Synthesis and Characterization of Novel High-Nitrogen Secondary Explosives

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TKX-50 (bis(hydroxylammonium) 5,5'-bis(tetrazolate-1*N*-oxide)) is one of the most promising ionic salts as a possible replacement for RDX. It can be prepared on a multigram scale by the reaction of 5,5'-(1-hydroxytetrazole) with dimethyl amine forming the bis(dimethylammonium) 5,5'-(tetrazolate-1*N*-oxide) salt which is then isolated, purified and subsequently reacted in boiling water with two equivalents of hydroxylammonium chloride to form TKX-50, dimethylammonium chloride and HCl.

The thermal behavior of TKX-50 (bis(hydroxylammonium) 5,5'-(tetrazolate-1*N*-oxide)) and the kinetics of its thermal decomposition were studied using differential scanning calorimetry (DSC) and thermogravimetric analysis (TGA). The thermal decomposition of TKX-50 starts within the range 210-250°C depending on the heating rate used, and is preceded by an endothermic process in the range 130-200°C.

The enthalpy of formation of TKX-50 was calculated to $\Delta H_f°$(TKX-50) = + 109 kcal mol^{-1}. The experimentally determined value based on bomb calorimetry is $\Delta H_f°$(TKX-50) = + 113 ± 2 kcal mol^{-1}.

The calculated results of the detonation parameters and equations of state for the detonation products (EOS DP) of explosive materials TKX-50 and MAD-X1 and several of their derivatives were obtained using the computer program EXPLO5 V.6.02. These values were also calculated for standard explosive materials which are commonly used such as TNT, PETN, RDX, HMX as well as for the more powerful explosive material CL-20 to allow comparisons to be made. The determination of the detonation parameters and EOS DP was conducted both for explosive materials having the maximum crystalline density and for porous right up to 50 % in volume materials. The influence of the content of plastic binder polyisobutylene used (up to 20 % in volume) on all of the investigated properties was also examined.

Calculated results on shock wave loading of different inert barriers in a wide range of their dynamic properties under explosion on their surfaces of concrete size charges of different explosive materials in various initial states were obtained with the use of the one-dimensional computer hydrocode EP. Barriers due to materials such as polystyrene, textolite, magnesium, aluminum, zinc, copper, tantalum or tungsten were examined (Fig. 1). Initial values of pressure and other parameters of loading on the interface explosive-barrier were determined in the process of conducted calculations. Phenomena of propagation and attenuation of shock waves in barrier materials were considered too for all possible situations.

From these calculations, an essentially complete overview of the explosion properties and characteristics of shock wave action onto barriers was obtained for several new and also for several standard explosive materials as a comparison. The results obtained suggest that in a wide range of their initial states (porosity, inert binders), the new explosive materials TKX-50 and MAD-X1 possess better explosive properties and shock wave action on practically every compact barrier which was considered, in comparison with several standard explosive materials, including the widely used military explosive RDX. A great volume of obtained calculated results can be used for subsequent more detailed analysis of the influence of different factors on the explosion and shock wave action characteristics of new explosive materials, and some of these results can be used for planning experimental confirmation of the ascertained regularities.

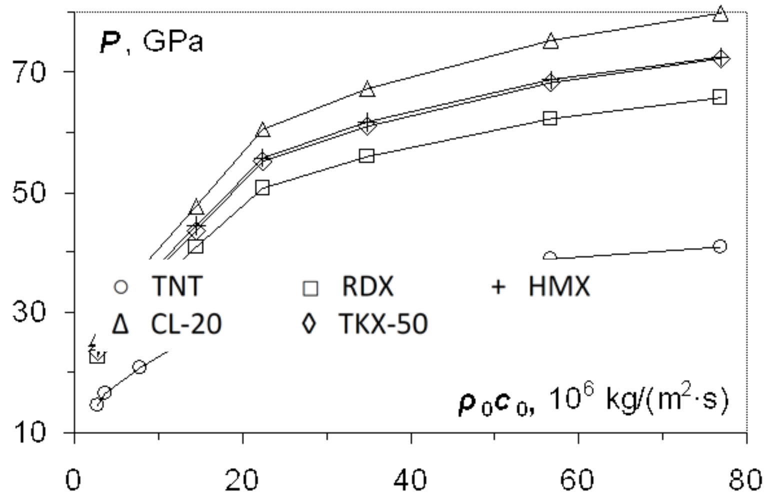

Fig. 1 The initial pressure on the interfaces of explosive-barrier from different materials (from polystyrene to tungsten).

