Density functional theory for dielectric properties of warm dense matter.

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The reflectivity of shocked xenon was measured in the experiments of Mintsev and Zaporoghets for wavelength $\lambda = 1064\,\text{nm}$ [1]. But there is no adequate theoretical explanation of these reflectivity results in the framework of the standard methods of nonideal plasma theory. The Drude model with static collisional frequency and in Born approximation gives reflectivities, which are 2.5 – 3 times larger than the measured values at low densities. The assumption of significant width to the shock front gives a good agreement with the experimental data. However, there are no evidences of this effect in experiment. One of the main goals of experiment [1] was estimation of free electron density and plasma frequency in shocked xenon. The absence of adequate theoretical explanation of the experimental results did not allow obtaining reasonable estimation for these parameters. We use method of estimation of plasma frequency, which is based on DFT calculation of dielectric function and reflectivity from shocked xenon. The imaginary part of the dielectric function is evaluated using the longitudinal expression for dielectric tensor. The real part is obtained by the Kramers-Kronig transformation. Quantum molecular dynamics simulation and VASP are used as in [2]. The better agreement with the results for the wavelength 1064 nm [1] is obtained. No arbitrary width correction of the energy gap between bound and free states like in [2] is made. To estimate the value of the plasma frequency within the DFT the method based on using of sum rules is suggested. This method allows to associate directly the calculated values of the plasma frequency and the reflection coefficient.

1. V.B.Mintsev, Yu.B.Zaporogets. Contrib. Plasma Phys. **29**, 493 (1989).
2. M.P.Desjarlais. Contrib. Plasma Phys. **45**, 300 (2005).