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Computer modeling of radiation processes in energetic materials

Abstract. The fundamentals of computer simulations of physical and chemical processes in the energetic substances (azides, etc.) when irradiated with electrons, ions and gamma-ray are developed. The basics of radiation technology for these materials with a high degree of combustion according to their specific application are developed.
Keywords: modeling, defects, ions, steel, azide, picrate, fulminate.

Introduction

The materials with high power characteristics are azides, picrates, fulminates, and other materials. Azides are organic compounds consisting of the system -N=N$^+$=N$^-$ (one or more groups of N_3) and M is the metal atom. The simplest of azides are compounds M $(N_3)_n$ (n - oxidation state, and M is metal). It is easy to show that this is nothing more than salt hydrazoic acid (HN_3). In addition it is also a double compound. The groups N_3 in them are connected with the atoms of two or more metals (in particular, K_2 $Cd(N_3)_4$). Mixed systems contain N_3, and the anion (in particular Zn (N3) Cl). The complex azide groups contain inner coordination sphere of the metal (in particular, Mn $(N_3)_4$/OR). In the present, the significant practical applications in research and industry have received azides of alkali and alkaline earth metals, for example Ag, Tl, Cu, Pb, Li, K, Na, Rb, Cs, Sr, Ca, Ba and some other materials. It should be borne in mind that the group N_3 is linear. In this type of communication compounds MN_3 is mainly ionic and ionicity increases in the transition from heavy metals (Pb, Ag, Tl) to the 3d metals, and then to the alkaline earth and alkali metals [1,2]. The table 1 shows the type of the crystal lattice, and some properties of the series azides on the basis of metal (table 1).

Table 1 – The structure and properties of some metal-based azides

Azid	Crystal lattice	Spatial group	Melting temperature, °C	Solubility, g in 100 g of water	ΔH^0 sample, kJ/mol
LiN_3	Geksagonalny.	*R 3m*	813	66,41 (18 °C)	7,3
NaN_3	Geksagonalny.*	*R3m*	—	28,0 (0-C)	21,3
KN_3	tetragonal.	*14/mcm*	354-	107,1 (16°C)	-1,7
RbN_3	tetragonal.	*14/mcm*	321	—	4,2
CsN_3	tetragonal.	*14/mcm*	326	224,2 (0°C)	-19,6
$Ca(N_3)_2$	rhombic.	*Fddd*	140-160**	45,0 (15°C)	14,2
$Sr(N_3)_2$	rhombic.	*Fddd*	—	45,83 (15°C)	2,5
$Ba(N_3)_2$	Monoklinny	*njm*	220**	17,0 (17°C)	22,2
α-$Pb(N_3)_2$	rhombic.	*Pnma*	350**	0,023 (18°C)	482,0

* are the parameters of the lattice: a = 0, 3646 nm, c = 1, 5214 nm. In this case the number of formula units in the cell 2 – 3. ** is the decomposition temperature (with explosion).

As seen from Table 1, the heavy metal azides are unstable at friction, impact, heat, etc. The exceptions are the alkali metal azides (except Li) that can decompose when heated without explosion. It is known that heavy metal azides are poorly soluble in water and alkali good. They possess the same properties as that of the salts of weak monobasic acids. The metal azides are decomposed under the scheme during the oxidation in particular: NaN_3 + NOCl → NaCl + N_2O + N_2. In the interaction of hydrogen with metal azides is their recovery (in the presence of catalysts, such as Pt, A1 amalgam, etc.) to a metal amides and N_2 or up to the free metal NH_3 and N_2. The original material for the production of most metal azide is sodium azide, obtained under the influence of nitric oxide (N_2O) in the melt $NaNH_2$ at 200^{o}C for the reaction: 2$NaNH_2$ + N_2O → NaN_3 + NaOH + NH_3. Sodium azide is obtained and the interaction of $NaNO_3$ with $NaNH_2$ or Na_2O, as well as with a mixture of gases N_2O and NH_3. Azides other metals are synthesized by reactions of metal salts with sodium nitrate in aqueous solution. The analysis of metal azides is carried out by oxidation of N_3 iodine in aqueous solution of nitrogen. Such an operation can be carried out on receipt of silver nitride or HN_3. The use of azide is widely used. Such as lead azide used in initiating powerful energy, and sodium azide for the synthesis of organic and inorganic azides, high-purity nitrogen, azides cesium, barium, strontium, etc. and high-purity metals. It should be noted that with increasing temperature azides of alkali metals (except lithium) and heavy metals begin to decompose the metal and nitrogen. An important characteristic of azides is their stability and reactivity under the action of various external mechanical and power loads, especially when targeted regulation reactivity and controlling the speed of chemical reactions energetic substances that form the basis of solid propellants, pyrotechnics, etc. n this case, the storage and use of these materials are presented fairly stringent requirements, especially when exposed to electromagnetic fields, temperature, radiation, pressure, stress, etc., leading to an irreversible process and a significant change in many physical and chemical properties and characteristics of materials. Solid-phase gradual decomposition of energetic materials under the influence of external factors can lead to a significant release of energy and fast self-sustaining chain reaction (eg, in the case of potassium azide, etc., is a typical representative of alkali metal azides).

