

## **Non-classical diffraction regimes of combustion and detonation waves**

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### **Abstract**

The classical regimes of diffraction in chemically active mixtures were investigated quite explicitly by many authors for the self-sustaining detonation wave (DW) passing from the tube into half-space (or from the narrow channel into sharply expanding channel). It was established, that in dependence on relation of the channel size with the characteristic size of DW-structure (cell size) the reinitiation of divergent DW (spherical or cylindrical) or failure of detonation regime and consequent transformation to regime of high-speed turbulent combustion of mixture are registered after DW-exit. The non-classical regimes of diffraction presented in this report are examined with stationary and non-stationary flames, including the regimes of transition of combustion into detonation (DDT). At variations of an energy of the initiator, initial pressure of a mixture, length of initiating section etc. it is possible to achieve a situation, when the point of DDT will be located near to cross-section with sharp expanding. The non-traditional behavior of diffracted wave in this case represents the special interest, as at DDT the maximum pressure are realized at the expense of strong DW-overdriven, much more exceeding pressure of products of self-sustaining DW. It is marked, that the non-traditional regimes of diffractions, investigated in the given work, represent a good test material for future numerical modeling. Such modeling was not realized by anyone up to day.

### **Introduction**

The classical diffraction of multifront detonation wave (DW) is complicated unsteady gasdynamic phenomenon comprising destruction and recovering of the ordered structure of multifront DW, which arise at sharp change of the geometric size of the gas charge (for example, when the self-sustaining DW passes from the tube into half-space ( $v=3$ ) or from the narrow channel into wider ( $v=2$ ) with diffraction angle  $\alpha=90^\circ$ ). Previous investigations (starting from pioneering investigations of [1-7]) revealed two qualitatively different propagation modes of DW-diffraction, depending on the ratio of characteristic sizes of initial charge (e.g., its diameter  $d$  at transformation to quasi-spherical wave or channel width  $l$  at transformation to quasi-cylindrical wave) and on the physicochemical parameters of the explosive mixture (cell size  $a$ ). These modes are the next: 1) initially self-sustaining DW decays after beginning of interaction with the expansion area and degenerates to form of nonsteady complex comprising an attenuating shock wave and trailing turbulent flame; 2) after interaction and quasi-steady transition period the DW-reinitiation is observed (Fig.1).

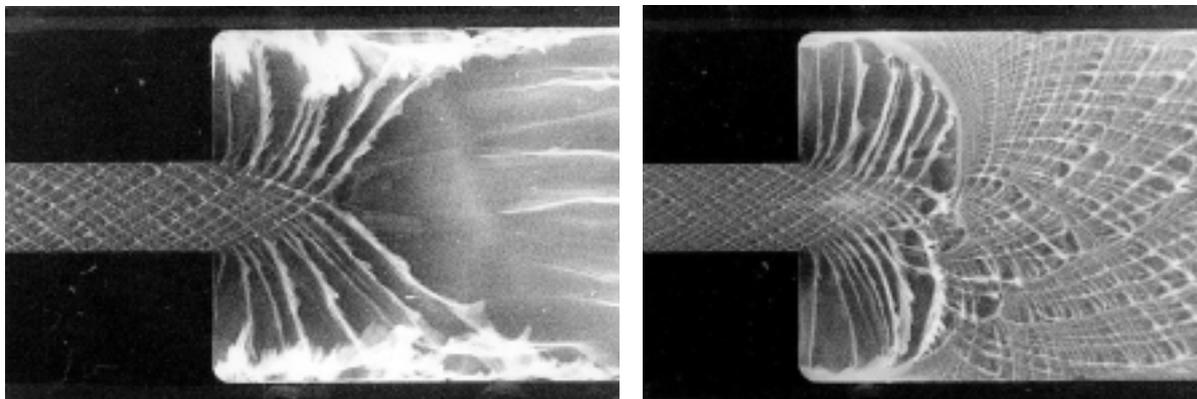


Figure 1. Self-luminosity photographs of diffraction of self-sustained DW: left – DW-decay, right – reinitiation.

Based on the firstly results of DW-diffraction the following relation was suggested in [3-7]:

$$d_{**} = 13 a = \text{const} \quad (1)$$

as the criteria for estimating of the critical diameter  $d_{**}$  of DW-transition from a tube to unconfined space. At this the self-sustaining DW equiprobably decays or transforms into a quasi-spherical DW after exit from tube into mixture space (diffraction angle  $\alpha=90^\circ$ );  $a$  is the characteristic cell size of multifront DW.

