Ab initio calculation of dielectric properties of shocked xenon.

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The reflectivity of shocked xenon was measured in the experiments of Mintsev and Zaporoghets in 1989 for wavelength $\lambda = 1064$ nm [1] and further for $\lambda = 694$ nm and $\lambda = 532$ nm [2]. But there is no adequete theoretical explanation of these reflectivity results in frames of the standard methods of nonideal plasma theory. As it was shown in [3], the Drude model, with collisional frequency in Born approximation, gives reflectivities that are 2.5 – 3 times larger than the measured values at low densities. The results of other approaches to the collision frequency calculation also can't provide better explanation of steep slope of reflectivity drop with decreasing of density. As it was shown in [3] 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. The values of reflectivity of xenon plasma, calculated by Desjarlais [4], are obtained in frames of the approach of quantum molecular dynamics, based on the finite temperature density functional theory; Kubo-Greenwood formalism is used for calculation of the optical properties. In comparison with [3] in [4] shock has an ideal step profile. The approach, used in this work, is approximately the same with method in [4]. However, in contrast to pseupotential in [4] (PAW Xe 07Sep2000), in given work the improved Projector Augmented Wave (PAW Xe_GW 08Jan2009) pseupotential is used. The advantages of this potential in comparison with (PAW Xe 07Sep2000) for calculation of shocked liquid xenon Hugoniot were first shown in [5]. The formula for longitudinal part of the dielectric tensor [6] is used, which is more accurate than the Kubo-Greenwood formula for transverse part of the dielectric function in frames of PAW method. The agreement of obtained results in this work with experimental data [1, 2] is much better than in [4].

References

1. Mintsev V. B., Zaporogets Yu. B. //Contrib. Plasma Phys. 1989. V. 29. P. 493.

2. Reinholz H., Röpke G., Wierling A., Mintsev V., Gryaznov V. // Contrib. Plasma Phys. 2003. V. 43. P. 3.

3. Reinholz H., Röpke G., Morozov I., Mintsev V., Zaporogets Yu., Fortov V., Wierling A. // J. Phys. A: Math. Gen. 2003. V. 36. P. 5991.

4. Desjarlais M.P. //Contrib. Plasma Phys. 2005. V. 45. P. 300.

5. Mattsson T. R., Magyar R. J. // AIP Conf. Proc. 2009. V. 1195. P. 797.

6. Gajdoš M., Hummer K., Kresse G., Furthmüller J., Bechstedt F. // Phys. Rev. B 2006. V. 73. 045112