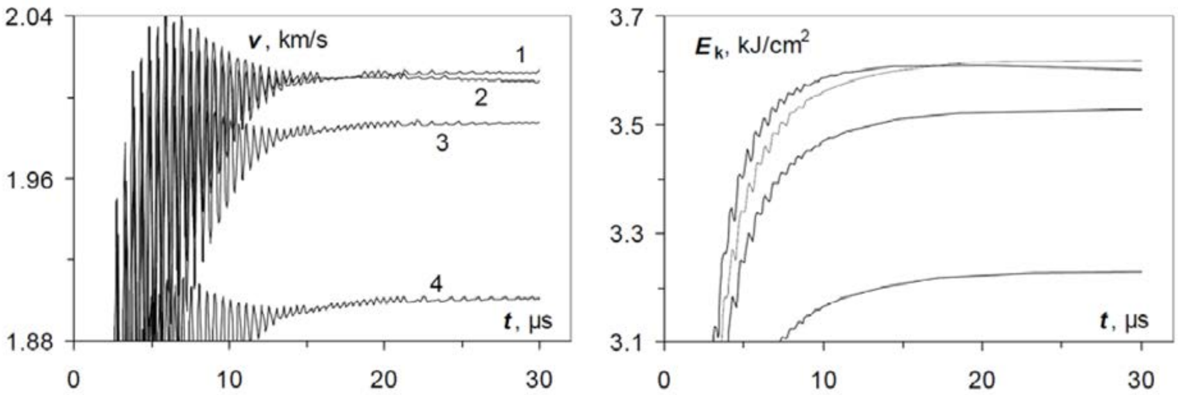

Fig. 2 Acceleration of plates by free charges of HMX (1), TKX-50 (2), MAD-X1 (3) and RDX (4).

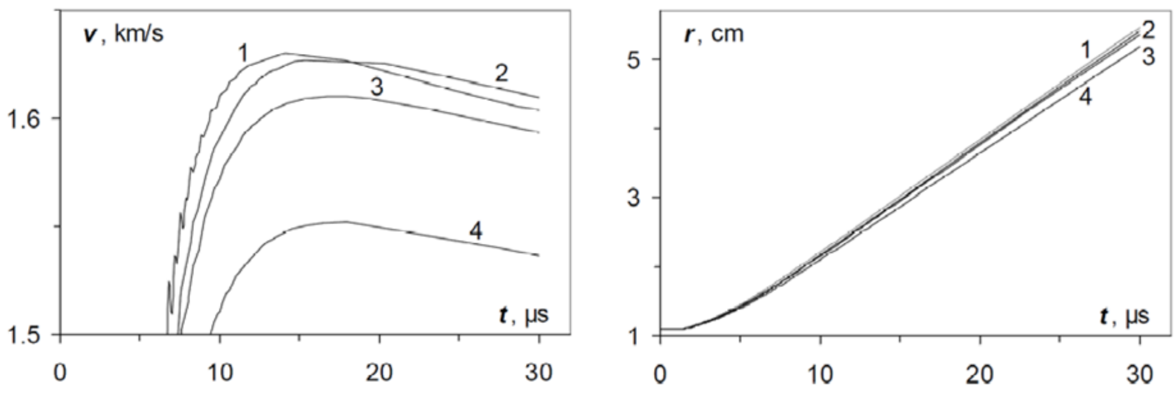

Fig. 3 Acceleration of Tantalum cylindrical layers by charges of HMX (1), TKX-50 (2), MAD-X1 (3) and RDX (4).

Tab. 1 Calculated cylinder energies for TKX-50 and RDX.

		% of standard			
compound V/V_0	E_C / kJ cm^{-3}	TATB	PETN	HMX	Cl-20
TKX-50					
2.2	-8.16	168	128	109	90
RDX					
2.2	-6.94	143	109	93	77

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