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X-ray absorption spectroscopy for industry: examples from Science Link project

K. Lawniczak-Jablonska[1]*, J. Libera[1], A. Chruściel [2] and M. Krasowska[3]

[1]Institute of Physics, Polish Academy of Sciences, Lotnikow Str 32/46, 02 668 Warsaw, Poland
[2]Scientific Consortium ADVANCE DMC, MEXEO, 47 225 Kędzierzyn-Koźle, Energetykow Str 9, Poland
[3]PPH Cerkamed, ul. Kwiatkowskiego 1, 37-450 Stalowa Wola

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*e-mail: jablo@ifpan.edu.pl

The x-ray absorption spectroscopy (XAS) is a synchrotron base technique widely used in solving scientific problems and offering unique possibility. Few examples will be shown how this technique can be applied for innovation in the industry. This is an example of “smart specialization” – a cooperation between Research & Development in companies and basic research. The examples are based on the results of Science Link project, which is a network between leading research infrastructure of photon and neutron and their users. The project aims to support and encourage innovation and entrepreneurship in the Baltic Sea Region. The scientific cases from three Polish companies were chosen. Synchrotron base techniques need advanced analysis of the results to get out useful for industry information. Therefore, the involvement of scientists is a must particularly for small companies without R&D department.

XAS technique can be considered as a finger print of chemical bonding of element under consideration. Therefore, can be used to find the neighborhood of given element (number, distances and kind of surrounding atoms), the location of given element in the crystal structure, it’s chemical bonding, and to estimate the proportion between few compounds of the same element in composite materials. This information can be of great importance in many technological problems.

One from investigated cases were the colored PVC materials used outdoor. In some of them, after two year exposure for the sunlight, the bleaching was observed. The PVC materials contain stabilizer with Zn element. The XANES and EXAFS measurements at the K-edge of Zn were performed and analyzed. The results indicated that the coordination of Zn atoms change after the exposure on light in the bleaching samples.

The other example are the pasts used in dental fillers. Products consist of amino and epoxy resin (filled with inorganic fillers), which react in the ratio of 1:1 in polyaddition process. The question was if the initial components remain in the final product. The K-edges of C, N and O were measured for each paste and compare with reference initial substances to decide if they can be distinguished in the paste after polyaddition process. The main conclusion was that no signs of any of the investigated initial materials could be clearly identified in the measured XANES spectra. New compound was formed in polyaddition process.

The next project was dedicated to the determination of structural characteristics of the non-stoichiometric composite transition metal complex salts, known as double metal cyanides (DMC), in order to correlate them with catalytic properties in the polyaddition of oxirane homologues used in manufacturing of important industrial polymeric materials (polyurethanes, surfactants etc.) as well as to compare synthesized catalyst with commercial reference one. The XANES and EXAFS spectra for Co and Zn elements were measured. It was shown that in all measured catalysts the neighborhood of Zn and Co centers were very similar and the atomic order around Co and Zn atoms was much closer to trygonal structure then cubic one.

Performed XAS measurements did not solve the technological problems reported by the companies but provide the suggestions where to look for the solution and usually were the beginning of scientific approach to the problem and need for further cooperation was clearly seen. They are a good examples how to initiate and maintain the useful cooperation between basic research and industry.

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