PREDICTION OF THE PROGRESS OF SOLID STATE REACTIONS UNDER DIFFERENT TEMPERATURE MODES

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Using a computational method (AKTS-TA-Software) [1] for the evaluation of the solid state kinetics, the calculations of the progress of solid state reactions are presented for temperature conditions different from those at which the experiments were carried out. The prediction of the solid state reaction extent is illustrated by the results obtained during decomposition of an inorganic pigment, polymer combustion and for the simulation of decomposition processes occurring at low temperatures. The applied method [2] was used for the prediction of the reaction progress under different temperature modes such as isothermal, non-isothermal, stepwise, adiabatic, modulated and, additionally for temperature profiles reflecting real atmospheric temperature changes. Adequate predictive examination of the scanned reactions requires at least five thermoanalytical measurements carried out with 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, DSC, EGA (MS or FTIR), TMA, can be applied for the calculations. The potential application fields of proposed method includes: chemicals, pharmaceuticals and food, material sciences, rubber, polymers, metallurgy and ceramics, safety analysis, self-reactive chemicals and explosives.

The prediction of the reaction progress for the complicated temperature programs will be illustrated by on-line calculations carried out during the lecture.

REFERENCES

[1] B. Roduit, Thermochim. Acta, 355 (2000) 171.
[2] B. Roduit, Thermochim. Acta, (2002) in press.