Structure of shock waves in noble gases under high density conditions.

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Abstract In the present paper we show the dependence of the shock structure in a dense, noble gas on each of the three non-dimensional parameters: non-dimensional initial density, non-dimensional initial temperature and non-dimensional shock velocity. It will also be demonstrated, that the length scale, most suitable for measuring the thickness of the shock wave in a dense gas, is the sum of the mean free path (calculated the same way as for a dilute gas) and the diameter of a single gas molecule.

1 Introduction

The research reported presently is a continuation of our earlier work on shock waves in dense media. In our paper [1] we argued, that for description of the shock wave structure in a dense, noble gas the following three non-dimensional parameters should be used:

- the non-dimensional density, $\rho = n\sigma^3$, (n is the number density of the molecules in the medium ahead of the shock wave, σ is some linear scale parameter connected with magnitude of the molecule, here assumed equal to the parameter in the Lennard-Jones interaction potential called "diameter of the molecule").
- the non-dimensional temperature, $\theta = TB/\varepsilon$, (T – temperature of the medium in front of the shock, ε – depth of the well of the interaction potential of the molecules, B – universal gas constant).
- the non-dimensional velocity, $\omega = U/c_m$, (U – shock velocity with respect to the medium in front of it, c_m – most probable molecular speed in the medium ahead of the shock).

In the present paper we show the dependence of the shock structure on each of these parameters separately. The results, for argon gas, were obtained numerically with the Molecular Dynamics technique [2]. For computations, the suitably modified program MOLDY [3] was used.

2 Molecular Dynamics Simulation

The program MOLDY [3], used in the present research, was originally designed for investigation of stationary phenomena. For the present research it was supplemented with additional procedures for calculation of the phenomena occurring in the medium in motion.
For description of the interactions between the molecules of the medium (single atoms) the Lennard-Jones potential [2] was applied.
The assumed shape of the calculation domain was that of a parallelpiped, whose length (in the x-direction) was equal to 50 or 100 average distances between the centers of the molecules in the undisturbed medium.
Before the actual simulation the medium was first equilibrated for a period equal to at least 10 picoseconds (10000 time steps). After that it was set in motion by adding the assumed

macroscopic velocity V to the x-component of the thermal velocity of each molecule. At the same time two impermeable, reflecting planes were inserted into the flow at the left and right borders of the calculation domain, thus generating the shock wave moving from the right border to the left and a rarefaction wave moving from the left border to the right.
The number of molecules taken for each simulation run ranged from 125000 to 500000. The time step assumed for simulation was equal to 0.001 picosecond. Each simulation run was finished after time period sufficiently long to evaluate the shock velocity and structure.

3 Results

3.1 Influence of the initial density

The influence of the initial density of the medium upon the structure of the shock has been presented in Figure 1. Fig. 1 – left shows this influence upon the density and temperature increase inside the shock, Fig. 1 – right shows this influence upon the shock thickness.

