Prediction of the progress of solid state reactions under different temperature modes

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Over last several years the research and development of new materials has accelerated significantly. This has resulted in increased interest in predicting their thermal stability both in extended temperature ranges and under temperature conditions at which the investigations of their properties is very difficult from the experimental point of view. These difficulties are prevalent at low temperatures (requiring very long investigation scanning times), as well when under specific temperature fluctuations.

A new method for predicting results from thermoanalytical scans has been developed (akts-ta-software). employing effective and efficient mathematical modeling, the method allows the calculations of the progress of solid state reactions under temperature conditions different from those at which the original scan investigations were carried out. the prediction of material properties can be undertaken for different temperature modes such as:

- isothermal
- non-isothermal
- stepwise
- modulated or periodic temperature variations
- temperature shock (rapid, short increase of the temperature)

Adequate predictive examination of the scanned reactions requires about six thermoanalytical measurements carried out with different heating rates, generally in the range of 1 to 20 K/min. The scans obtained by any thermal technique such as e.g. TG, DTA, EGA, TMA, can be applied for the calculations. The application of the new method for prediction of the solid state reactions will be illustrated during the lecture by the examination of the complicated progresses of the decomposition of an inorganic pigment and hydromagnesite (component of some pharmaceuticals). The potential application fields of proposed method include:

- Chemicals, pharmaceuticals and food
- Material sciences, rubber, polymers
- Metallurgy and ceramics
- Safety analysis, self-reactive chemicals and explosives

The features of the developed software will be presented and discussed