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Brewster angle of shock-compressed xenon plasmas

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Abstract. Experimental results for Brewster angle measurements are used to estimate the
width of the shock front in xenon. The possible influence of the shock front width on the dense
xenon reflectivity is discussed. The calculated values of the Brewster angle are shifted with
respect to the experimental values. It may be partially related to the nonzero width of the wave
front. The estimated values of the widths are 161, 154, and 145 nm for the wavelengths 1064,
694, and 532 nm respectively. These values are obtained within the framework of the Drude
theory of reflection in the optically nonuniform media. The density functional theory (DFT) is
applied to calculate values of the dielectric function and refraction. The effect is discussed if
the widths found could influence the normal reflectivity obtained in the framework of the DFT.

1. Introduction
The analysis of the response to the electromagnetic radiation is a conventional method for the
diagnostics of the dense plasmas. The polarized reflectivity measurements can be used for the
determination of the free-charge carrier density. The dependencies of reflectivities of s- and p-
polarized components ($R_s$ and $R_p$) of laser radiation on the incidence angle are measured for the
plasma densities 2.7 and 2.8 g/cm$^3$ for the wavelengths $\lambda= 1064$ nm, 694 nm and 532 nm [1–5].
The minimum value (at the Brewster angle) of $R_p$ is a nonzero one because the considered
medium is absorptive.

2. Calculation method
The Fresnel formulas are used for the calculation of the s- and p- polarized reflectivities

$$ R_s = \left| \frac{\cos \varphi - \sqrt{\varepsilon - \sin^2 \varphi}}{\cos \varphi + \sqrt{\varepsilon - \sin^2 \varphi}} \right|^2, \quad R_p = \left| \frac{\varepsilon \cos \varphi - \sqrt{\varepsilon - \sin^2 \varphi}}{\varepsilon \cos \varphi + \sqrt{\varepsilon - \sin^2 \varphi}} \right|^2. $$

(1)

The dielectric function (DF), which is included in (1) is a complex function and can be expressed
as $\varepsilon = \varepsilon^{(1)} + i\varepsilon^{(2)}$. The dependence on frequency $\omega$ of the imaginary part of the DF is defined
by the longitudinal expression in the long-wavelength limit [6–8]:

$$
\varepsilon^{(2)}_{L}(\omega, R_1) = \frac{4\pi^2 e^2}{3} \lim_{|q| \to 0} \frac{1}{|q|^2} \sum_{n,n',\alpha,k} 2w_k \left[ f(T,E_{n',k+q}) - f(T,E_{n,k}) \right] \left| \langle u_{n',k+q+e_\alpha} | u_{n,k} \rangle \right|^2 \times \delta(E_{n',k+q} - E_{n,k} - \hbar \omega)
$$

(2)
at a given ion configuration $R_I$, where $e$ is the elementary charge, $\Omega$ is a system volume, $q$ is a wave vector of the incident radiation. The summation is carried out over all electron states $n, n'$. The contribution of the sum terms with $n = n'$ (intraband transitions) are taken into account as well as contribution of terms with $n \neq n'$ (interband transitions). The summation over index $\alpha$ multiplied by $1/3$ is averaging over three spatial coordinates. The unit vector $e_\alpha$ determines a direction of the cartesian axis, corresponding to the coordinate $\alpha$. The summation is also carried out over all $k$-points in the Brillouin zone with taking into account of weight $w_k$ of a $k$-point. The factor 2 before the weights takes into account spin-degeneracy of the system considered. $f(T, E_{n,k})$ is the Fermi-Dirac distribution function, which defines the occupation of state $n$, at temperature $T$. $E_{n,k}$ is the eigenvalue (energy level) corresponding to the wave function $\psi_{n,k}$. $u_{n,k}$ is the cell periodic part of the Bloch function $\psi_{n,k} = e^{ikr}u_{n,k}$, which is a solution of the Schrödinger equation. $\hbar$ is the Plank constant.

The eigenvalues and the wave functions are calculated within the framework of the Kohn-Sham DFT approach. VASP (Vienna Ab initio Simulation Package) [9–12] plane-wave code is used in this work for DFT modeling. The type of the exchange-correlational functional is PBE [13]. It is shown in [14, 15] that the longitudinal expression (2) gives more correct result in comparison with the widely used Kubo-Greenwood formula [16, 17] within the framework of the projector augmented wave (PAW) approach. The correctness of the expression (2) is confirmed in [18, 19] where it is shown that using of (2) provides better explanation of the experimental dependence [20–23] of the shocked xenon reflectivity for normal incidence on density in comparison with the Kubo-Greenwood formalism used in [24].

The real part of the DF is obtained by the Kramers-Kronig transformation

$$\varepsilon^{(1)}(\omega, R_I) = 1 + \frac{2}{\pi} P \int_0^\infty d\omega' \frac{\omega' \varepsilon^{(2)}(\omega', R_I)}{(\omega')^2 - (\omega - i\eta)^2},$$

(3)

where $P$ denotes the principle value (in the limit $\eta \to 0$).