Experiment

In the simulation of processes occurring in energetic materials at various influences are often using methods of molecular statics and molecular dynamics. Apply different potentials, in particular the Coulomb (for electrostatic interactions), Buckingham (taking into account the electron shells of atoms and instantaneous induced dipoles), Aksilorda-Teller (taking into account the three-particle interactions), Spring (taking into account the core-shell interactions) etc. Give a series of calculated physical properties of potassium azide (constant elasticity): C11 = 40, 91 GPa, C12 = 22,89 GPa, C13 = 11,43 GPa, C33 = 40,38 GPa, C44 = 7,44 GPa and C66 = 20,20 GPa; bulk modulus of 23.58 GPa and the shear modulus of 11.15 GPa, which are in good agreement with the experimental data. The energy of formation of point defects in a crystal of potassium azide is 2.06 eV. It is found that the explosives are widely used in industry and in various sectors of the economy, particularly used in agriculture, where they facilitate the work of the person and accelerate the production of works, tunneling and channels in hard rock and the destruction of the underwater rocks (that elusive and sometimes impossible without the use of explosives), in procuring coal, building materials from rocks, various ores and minerals (much easier and faster using explosives). We have analyzed characteristics of such materials. For example, in agriculture, such explosives are used for uprooting stumps and boulders destruction. To enhance the energy characteristics of the materials we use different streams of particles (pre-exposure to different doses). We have analyzed characteristics of such materials. For example, in agriculture, such explosives are used for uprooting stumps and boulders destruction. To enhance the energy characteristics of the materials we use different streams of particles (pre-exposure to different doses). Advantages of the main explosives to other energy sources (excluding nuclear) is the enormous power of the explosive transformation, produce more work in an extremely short period of time, which is especially important in production, where the payoff time is very important in terms of cost. In this regard, a comprehensive technology and cooling system are developed designs to avoid fire material, which is also very important in the safety of modern technology. The method is proposed for producing new materials using a variety of polymers (PTFE, etc.). We found that radiation exposure significantly increases the combustion of material (20-30%).

The computer simulation radiation-induced defects in energetic materials (silver azide, lead, etc) were held by their irradiation with high-energy electrons, ions, and gamma rays. The physical model for the generation of cascade regions and their spatial distribution was developed. The model is based on the following approximations: 1. Charged particles and photons propagate in a medium straight without changing its direction 2. Differential and integral cross sections (and correspondingly the mean free path) interactions are selected for the electrons in the form of cross section McKinley-Feshbach (or Mott), and for the ions in the form of the cross section of Rutherford. 3. The ionization losses were calculated by the formula Beta-Bloch (for electrons) and the tables Kumakhov-Komarova (for ions).

