Combinatorial Chemistry of Materials, Polymers and Catalysts

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ABSTRACT:
The need for new materials and catalysts has never been satisfied by conventional methods. Chemical diversity is much too large to be explored systematically. Combinatorial chemistry applied to the discovery of new materials and catalysts can provide new lead structures, which has already been demonstrated by pioneers in the field. Combinatorial chemistry is much more than just a multiplication of experiments. In order to provide the results expected, combinatorial chemistry requires the combination of library preparation, characterization, identification of the desired properties and retrievable collection of the accumulated data in an intelligent data base. The state of the art of combinatorial chemistry in materials, polymer and catalysis research is reviewed.
We have been engaged in the manual and automated preparation of catalyst libraries by liquid phase techniques (sol-gel-process and hydrothermal synthesis) for a variety of applications. The chemical nature of the components prepared on the library is not only a product of the liquid phase reaction conditions, but also of the drying and calcination process. High-throughput characterization of the library components is therefor as important as the identification of desired materials properties. Automated micro-X-ray-fluorescence spectrometry with a commercial instrument has been used successfully to identify chemical compositions of library components. Automated microdiffraction has been used to characterize the microstructure of the materials prepared. For the sensitive detection of reaction energies on catalyst libraries emissivity corrected IR-thermography has been developed. It is used to identify catalytic activity of library components through the heat of reaction with high efficiency. This method has been applied to total oxidation, selective oxidation and hydrogenation reactions. Although much slower, but more detailed information was obtained with spatially resolved mass spectrometry. In a simple set-up product composition of selective oxidation reactions have been scanned with the help of a simple gas analyzer (quadrupole mass spectrometer). A remarkable discrimination of product selectivity was recorded on a diverse library containing amorphous microporous mixed oxide catalysts. With high resolution MS more difficult problems, such as the differentiation of products of the same unit mass, such as CO, N_2 and ethylene can be solved in high throughput modes. The selectivities observed correlate well with the behaviour of the materials under conventional reaction conditions.

References:
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