3. Width of the wave front

The measured and calculated values of the $R_s$ and $R_p$ reflectivity dependence on incident angle $\varphi$ are shown in figure 1 for the wavelengths of laser radiation 1064, 694 and 532 nm and densities 2.7 and 2.8 g/cm$^3$. The experimental data [1–5] are depicted by squares ($R_s$) and circles ($R_p$). The solid lines correspond to the calculated results obtained in this work within framework of the DFT with the longitudinal expression (2) for the imaginary DF and without introduction of the broadening of the wave front. Dashed lines correspond to the results calculated with introduction of the wave front broadening. The upper lines (solid and dashed) correspond to $R_s$ and lower ones to $R_p$. The calculated minimum of the dependence $R_p(\varphi)$ is shifted relatively the experimental one. It can be considered as notification of existence of the transitive region with finite width, where the plasma density increases smoothly to a final value.

The assumption that the broadening of the shock front width could improve the agreement of the Drude formula with static collisional frequency with the experimental data is introduced in [23, 25–27] for the normal incidence of laser radiation. The wave front width depends on the xenon ionization rate and its magnitude, estimated in [20], is $\hbar \approx 100$ nm. However, the suggested width of the wave front [23, 25–27] is approximately 800 nm, which considerably exceeds theoretical estimation. The satisfactory agreement of theoretical results with the experiment for the dependence of polarized reflectivity on the incident angle is obtained for the wave front width 220 nm in the framework of Drude model [5] with the electron density profile suggested in [28].
3.1. Helmholtz equations.

For the normal incidence of the radiation in [23, 25–27], the method of estimation of the wave front width is based on the solution of the Helmholtz equation for the of complex amplitude of the electric field $E(z)$ with wavelength $\lambda$, which propagates along the axis $z$ in the medium with nonuniform DF $\varepsilon_\lambda(z)$

$$\frac{d^2E(z)}{dz^2} + \frac{4\pi^2}{\lambda^2} \varepsilon_\lambda(z)E(z) = 0.$$ (4)

The reflectivity is found from the corresponding boundary conditions. The magnitude of the width obtained using this method is 95 nm at $\rho = 2.8 \text{ g/cm}^3$ for DF calculated within the framework of the DFT [18, 19]. It is much closer to the theoretical estimation [20].

For the calculation of the dependence of the s-polarized wave amplitude on incident angle $\varphi$, the expression $\varepsilon_\lambda(z) - \sin^2 \varphi$ has to be substituted in (4) instead of $\varepsilon_\lambda(z)$. The amplitude of p-polarized wave is determined by the following expression for the magnetic field $H(z)$

$$\varepsilon_\lambda(z) \frac{\partial}{\partial z} \left( \frac{1}{\varepsilon(\lambda, z)} \frac{\partial H(z)}{\partial z} \right) + (\varepsilon(\lambda, z) - \sin^2 \varphi) H(z) = 0.$$ (5)

3.2. Drude approach

The depth of the wave front $h$ can be also estimated within the framework of the Drude theory [29–31] for the polarized reflection of the electromagnetic wave using the experimental dependence of $R_s$ and $R_p$ on the incident angle $\varphi$. For this approach, the magnitude of $h$ can evaluated from following equation

$$\frac{R_p}{R_s} = \frac{\pi^2 h^2}{\lambda^2} \frac{n^2 + 1}{(n^2 - 1)^2 \eta^2},$$ (6)

where $\eta = \sqrt{N^2 + n^2 (1/N^2)} - 1 - n^2$, $N = N(z) = \sqrt{\varepsilon_\lambda(z)}$ is a nonuniform refraction coefficient, overline is a symbol of averaging over the width of the transitive layer (wave front), $n$ is a refraction coefficient of the plasma. The ratio $R_s/R_p$ is found at the value of angle $\varphi$ where $R_p$ reaches the minimum (Brewster angle). For the linear dependence of $N(z)$ the expression (6)
gives the following result for $h$:

$$h = \lambda \left[ \left( \frac{3}{2\pi} \right) \left( \frac{R_p}{R_s} \right)^{1/2} \left( R |n|^2 + 1 \right)^{-1/2} \right]$$

where $R$ is a reflection coefficient for the normal incidence. The refraction coefficient $n = \sqrt{\varepsilon}$ is calculated in the framework of the DFT.

3.3. Results

The estimated values of the widths are presented in Table 1. The upper values ($h_1$) correspond to the values of the shock wave width calculated as parameters of the equations (4) and (5), which give the experimental Brewster angles. The polarized reflectivities with the wavefront widths $h_1$ are also shown in Figure 1 by dashed lines.

The lower values $h_2$ are obtained within the framework of the Drude theory of reflection. As one can see, Helmholtz and Drude approaches give estimations of the width, which are less than the estimations of [5] and closer to the theoretical value.

Table 1. The width of the wave front. The values are obtained as parameter of solution of Helmholtz equations ($h_1$) and from the Drude theory ($h_2$).

| $\lambda$, nm | $\rho$, g/cm$^3$ | $h_1$, nm | $h_2$, nm |
|----------------|-----------------|-----------|-----------|
| 1064           | 2.7             | 80        | 161       |
| 694            | 2.8             | 100       | 154       |
| 532            | 2.8             | 100       | 145       |

4. Conclusions

In this paper, we have suggested two methods of estimation of the width of the wave front based on the calculation of the dielectric function using density functional theory approach. The first method is based on the evaluation of the wave front width as a parameter of the solution of the Helmholtz equation. The second method allows estimating the wave front width from the experimental ratio of $s$- and $p$-polarized reflectivities within the framework of the Drude theory of refraction from optically nonuniform medium. Both values of the wave front width are close to the physically justified width of the nonstationary ionization [20], in comparison with the results of [1–5, 23, 25–27].

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