GROWTH OF CARBON PARTICLES IN A DETONATION WAVE

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When condensed explosives explode, excess carbon is released in the form of atoms or small clusters, which then combine into larger particles, up to several nanometers [1–3]. Brownian coagulation should lead to significantly larger sizes (tens of nm). Naturally, the idea arose of limited growth of particles due to their exit from a quasi liquid state with increasing size [4, 5]. Later, particles hundreds of nanometers in size were discovered in the explosion products of the hydrogen-free explosive benzotrifuroxane (BTF) [6], which were clearly not subject to size restrictions (presumably due to the higher explosion temperature). For such particles, Brownian coagulation turned out to be too slow. In [7], the importance of turbulence (or shear flows) in detonation products, which arise due to the heterogeneity of the substance and can sharply accelerate coagulation, was noted.

Data on the dynamics of particle growth in real time, obtained by the method of small-angle scattering of a beam of synchrotron radiation (SR) [8], make it possible to compare the predictions of growth models with experiment. We take the kinetics of unlimited particle growth taking into account the shear in the form

$$v\frac{\mathrm{d}N}{\mathrm{d}t}=\frac{1}{\tau_B}+\frac{Nv^{-2/3}}{\tau_S},\quad \tau_B=\frac{3\eta}{4kTn_0},\quad \tau_S=\frac{0.49}{\alpha\Gamma},$$

here N is the average number of carbon atoms in a particle, constants τ_B, τ_S are the characteristic times of Brownian and shear coagulation, η, T are the viscosity and temperature of the medium, n_0 is the initial concentration of carbon atoms, α is the volume fraction of carbon, Γ is the velocity gradient in the detonation products (when the reaction develops from hot spots, Γ is approximately equal to the inverse reaction time). The expansion of detonation products, which slows down growth, is taken into account by the multiplier $v=V/V_0$ on the left side of the equation. On the right side, the effect of expansion on the gradient is highlighted: $\Gamma\propto v^{-2/3}$. Expansion for cylindrical charges occurs primarily in the radial direction. The estimated dependence $v=(1+t/\tau_H)^2$. was accepted. The times τ_B, τ_S and τ_H were adjusted to reproduce the data [8]. The calculation results for $\tau_B=4$ ps, $\tau_S=0.11$ μs, $\tau_H=2{,}1$ μs are presented in Fig. 1. These times are consistent with theoretical estimates of detonation parameters within the binary order of magnitude.

During the first microsecond, the calculation overestimates the particle size by approximately two times to compensate for the initial underestimation of the experimental data. The SR scattering signal depends on the contrast – the difference in the densities of the medium and particles. The expansion of matter during detonation begins from the surface of the charge, where the density contrast will be strongest. The outer regions where relatively small particles can be expected to form will be overrepresented in the scattered radiation, giving the appearance of slow particle growth in the initial stage.

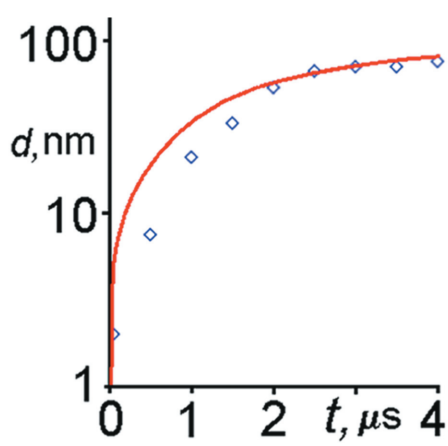

Fig. 1. Comparison of the calculated dynamics of particle sizes in BTF with experiment. Points – data [8]

During the detonation of “ordinary” explosives, such as the TNT/RDX composition, upon reaching a size of about 5 nm, the particles stop merging and their aggregation into fractal clusters begins [4]. Recently this fact was confirmed in works [9,10]. Sparse fractal aggregates cover the entire space, forming a kind of aerogel, which additionally blocks the growth.

However, due to gas-dynamic expansion, the weak bonds of gel are constantly broken, which creates the possibility of further slow growth of compact particles. Such growing was noted in [10] and can be produced, in particular, by the resonance of optical and acoustic modes of elastic waves caused by particle collisions [11]. In substances like BTF, the gel does not have time to form, since the particles continue to unite until the stage of noticeable expansion.

References

1. **Volkov, K. V.** Synthesis of diamond from the carbon in the detonation products of explosives [Text] / K. V. Volkov, V. V. Danilenko, V. I. Elin // Combust., Explos. and Shock Waves. – 1990. – Vol. 26, No. 3. – P. 366–368.
2. **Greiner, N. Roy** Diamonds in detonation soot [Text] / N. Roy Greiner, D. S. Phillips, J. D. Johnson, F. Volk // Nature. – 1988. –Vol. 333 – P. 440–442.
3. **Lyamkin, A. I.** Diamonds obtained in explosion [Text] / A. I. Lyamkin, E. A. Petrov, A. P. Ershov et al. // Soviet Physics Doclady. – 1988. – Vol. 33. – P. 705–707.
4. **Ershov, A. P.** Fractal structure formation in explosion [Text] / A. P. Ershov, A. L. Kupershtokh // Combust., Explos. and Shock Waves. – 1991. – Vol. 27, No. 2. – P. 231–236.
5. **Danilenko, V. V.** Synthesis and sintering of diamond by explosion [Text]. – M. : Energoatomizdat, 2003. – 272 p.
6. **Mal'kov, I. Yu.** Formation of diamond from the liquid phase of carbon [Text] / I. Yu. Mal'kov, V. I. Filatov, V. M. Titov et al. // Combust., Explos. and Shock Waves. – 1993. – Vol. 29, No. 4. – P. 542–544.
7. **Mal'kov, I. Yu.** Carbon coagulation in a nonstationary detonation-product flow [Text] // Combust., Explos. and Shock Waves. – 1994. – Vol. 30, No. 5. – P. 155–157.
8. **Ten, K. A.** Carbon condensation in detonation of high explosives [Text] / K. A. Ten, V. M. Titov, E. R. Pruuel et al. // Proc. 15th Symposium (Internat.) on Detonation. San Francisco, CA, USA, 2014. – P. 369–374.
9. **Hammons, J. A.** Submicrosecond Aggregation during Detonation Synthesis of Nanodiamond [Text] / J. A. Hammons M. H. Nielsen, M. Bagge-Hansen et al. // The Journ. Phys. Chem. Letters. – 2021. – Vol. 12 (22). – P. 5286–5293.
10. **Rubtsov, I. A.** Two-stage model of carbon condensation during detonation of condensed explosives [Text] // Siberian Physical Journal. – 2022. – Vol. 17, No. 2. – P. 48–55.
11. **Anisichkin, V. F.** The phenomenon of resonant solid-phase coalescence of small diamond particles in explosion products [Text] // Russ. Journ. of Phys. Chem. B. – 1993. – Vol. 12, No. 5. – P. 605–608.