THE MECHANISM OF AMMONIUM PERCHLORATE DECOMPOSITION INITIATED WITH VARYING INTENSITY OF THERMAL ACTION

A. Kh. Rudina, A. V. Stankevich, A. V. Sobolevskaya, I. V. Chemagina

FSUE «RFNC – VNIITF named after Academ. E. I. Zababakhin», Snezhinsk, Russia

The study of the processes of thermal decomposition of chemicals and materials based on them is a key issue of safety in chemical engineering and product design. The kinetics and mechanisms of chemical reactions make a significant contribution to the observed processes and the transition from one decomposition mode to another. Ammonium perchlorate (PCA) is a component of highly flammable fuels and energetic materials. The PCA thermal decomposition has been studied by multiple research groups (see, for example, [1–4]). The PCA thermal decomposition is preceded by the phase transition of the second kind (the $\alpha \rightarrow \beta$ transition) [5], which is accompanied by oscillation of the crystal lattice and phase equilibrium.

Together with the kinetics of chemical reactions, the study of thermal decomposition reactions makes it possible to determine:

1. The chemical reaction order at each decomposition stage;
2. The chemical activity of the gas phase in relation to the condensed one;
3. The localization of chemically active centers in crystals; and
4. The chemical composition of the material.

Objectives

1. Conducting thermal decomposition experiments using the combined DTA-TGA-IR methods at various heating intensities and PCA masses;
2. Preprocessing of experimental data and determining heat resistance;
3. Construction of models of thermal decomposition kinetics and assessment of reaction mechanisms by various methods; and
4. Comparative analysis of the results obtained by various methods.

Conclusion

It has been shown that at low thermal exposure rates in small masses no active Cl and HNO_3 are formed. As the mass and the intensity increase, concentrations of HNO_3 and active Cl in the gas phase increase. An increase in mass of the sample leads to a shift in the phase equilibrium from 40/60 to 20/80, a decrease in the reaction onset temperature by 15–25%, and an earlier development of autocatalytic processes. An increase in thermal exposure intensity has a similar effect.

The authors make assumptions about the change in the probability of a shift in the threshold pressure for initiating chemical reactions depending on the exposure intensity and the mass of the material.

References

1. **Manelis, G. B.** Thermal Decomposition and Combustion of Explosives and Powders [Text]. / G. M. Nazin, Yu. I. Rubtsov, V. A. Strunin. – M. : Nauka, 1996.
2. **Oxley, J. C.** Ammonium perchlorate decomposition: Neat and solution [Text] / J. C. Oxley, J. L. Smith, B. R. Valenzuela // Journal of Energetic Materials. – 1995. – Vol. 13. – Iss. 1–2. – P. 57–91.
3. **Mallick, Lovely** Thermal Decomposition of Ammonium Perchlorate – A TGA-FTIR-MS Study [Text] / Lovely Mallick, Sudarshan Kumar, Arindrajit Chowdhury // Thermochimica Acta. – 2015. – Part I; 2017. – Part II.
4. **Zhu, Yan-Li** Kinetics of Thermal Decomposition of Ammonium Perchlorate by TG/DSC-MS-FTIR [Text] / Yan-Li Zhu, Hao Huang, Hui Ren, Qing-Jie Jiao // Journal of Energetic Materials. – 2014. – Vol. 32. – Iss. 1. – P. 16–26.
5. **Gretsova, A. N.** Phase equilibrium and oscillation of crystal-structure parameters of ammonium perchlorate in the polymorphic transition region [Text] / A. N. Gretsova, A. V. Stankevich, B. G. Loboilko, D. V. Petrov, A. Yu. Garmashev, O. V. Kostitsyn and N. P. Taibinov // J. Phys.: Conf. Ser. 946. – 2018. – 012103.