On this Colloquium in memory of Prof. R.I.Soloukhin it is necessary emphasized specially that R.I.Soloukhin with V.V.Mitrofanov were the first investigators who used the cylindrical symmetry for DW-diffraction. Moreover, they formulated firstly in [7] the numerical estimation of the criteria of DW-diffraction.

Equation of type (1) was checked carefully in numerous following experiments (for example, [3-21]). Some schemas of DW-diffraction and its optimization are demonstrated on Fig. 2. The diffraction angle, relation of sizes of narrow and wider channels, degree of a wave overdriven, boundary type (linear or curvilinear, expanding or converging) a.o. influence on conditions of DW-reinitiation.

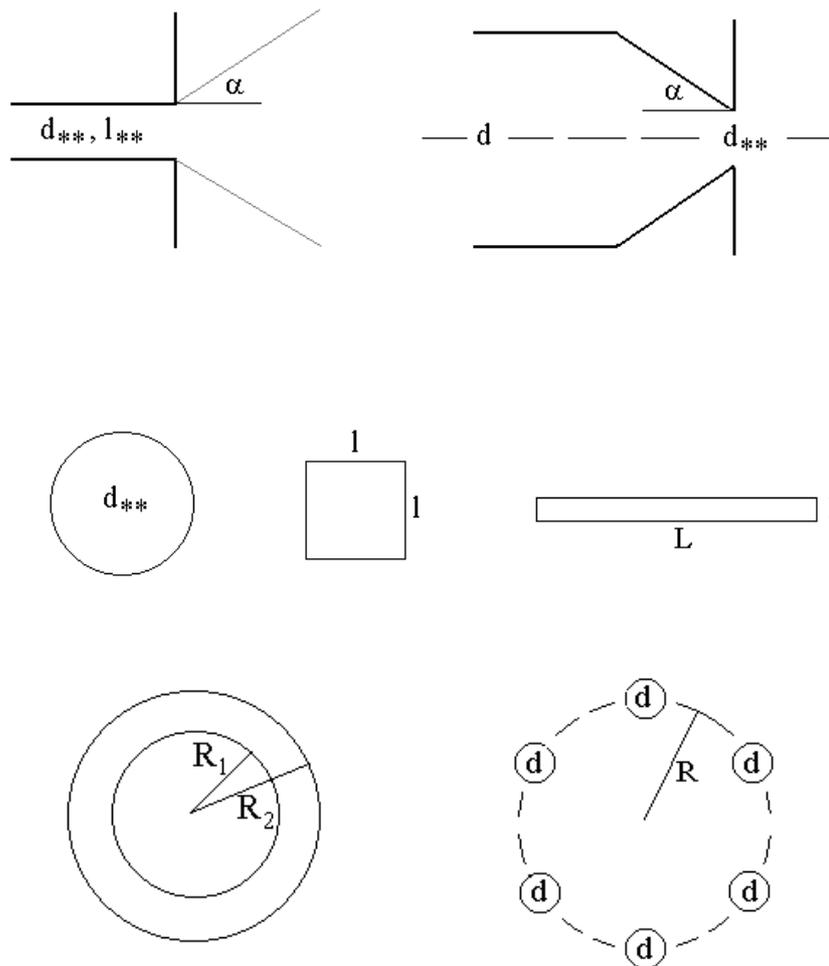


Figure 2. Some diffraction schema: upper – exit of self-sustaining DW in expanding channel (with rectilinear  $y=x \operatorname{tg} \alpha$  (diffraction angle  $\alpha=0 \div 90^\circ$ ) or curvilinear  $y=f(x)$  boundary); creation of overdriven DW with the help of converging system and subsequent exit of overdriven DW; middle and lower – variation of charge form of diffracted DW (circle, square, linear, ring, multi-charges schema).

Such examination was provoked not only scientific interest to phenomenon of DW-diffraction, but also its practical application (as initiation method of combustible mixtures) and from hazards point of view especially.