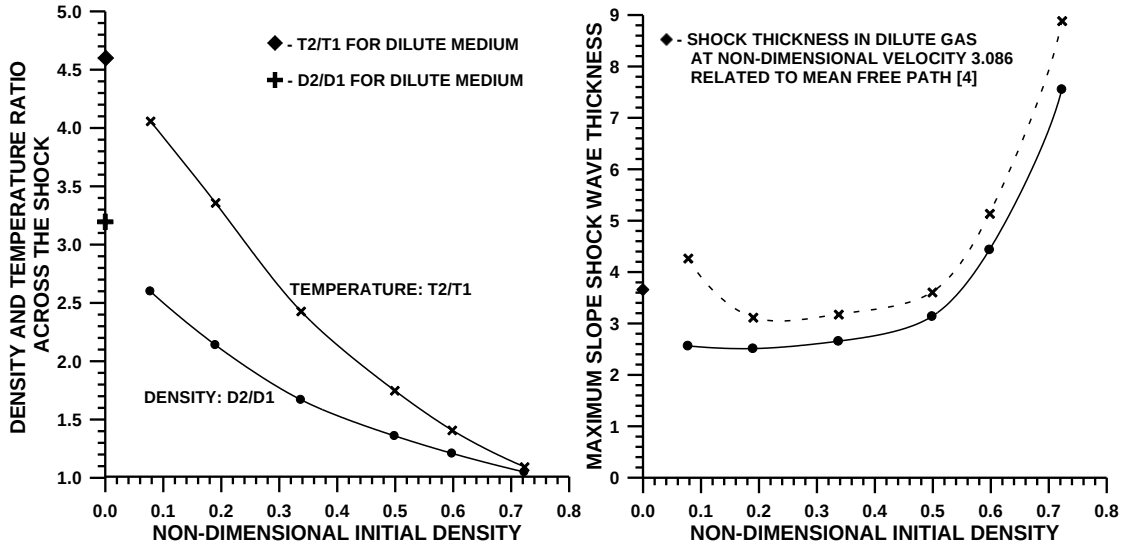

Fig. 1. Density and temperature ratios across the shock (left) and the maximum slope shock thicknesses (right) in argon, in terms of the non-dimensional initial density $\rho = n\sigma^3$, for the non-dimensional initial temperature $\theta = T_1 B/\varepsilon = 2.5042$, ($T_1 = 300K$) and non-dimensional velocity $\omega = U/c_m = 3.165 \pm 0.04$, ($U \approx 1118.45 m/s$)

Broken line – shock thickness related to $\sqrt[3]{n}$ (where n – number density of the molecules). Solid line – shock thickness related to the sum of the mean free path and the diameter of a molecule.

From Fig. 1 – left it is evident, that the initial density influences strongly the density and temperature increase inside the shock. The reason seems to be obvious: the molecules, whose volume practically cannot be compressed, with increasing density occupy relatively larger and larger part of the total volume of the medium. Similarly, at higher densities the free thermal motion of the molecules is obstructed by lack of space.
Fig. 1 – right contains two lines: the broken one, presenting shock wave thickness related to the average distance between the centers of the neighbouring molecules (as suggested by Bridgman [5], taken equal, approximately, to $\sqrt[3]{n}$, where n – number density of the molecules), and the solid line, presenting shock wave thickness related to the sum of the mean

free path and the diameter of a molecule. Both lines are approximately parallel at initial densities above $\rho = n\sigma^3 = 0.2$, however at densities lower than that the broken line turns unexpectedly up. To explain such behaviour one should note, that at densities higher than $\rho = 0.2$ the distances between the neighbouring molecules are smaller than the diameter of a molecule and the collisions occur only between the closest neighbours. At lower densities the moving molecule may squeeze between its closest neighbours and collide with some molecule at larger distance. Under such circumstances the absolute value of the shock wave thickness will be correspondingly larger, however this value related to the sum of the mean free path and the diameter of a molecule may remain constant. It seems therefore obvious, that the average distance between the centers of the neighbouring molecules may be used as the dimension characteristic for the shock wave structure only for the most dense media, at non-dimensional densities $\rho \geq 0.2$. The sum of the mean free path and the diameter of a molecule seems to be applicable in this respect in much broader range of densities. In the subsequent considerations the shock thickness will always be related to this sum of the mean free path and the diameter of a molecule.

One additional point should be noted here: in the range of densities considered the non-dimensional shock wave thickness increases with increasing density. This increase, very slow for non-dimensional density below 0.5, is much faster above this value. As a result, the non-dimensional shock wave thickness is about 3 times larger at density $\rho = 0.7$ than that at density $\rho = 0.2$.

3.2 Influence of the initial temperature

The influence of the initial temperature of the medium upon the structure of the shock has been presented in Figure 2. Fig. 2 – left shows this influence upon the density and temperature increase inside the shock, Fig. 2 – right shows this influence upon the shock thickness.

