

## Chain-Thermal Model of Silver Azide Explosive Decomposition Pulse Initiation

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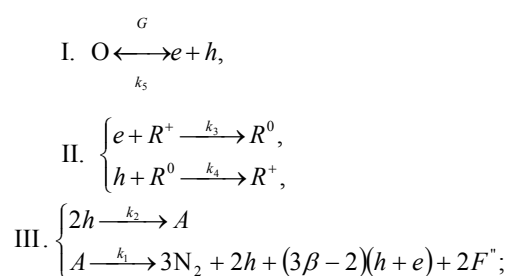
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**Abstract – The chain-thermal model is formulated on the basis of heavy metal azide explosive decomposition solid-state branching-chain reaction kinetic model proposed previously. It is shown that at the stage of reaction induction period the temperature practically is not changed, the temperature rises with a certain lag in relation to the chain reaction rate increase. At early stages of the reaction propagation kinetics of process is the same with the usage of both the chain explosion model and the chain-thermal explosion model. Regard for the heat evolution influences later stages of the explosion decomposition propagation. The activation energy of the chain propagation stage is estimated. It is shown that regard for the heat evolution results in the increase of the reaction propagation rate along the crystal.**

Heavy metal azides and compositions based on them are regular priming explosives and are classified as energetic materials. The key feature of energetic materials, that is, their high energy richness causes transition of slow decomposition to spontaneous explosive decomposition either due to various external effects or during operation, transportation and storage. In the work [1] branching chain solid-state initiation reaction model of heavy metal azide explosive decomposition has been formulated.

In order to describe total kinetic dependence of  $\text{AgN}_3$  pulse initiation explosive decomposition it is necessary to take into account the sample self-heating during the chemical reaction. The main objective of this work is formulating the chain-thermal initiation model of heavy metal azide explosive decomposition.

In the bimolecular model of heavy metal azide chain initiation reaction the stage of the chain propagation is in interaction of two holes localized on adjacent sites of the crystal lattice, with the formation of the intermediate complex  $\text{A}(\text{N}_6)$  as the result and its consequent destruction with the molecular nitrogen ( $\text{N}_2$ ) formed and energy evolved, the latter is used for current carrier generation [1].



$\beta = (L - p - 1,5[\text{N}_2] - 2A)/L$  is the coefficient determining the portion of non-excited sites in anionic sublattice,

$L = 2 \cdot 10^{22} \text{ cm}^{-3}$  is the concentration of silver azide lattice sites, where  $R^0$ ,  $R^+$ ,  $N_R^0$ ,  $N_R^+$ , are the recombination centers and their concentrations in various charging states, and  $N_R$  is the total concentration of the recombination centers.

$k_1$  and  $k_2$  are formation and destruction constants of complex A,  $k_3 = 1,95 \cdot 10^{-7} \text{ cm}^3/\text{s}$  is the constant of the carrier capture on the attracting recombination center,  $k_4 \cong 0,81 \cdot 10^{-8} \text{ cm}^3/\text{s}$  is the constant of the carrier capture on the neutral recombination center,  $k_5$  is the constant of bimolecular recombination of electron-hole pairs (in the calculations  $k_2/5$  was taken).

In the result of processing the experimental dependence of the threshold energy density on pulse effect duration the following constants have been determined:

$k_R = 5 \cdot 10^6 \text{ s}^{-1}$  is the constant of recombination,  $k_1 = 3 \cdot 10^7 \text{ s}^{-1}$  is the constant of complex A destruction,  $k_2 = 0,5 \cdot 10^{-11} \text{ s}^{-1} \text{ cm}^3/\text{s}$  is the constant of complex A formation.

During the sample self-heating calculation an instantaneous ordering of heat balance in the system was assumed as well as that direct and trapped recombination stage and complex A destruction stage pass with the energy evolving. From the silver azide thermal capacity and energy evolving of the respective stages a proportionality coefficient within energy evolving rate and heating rate ( $k_6 = 2 \cdot 10^{-19} \text{ cm}^{-3}$ ) has been determined. The constant of complex A formation and electron-hole pair recombination constants depend on temperature weakly, whereas the constant of complex A destruction depends on temperature exponentially  $k_1 = k_1^0 \cdot \exp(-E_a/kT)$ . For kinetic calculation the system of differential equations has been drawn:

$$\begin{cases} \dot{p} = G - 2k_2 p^2 - k_R p - \frac{k_2}{5} p(p + 2A) + \\ 3k_1^0 \cdot \exp(-E_a/kT)A \\ \dot{A} = k_2 p^2 - k_1^0 \cdot \exp(-E_a/kT)A \\ \dot{N}_2 = 2k_1^0 \cdot \exp(-E_a/kT)A \\ \dot{T} = \left(\frac{k_2}{5} p(p + 2A) + k_R p + \right. \\ \left. k_1^0 \cdot \exp(-E_a/kT)A \right) \cdot k_6 \end{cases},$$

where  $p$  is the concentration of holes.

The kinetic analysis of the system has been carried out, the phase-plane portrait of the system after pulse effect has been drawn, stability domain boundaries and coordinates of the critical point have been found. It is shown that at the induction period stage a sample self-heating can be neglected.

The software package for simulation of heterogeneous solid-state chain reaction propagation of heavy metal azide explosive decomposition with regard for heat evolving has been developed.

The results of the previous investigations show that branching-chain mechanism is a determinative factor for gas-phase inflammation of the whole series of compositions under lower, atmospheric and high pressures. Self-heating becomes significant only during the developing chain burning and enters into a positive feedback coupling with the chain avalanche. It has been determined that in the whole pointed area of pressures, the burning depending on initial concentrations of the components may be caused either by the chain avalanche only or by the chain avalanche and avalanche-like accumulation of thermal energy simultaneously in the reaction system. The main objective of this work is investigation into non-

isothermal modes of solid-state branching-chain reaction propagation. On the basis of the previously proposed kinetic model of heavy metal azide explosive decomposition the model of chain-thermal reaction has been formulated for the first time. It is shown that at the initial stages of the process temperature practically does not change, a temperature rise takes place with a certain lag in relation to the chain reaction rate, at early stages of the explosive decomposition initiation, kinetics of the process is the same with the usage of both the chain explosion model and the chain-thermal explosion model, at later stages kinetics of the explosive decomposition increases faster.

It is shown that regard for the heat evolution results in the reaction propagation rate increase along the crystal.

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### References

- [1] V.G. Kriger and A.V. Kalenskii, *Khim. Fiz.*, 14, № 4, 152 (1995). V.G. Kriger and A.V. Kalenskii, *Khim. Fiz.*, 15, № 3, 40 (1996).