Moreover, the relation as type (1) is very important in connection with hypothesize on the key role of the cellular front structure in DW-initiation and propagation, and also with the possibility of estimation through  $a$  of great number of critical parameters of multifront DW, namely, the initiation energy for various flow symmetries, geometrical sizes critical for DW propagation and transformations in channels of different configurations, size of a projectile capable of detonation excitation in the mixture, critical sizes of unconfined gaseous charges, critical constants characterizing the induction period, a.o. The review of modern state of diffraction problem was published in [22].

It was established up to now that relation (1) with constant value can be used only for approximate estimation of critical diffraction diameter,  $d_{**}/a$  value for different mixtures is not constant and varies double as minimum in both side.

Numerical modeling of DW-diffraction in the rigorous multidimensional formulation is an extremely complicated problem. Some Codes for DW-diffraction are known (for example, [23-25]), but the critical  $d_{**}/a$  value, consisting with experimental data, not calculated yet.

### **Non-classical regimes. Results and discussion**

Non-classical regimes of diffraction of stationary and non-stationary laminar and turbulent flames, including the regime of transition of combustion (deflagration) in detonation (DDT) are less investigated. In the given paper some results of such researches are represented, when the range of characteristic velocities of propagation of front of a chemical reaction in a combustible mixture reaches from centimeters per one second (laminar flame) up to kilometers per one second (detonation, including high overdriven).

The main experiments were carried out on mixtures of acetylene  $\text{H}-\text{C}\equiv\text{C}-\text{H}$  and cyanogen  $\text{N}\equiv\text{C}-\text{C}\equiv\text{N}$  (fuels with triple chemical bonds) with oxygen. The choice of these fuels is connected with their easy-to-use spectral characteristic (luminescence of CH radical in blue spectral region). Acetylene is interesting fuel also because of possibility of carbon condensation in products with formation of nanoparticles, fullerenes, nano-tubes, a.o. Cyanogen has similar peculiarities. The registration was carried out with the help of schlieren streak-recorders, luminosity photo and pressure transducers in different tubes and channels.

The parameters of combustion and detonation of these mixtures were calculated with the help of computer Program «SAFETY» [26] and some results are presented on Figs.3-7.

At initial pressure - 1.0 atm and temperature - 298 K the basic parameters for fuel-oxygen and fuel-air mixtures are the next. For fuel-oxygen mixtures the detonation temperature is maximal at equimolar composition: acetylene - 4507 K, cyanogen - 6178 K (the highest value among gaseous fuels). At this the detonation velocities are 2934 and 2732 m/s (to be close observed in experiments of [27]), the detonation pressures ratio - 46.1 and 59.1, the cell sizes are 0.08 and 0.15 mm, the critical diameters of detonation reinitiation («exit» diameter) - 1.0 and 1.9 mm...

A condense carbon formation takes place at next concentrations of acetylene and cyanogen - about 60% in oxygen (and about 20% in air) up to 100 %. In this concentration range the energy of carbon condensation plays the important role for stationary propagation of detonation wave, without C-condensation an intensity of DW is sufficiently lower. For clean acetylene and cyanogen (upper limit, without oxygen or air) the detonation velocities are 1977 and 1591 m/s, temperatures - 3130 and 3746 K, pressures ratio - 20.4 and 26.0, the condense carbon in products - about 87.5 and 89.4 % from initial quantity...

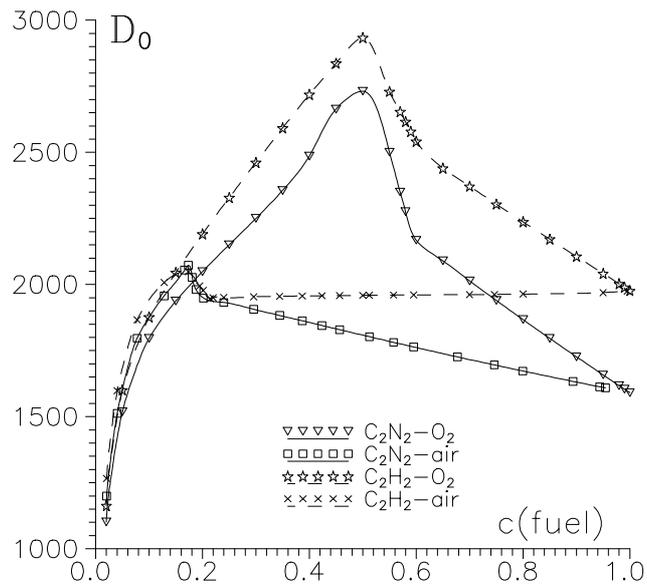


Figure 3. Velocity of DW (m/s) on molar fuel concentration for fuel-oxygen and fuel-air mixtures (calculation with taking into account of possibility of carbon condensation in detonation products).