For electrons, forming primary knocked-out atoms, the dependence of the approximation function (cross section) of energy, which in turn depends on the penetration depth, is as follows:

$$\sigma = \sigma_0 \left(1 - \frac{1}{a\left(E_0 - kh\right)} \right).$$

The cascade-probability function for charged particles was used in

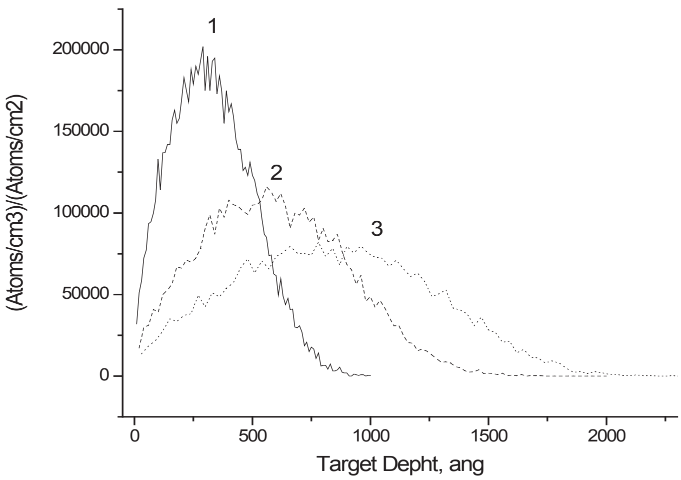
$$\psi_n\left(N, h, E_0\right) = \frac{1}{n!\lambda_0^n} \left(\frac{E_0 -}{} \right)$$

the form of N from the recurrence relations for Ψ_1, Ψ_2,,,,,,, Ψ_{n-} and here a, k, σ_0 are the approximation parameters. The calculations show that for all types of targets the cascaded probability functions first increase, reach a maximum and then slowly decrease to zero. With increasing energy of the primary particles of the maxima of the distributions are shifted to the right and decrease. Then it was found that irradiation led to a significant increase in the degree of combustion.

Results and Discussion

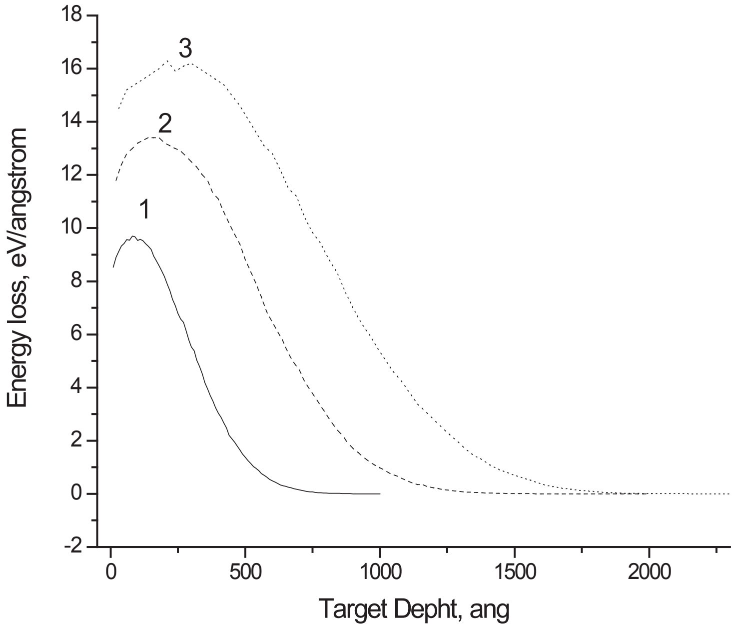
Further modeling of the distribution of implanted impurities (nitrogen ions in lead azide and silver) and the distribution of energy loss in depth was conducted. The calculations were made on the basis of programs "TRIM" and "Cascade". The "Trim" has a wide range of settings.

The type of material, the proportion in it of different elements is being established; the thickness of the material, the energy of the beam and the type of incident ions, as well as the angle of entry of the beam relative to the material surface is being given. You can specify multiple layers of different materials (the study of coatings and films.) Nitrogen ion beam energy was 10-30 keV. As a result the distribution curves of the ions and the profiles of the energy loss by ionization in depth of the sample, depending on the energy of the incident ions were obtained. The "cascade" allows counting the distribution of cascade areas in depth material. The most interesting results are the distribution of nitrogen ions in silver azide and lead as additional nitrogen can lead to a significant change of the processes. Figure 1-6 shows the profiles of implanted particles, energy loss and sputtered atoms in depth PbN_3 and AgN_3.



