plasma up to the region where the density approaches the critical value. Here the wave will be reflected.

To perform an exploratory calculation, a density profile was assumed where the electron density increases linearly with distance \( z \) from zero up to the saturation value \( n_e \) at the distance \( d \). We assume the following linear dependence of the dielectric function on the distance of the shock wave front \( z \)

\[
\epsilon(z) = 1 - \frac{z \omega^2_{pl}}{L \omega^2 \left(1 + \frac{n_e}{n_{cr}} \right)},
\]

(16)

\( L \) is the depth where the critical density \( n_{cr} \) is reached and the radiation is assumed to be reflected. The total width of the shock wave front is then determined by

\[
d = \frac{n_e}{n_{cr}} L .
\]

(17)

The collision frequency \( \nu_{cr} = 4.09 \times 10^{14} \text{ s}^{-1} \) was determined from the static collision frequency at the critical density using the interpolation formula for the static
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Tab. 4: Calculation of the width $d$ of the shock wave front from the reflectivity $R$, assuming a linear density profile. The critical density $n_{\text{cr}}$ is reached at depth $L_{\text{cr}}$. $d_{\text{cr}}$ according to Eq. (17), $d_{\text{lin}}$ solving the propagation of radiation in a linear density profile.

Conductivity (15). The reflectivity can be calculated via (see [11])

$$R = \exp \left( -\frac{8\nu_{\text{cr}}L}{3c} \right). \quad (18)$$

Taking the experimental values $R$ for the reflectivity, the width $d_{\text{cr}}$ of the shock wave front according to (18) is given in Tab. 4.

Compared with the value given in [1], see also Sec. 1 above, our estimation of the width of the shock wave front is larger by about one order of magnitude and almost independent of the thermodynamic parameters. Only the value at the lowest density value comes out to be smaller.

A more rigorous treatment of the propagation of laser radiation through a shock wave front should take into account the dependence of the collision frequency on the local electron density. An arbitrary density profile $n_e(z)$ can be approximated by a sufficiently large number of thin layers with constant electron density, and solving the boundary conditions when going from one slab to the next one. In such a way, any arbitrary density profile $n_e(z)$ can be calculated.

We have considered a linear dependence of the electron density on the distance $z$ within the shock wave front of width $d$, $n_e(z) = n_e z/d$, with $n_e$ being the electron density behind the shock front. The subdivision of the width $d$ into equidistant slabs has been increased until convergence was reached. For given density $n_e$, the interpolation formula for the dc conductivity $\sigma_{\text{ERR}}$ has been used to find the dielectric function of the corresponding slab according to the Drude formula (3). Results $d_{\text{lin}}$ reproducing the experimental reflectivity values $R$ are shown in Tab. 4. Convergence was reached by dividing $d_{\text{lin}}$ into 16 equidistant slabs.

## 4 Conclusion

In order to infer plasma parameters from optical reflection coefficient measurements of dense Xenon plasmas, we propose a width of the shock wave front of about $2 \cdot 10^{-6}$ m. Only at the lowest density measured, the value for $d$ may be smaller. The linear density profile should be considered as a model only to estimate the width of the shock wave front. Our method to approximate a given density profile by a sufficiently large number of thin layers with constant electron density can be applied to any $n_e(z)$ which, in general, could be obtained by determining the distribution function for the non-equilibrium process of the shock wave propagation.
Our calculations are based on an interpolation formula for the dc conductivity, obtained from a systematic quantum statistical treatment of limiting cases. In particular, the account of the renormalization factor and of strong collisions is essential to obtain the correct low-density limit. The uncertainty in using the interpolation formula increases for $\Gamma \leq 1$. The values for the plasma parameter $\Gamma$ for the dense Xenon plasmas considered here are in the region $1 < \Gamma < 2$, and $5 > \Theta > 1.5$ and we estimate the error of about 30 %. Furthermore, the dynamical collision frequency should be used instead of the static one. Using the Gould-DeWitt approach, the dynamical collision frequency was investigated in [5], and minor modifications (about one half of that given above) are expected. The effects of non-locality can be neglected in the region of plasma parameters considered, as shown above for the Born approximation.

Xenon under the conditions considered is a partially ionized plasma. The composition is shown in Tab. 1. The conductivity as well as the related quantities are influenced by the neutral component, which leads to a modification of the reflection coefficient. However, at the temperatures of about 30 000 K the contribution of the neutral component to the conductivity is small and will not be considered here. Similarly, the role of non-equilibrium effects such as relaxation of the composition will also not be considered here.

Shock wave front investigations may be the subject of forthcoming experimental work. An interesting point would be the simultaneous determination of reflectivities at different frequencies. It is expected that in this way more information about the density profile of the shock wave front can be obtained.

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