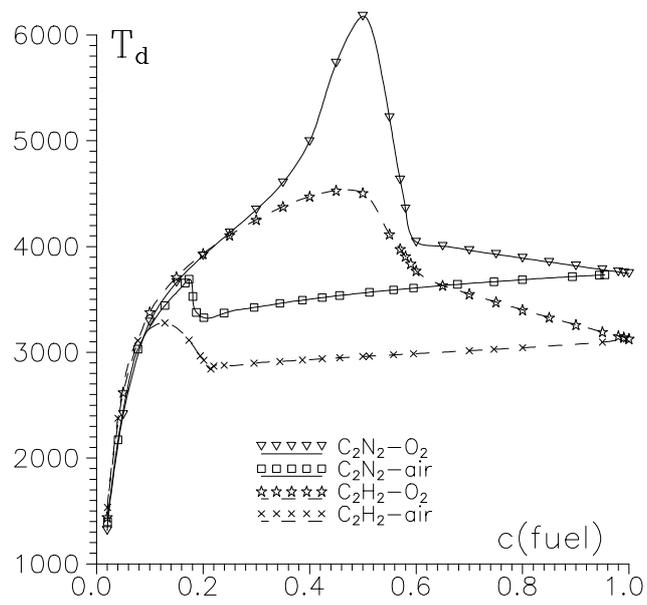


Figure 4. Temperature in detonation products (K) on molar fuel concentration for fuel-oxygen and fuel-air mixtures (calculation with taking into account of possibility of carbon condensation in detonation products).

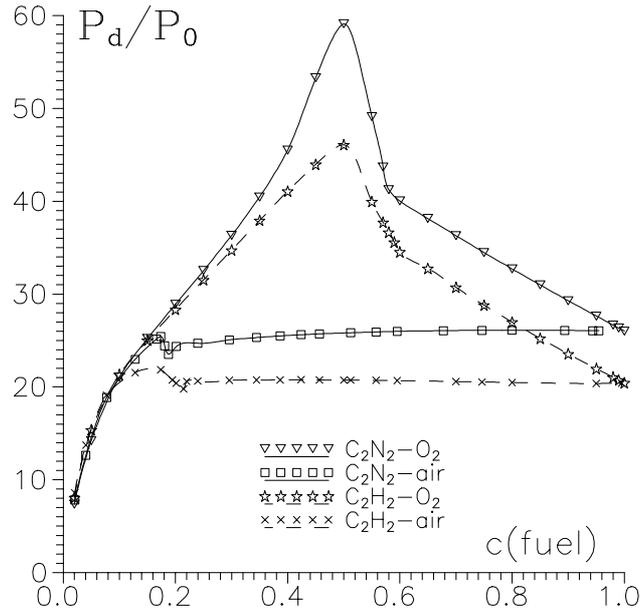


Figure 5. Pressure of detonation products on molar fuel concentration for fuel-oxygen and fuel-air mixtures (calculation with taking into account of possibility of carbon condensation in detonation products).

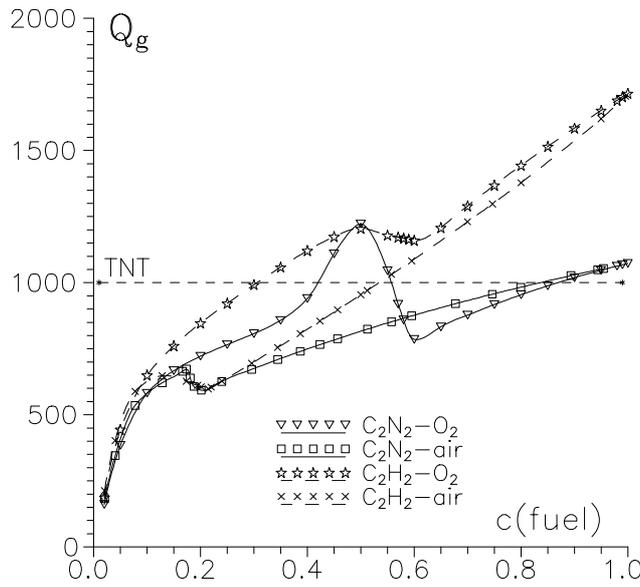


Figure 6. Energy-release of DW (call/g) on molar fuel concentration for fuel-oxygen and fuel-air mixtures (calculation with taking into account of possibility of carbon condensation in detonation products). Horizontal dotted line corresponds to standard TNT value.