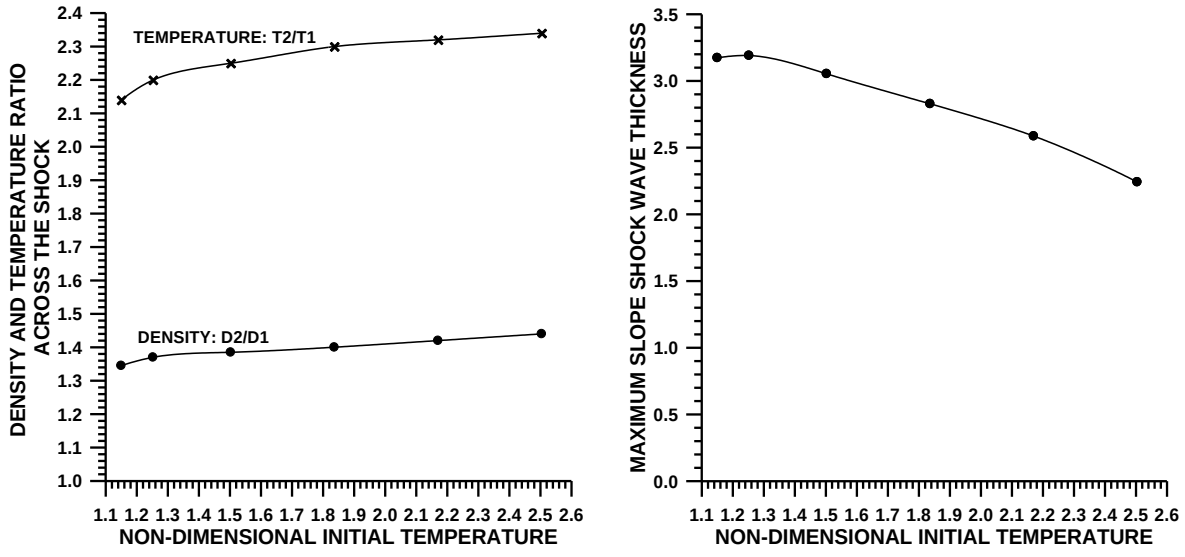

Fig. 2. Density and temperature ratios across the shock (left) and the maximum slope shock thicknesses (right) in argon, in terms of the non-dimensional initial temperature $\theta = T_1 B / \varepsilon$, at initial density $\rho = n\sigma^3 = 0.5978$, (mass density of argon equal to mass density of water) and non-dimensional velocity $\omega = U / c_m = 4.656 \pm 0.07$.

In the considered temperature range (from 137.75 K to 300 K) the influence of the initial temperature upon structure of the shock wave in argon under high density conditions is weak. With increasing temperature, the density ratio across the shock increases from 1.345 to 1.44 (about 7 per cent) only. The temperature ratio increases from 2.14 to 2.34 (about 9 per cent). The non-dimensional value of the maximum slope shock thickness decreases from 3.17 to 2.24 (about 30 per cent), which is a bit more significant.
It should be noticed here, that in dilute argon, at the same non-dimensional velocity, the density ratio across the shock equals 3.59, independently of initial density and temperature. Similarly, the temperature ratio, which equals 8.97. Both values are much higher than those at high density conditions.

3.3 Influence of the shock velocity

The influence of the shock velocity upon its structure has been presented in Figures 3 and 4. Fig. 3 – left shows this influence upon the density increase inside the shock, Fig. 3 – right shows this influence upon the temperature increase.