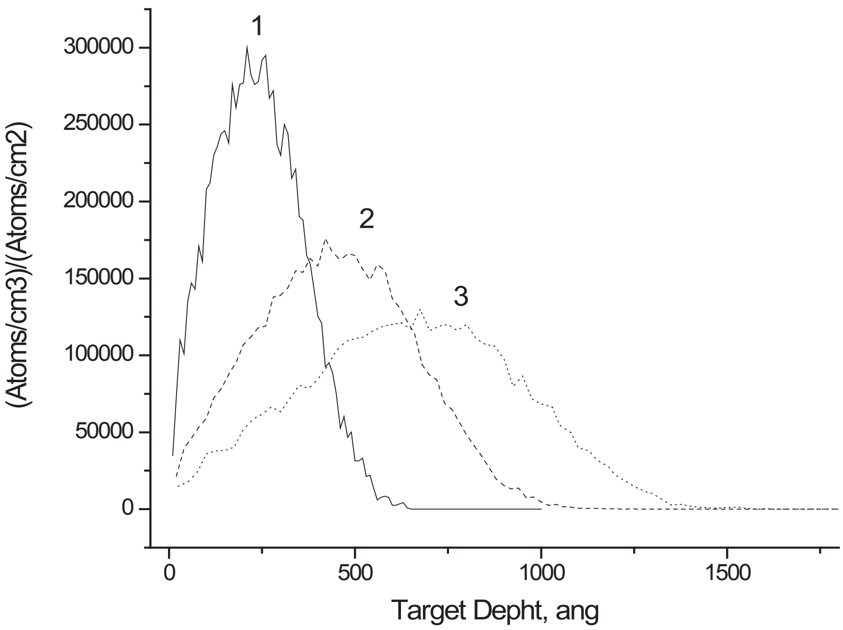
1 – 10 kEv; 2 – 20 kEv; 3 – 30 kEv

Figure 1 – Distribution of N on irradiation by PbN_3



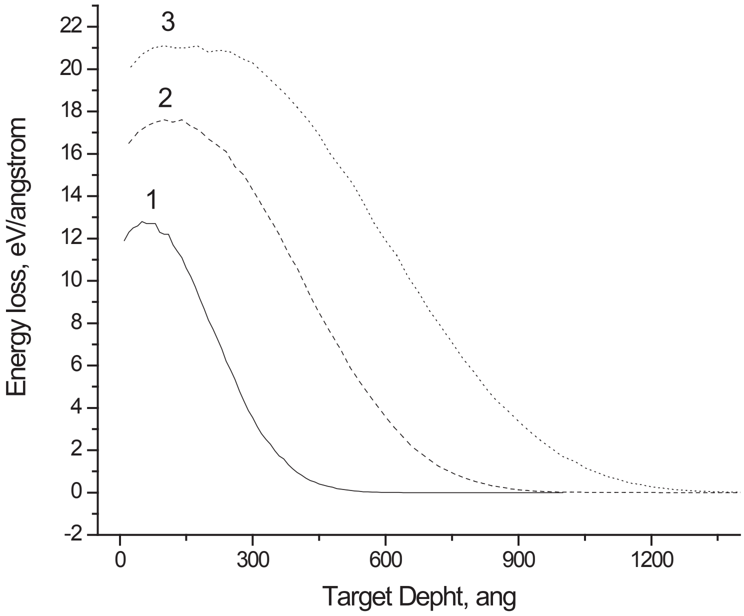
1 – 10 kEv; 2 – 20 kEv; 3 – 30 kEv

Figure 2 – Distribution of ionization losses on irradiation PbN_3 by flux of N ions