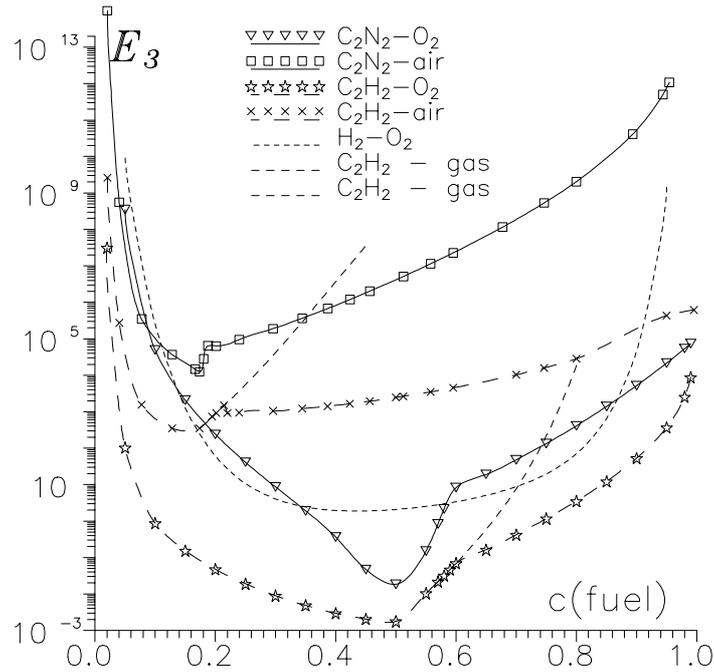


Figure 7. The critical initiation energy of spherical DW (J) on molar fuel concentration for fuel-oxygen and fuel-air mixtures (calculation with taking into account of possibility of carbon condensation in detonation products). Such graph illustrates the comparative efficiency of initiation of different mixtures (hazard problem).

The critical initiation energies for spherical detonation are demonstrated on Fig.7 for example. For fuel-oxygen mixtures at equimolar concentration they are the next: acetylene - 0.0018 J, cyanogen - 0.018 J. For fuel-air mixtures the minimal energies are 350 and 12500 J (the cell sizes - 4.7 and 13.5 mm), for stoichiometric acetylene-air mixture the cell size equals 8 mm, the critical diameter - 144 mm, the critical initiation energy - 1600 J. The data for nonequimolar cyanogen-oxygen mixtures are similar approximately to hydrogen-oxygen system (see Fig.7 and all lines for comparison).

At experimental investigations the large variety of regimes of propagation of waves of combustion and detonation as in the initial channel (pipe) of a constant cross-section, and as after diffraction is revealed. For example, together with predictable cases of DW behavior after a diffraction – DW reinitiation or transformation to a combustion regime – the regime of whole failure not only

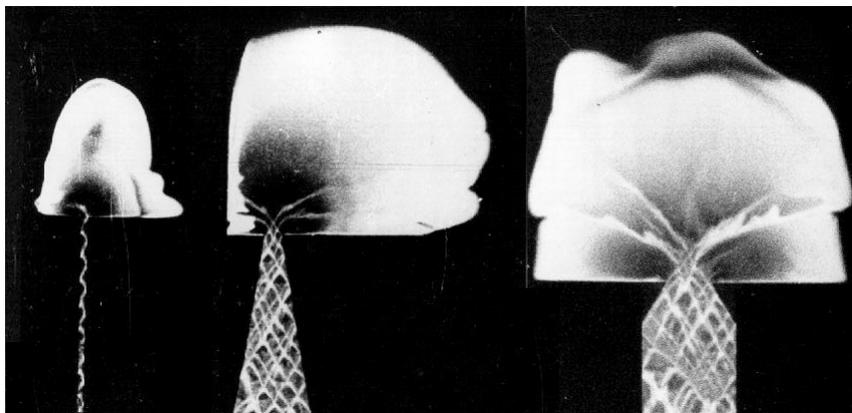


Figure 8. The effect of whole destruction of detonation and combustion at diffraction of marginal detonation (left) and even over-driven DW (middle and right).

detonations, but also combustions is observed under certain conditions, exhibited in full vanishing of products luminescence. The similar effect is revealed not only for self-sustaining, but also for overdriven DW – a few photos are demonstrated on Fig.8.

