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im. Ignacego Łukasiewicza

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STRUKTURA FAL UDERZENIOWYCH W GĘSTYCH GAZACH I CIECZACH - SYMULACJA METODĄ DYNAMIKI MOLEKULARNEJ

STRUCTURE OF SHOCK WAVES IN DENSE GASES AND LIQUIDS - MOLECULAR DYNAMICS SIMULATION

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The structure of shock waves in dense media has already been investigated by a number of authors. The method used most frequently was the Molecular Dynamics simulation. The molecules of the medium were usually modeled as hard spheres, or as points interacting with Lennard-Jones potential. In our earlier work [1] we presented some results for argon, showing that the shock thickness decreases with increasing density when it is related to the mean free path for a dilute medium and to the mean distance between centers of the molecules for a dense medium, provided that the shock Mach numbers are similar (Fig. 1). As shown there, the maximum slope shock thickness in argon at initial mass density equal to the density of water (mean distance between centers of the molecules $\lambda = 4.048$ Å) and the shock Mach number Ms = 1.97 (curve 5 in Fig. 1) is equal to only $L = 2.9\ \lambda$, while for a dilute gas at similar Mach number and the mean free path $\lambda = 0.9$ mm the shock thickness is $L = 5\ \lambda$ (curves 1 and 2 in Fig. 1).

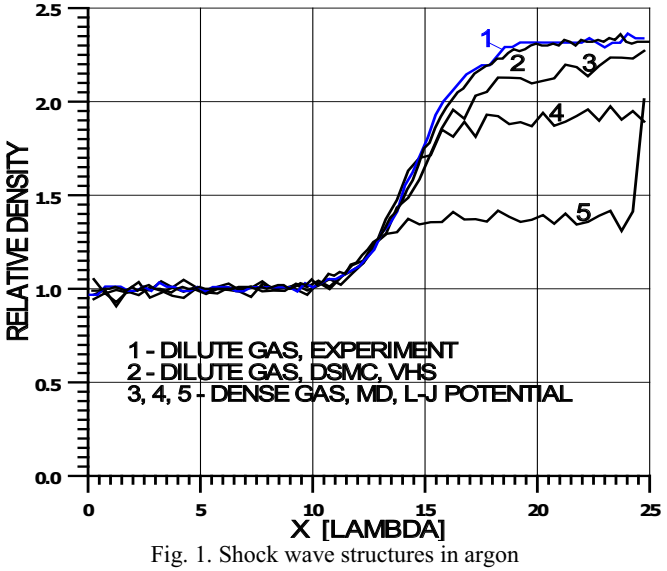

Fig. 1. Shock wave structures in argon

It seemed interesting to investigate the shock structure in more complex substances too. Water seemed appropriate for the first choice as its molecule was relatively complex and at the same time not too complex

to require excessive amount of computing time. Out of large number of the models of water molecule the TIP4P model was selected. This model consists of one oxygen atom, two hydrogen atoms, two positive electric charges placed at the centers of the hydrogen atoms and one negative charge placed close to the center of the oxygen atom. The molecules interact with each other with the Lennard-Jones potential and with Coulombic forces between the electric charges.
The Molecular Dynamics simulations were performed for two cases: full TIP4P model with electric charges taken into account and the same without electric charges. The shock wave was generated when a mass of water moving with velocity V = 620.86 m/s collided with a plane, perpendicular, impermeable wall. The Mach number of this shock was equal to Ms = 1.80.

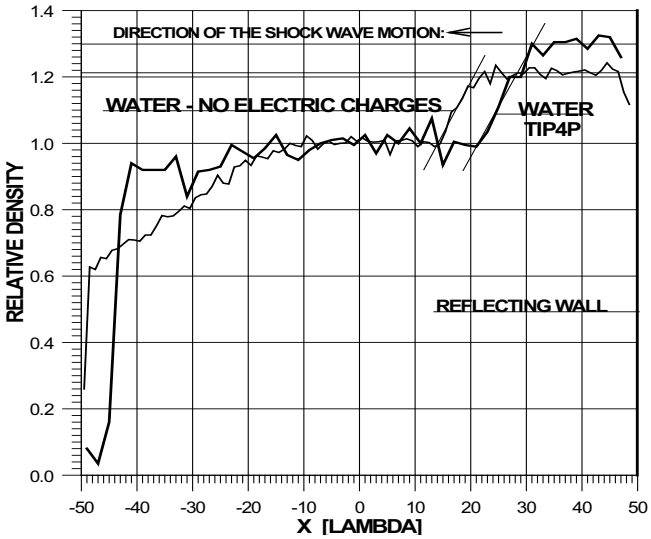

Fig. 2. Shock wave structures in water

Fig. 2 shows the density distributions along the axis perpendicular to the reflecting wall for the two simulated cases, for the same time after collision with the wall. It is evident, that lack of the electric charges makes water more "rigid" – the shock in such "water" moves faster than in real water and, at the same time, the amplitude of this shock is smaller. The thicknesses of the shocks in both cases are comparable, hence it may be concluded, that the electric charges do not influence them appreciably.
Comparing Fig. 2 with curve 5 of Fig. 1 one can conclude, that under comparable conditions the shock wave in water is much thicker than that in dense argon (in the case shown here about 3 times). This might suggest, that the thickness of the shock wave in dense medium is influenced mainly by the complexity of its molecules.
In the full paper some more results for molecular liquids will be presented. It seems interesting how the electric charges present in complex molecules influence the shock wave structure.

References:

[1] Walenta Z. A., Słowicka A. M., in: *Structure of shock waves in dense media,* Shock Waves, ed. K. Kontis, Heidelberg: Springer, 2012, ISBN:978-3-642-25687-5.