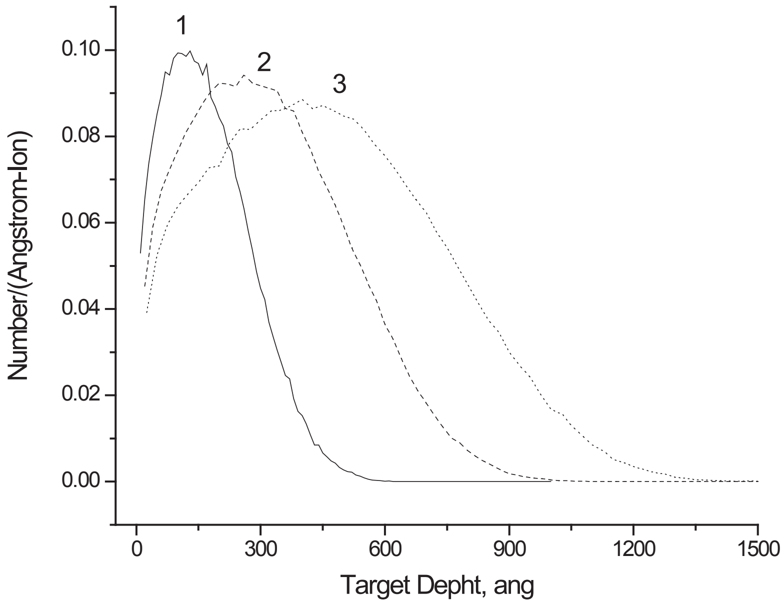
1 – 10 kEv; 2 – 20 kEv; 3 – 30 kEv

Figure 3 – Distribution of N on irradiation by PbN_3



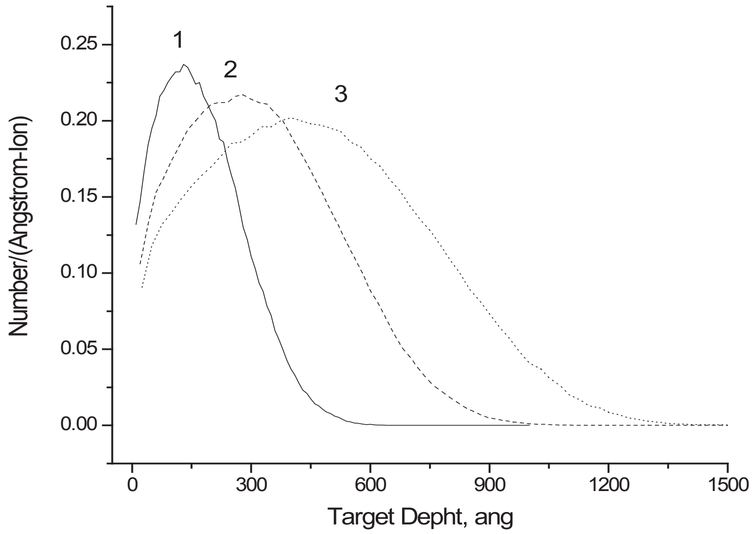
1 – 10 kEv; 2 – 20 kEv; 3 – 30 kEv

Figure 4 – Distribution of ionization losses on irradiation AgN_3 by flux of N ions



1 – 10 kEv; 2 – 20 kEv; 3 – 30 kEv

Figure 5 – Distribution of sputtered atoms Ag on irradiation AgN_3 by flux of N ions



1 – 10 kEv; 2 – 20 kEv; 3 – 30 kEv

Figure 6 – Distribution of the AgN_3 atoms ejected on irradiation by flux of N ions

Conclusion

From these data it is seen that in the azide with increasing of energy of the incident particles the peak of the distribution of implanted ions becomes more widespread. In this case, the average depth of deposition of particles decreases. In this case, the average depth of deposition of particles decreases. In this case, the average depth of deposition of particles decreases. With the growth of the mass of the ions the peak width increases and the particle distribution itself is shifted to the left. In good approximation, most of curves are described by a Gaussian distribution. Similar dependences are observed for other energetic materials.

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Энергетикалық материалдардағы радиациялық процесстерді эвм-мен моделдеу

ЭВМ-да модельдеу негізі энергетикалық заттардағы (азидтар т.б) физика-химиялық процесстерді электрондармен, иондармен және гамма квантармен шағылыстыру нәтижесінде құрылған. Радиациялық технология жоғары дәрежеде жандыру арқылы осы материалдарды алу және нақты қолдану негізінде құрылған.

Түйін сөздер: модельдеу, ақаулар, иондар, алмас, азид, пикрат, фульминат.

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Моделирование на ЭВМ радиационных процессов в энергетических материалах

Разработаны основы моделирования на ЭВМ физико-химических процессов в энергетических веществах (азиды и др.) при их облучении электронами, ионами и гамма-квантами. Разработаны основы радиационной технологии получения этих материалов с высокой степенью сгорания с учетом их конкретного применения.

Ключевые слова: моделирование, дефекты, ионы, сталь, азид, пикрат, фульминат.