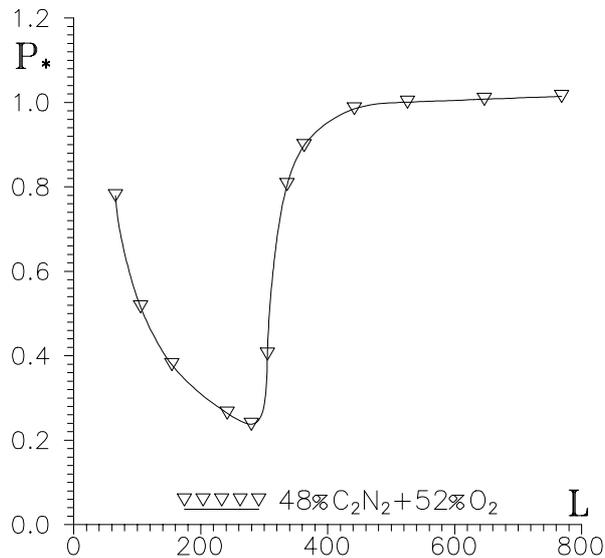


Figure 9.

At variations of an energy of the initiator, initial pressure of a mixture, length of initiating section etc. it is possible to achieve a situation, when the point of DDT will be located near to diffraction cross-section. The critical pressure (atm) of mixture 48% $C_2N_2$ +52% $O_2$  for successful DW-diffraction (at transition from tube of diameter  $d=6$  mm to  $d=44$ mm) on length  $L$  (mm) of initial tube is demonstrated on Fig.9 [28]. One can see that at  $L>400$  mm the diffraction conditions not depend on length of initial tube, because in this case the usual self-sustaining DW is diffracted. But at  $L<400$  mm the unusual behavior is observed – successful DW-diffraction at lower pressure with some optimal value, what is contradicted with classical results. The nature of this effect is connected with transition of deflagration to detonation near the diffracting cross-section.

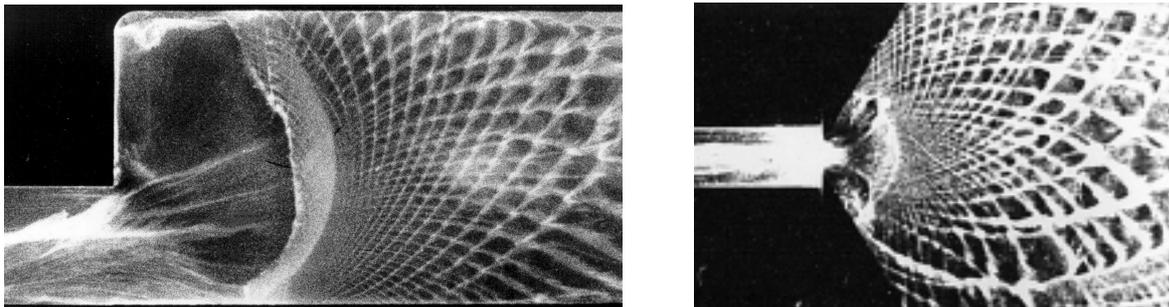


Figure 10. DDT at flame diffraction (left) at  $\alpha=90^\circ$ ; DDT at flame transition to expanding channel.

The non-traditional behavior of diffracted wave in this case demonstrates on two photos on Fig.10: the initiation of DW at flame diffraction. This case represents the special interest, because at DDT the maximum pressure is realized at the expense of strong DW-overdriven, much more exceeding pressure of products of self-sustaining DW. Moreover, the critical ignition energy is much lower (some orders) the critical energy of DW-initiation. So, diffraction of DDT can be considered as high effective method of optimization of initiation processes.

It is marked, that the non-traditional regimes of diffractions, investigated in the given work, represent a good test material for future numerical modeling. Such modeling was not realized by anyone up to day.

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