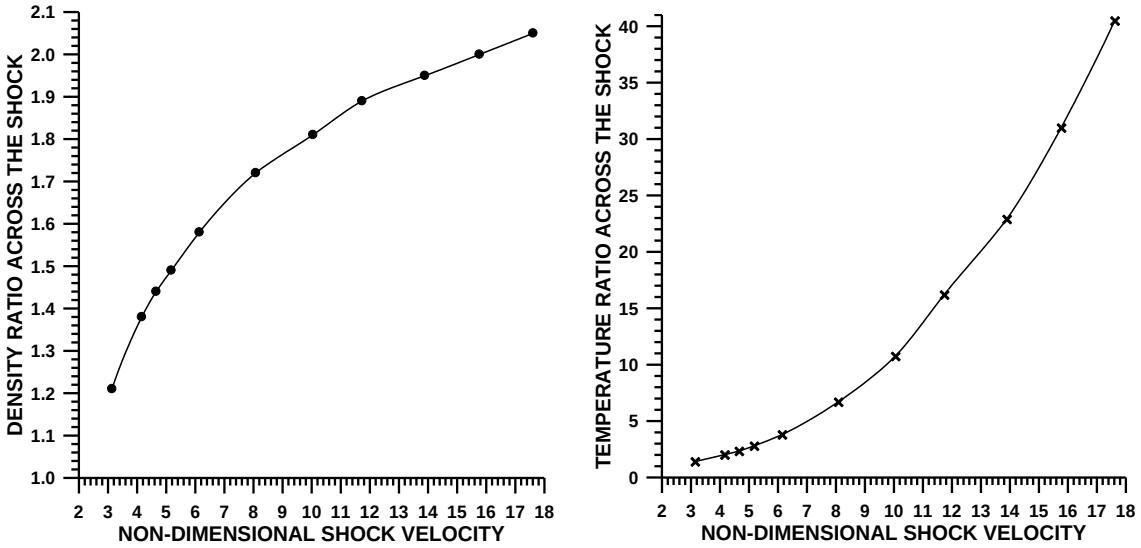

Fig. 3. Density ratio (left) and temperature ratio (right) across the shock in argon, in terms of non-dimensional velocity $\omega = U / c_m$, at non-dimensional initial density $\rho = n\sigma^3 = 0.5978$, (mass density of argon equal to mass density of water) and non-dimensional temperature $\theta = T_1 B / \varepsilon = 2.5042$, ($T_1 = 300K$).

The curves shown in Fig. 3 are similar to those for dilute argon at the same shock velocities, only the values of density and temperature ratios for the same shock velocities are lower.

Fig. 4 shows the dependence of the non-dimensional maximum slope shock thickness on shock velocity. Similarly to the case of dilute gas the slowest (the weakest) shock is the thickest. With increasing shock velocity the non-dimensional thickness of the shock decreases and tends to the value of about 1.8.
In a dilute gas this dependence has a minimum around the Mach number $Ms = 3$ [4] (non-dimensional velocity $\omega = U / c_m = 2.74$). Such minimum is not visible here.

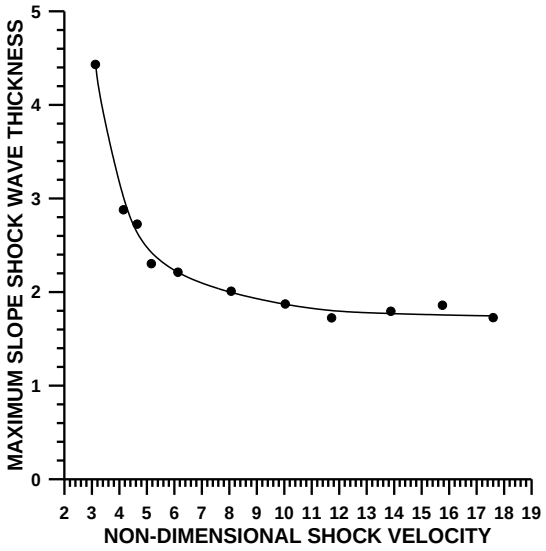

Fig. 4. Non-dimensional maximum slope shock thickness in terms of the non-dimensional velocity $\omega = U / c_m$ at non-dimensional initial density $\rho = n\sigma^3 = 0.5978$, (mass density of argon equal to mass density of water), and non-dimensional temperature $\theta = T_1 B / \varepsilon = 2.5042$, ($T_1 = 300K$).

4 Conclusions

- It has been found, that the average distance between the centers of the neighbouring molecules (as suggested by Bridgman [5]) may be used as a measure of shock thickness in the case of the highest densities only. The measure, which is appropriate in much broader range of parameters is the sum of the mean free path (calculated in a standard way) and the diameter of a single molecule.
- For a dense medium, the increase of the initial density causes decrease of density and temperature ratios across the shock propagating in this medium (which is different from the situation for dilute gases). The above is due to the fact, that at higher densities the molecules, which have finite and practically constant volume, occupy larger part of the total volume of the medium. Apart from that, at higher densities the free thermal motion is obstructed by lack of free space.
- For moderately dense medium the non-dimensional shock wave thickness is nearly constant. It then steeply increases with increasing density for the highest densities.
- The initial temperature has little influence upon the structure of the shocks in dense media. The increase of this temperature causes only slight increase of the density and temperature ratios across the shock, as well as decrease of the non-dimensional shock thickness.
- Influence of velocity of the shock upon its structure in a dense medium is qualitatively similar to that in a dilute gas. However the ratios of densities and temperatures across the shock, for the same non-dimensional shock velocities are smaller for dense medium than for dilute gas.

  Apart from that, the dependence of the thickness of the shock in a dilute gas on its velocity has a minimum for the shock Mach number about 3, while in a dense medium no minimum is present. When velocity of the shock is increased its thickness tends to some asymptotic value.

References

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