



Zdeněk Kožíšek

Na seminári sa zúčastnilo 52 účastníkov (14 účastníkov zo SR, 36 z ČR a 2 účastníci z Poľska) a odznelo 40 prednášok. Najviac boli zastúpené prednášky týkajúce sa bodu d), ale objavili sa zaujímavé príspevky z oblasti matematického modelovania vlastností materiálov a návrhy na nové zariadenia. Na druhej strane celkom absentovali prednášky týkajúce sa vyučovania materiálových vied na fakultách, čo je pre organizátorov signálom na úvahy o zmenách náplne ďalších seminárov. Táto situácia sa však môže zmeniť, keďže v súčasnosti sa tvoria nové študijné programy a určite bude zaujímavé získať prehľad o výučbe materiálových vied na jednotlivých univerzitách po reforme vysokoškolského štúdia. Témy prednášok sú uverejnené v zborníku zo seminára s názvom totožným s názvom seminára (ISBN – 80-89088-16-3).

V rámci kultúrneho programu seminára sa pre zdatnejších účastníkov seminára uskutočnil prechod hrebeňom Otrhancov a Jakubinej a menej zdatní účastníci absolvovali prehliadku skanzenu Liptovskej dediny v Pribyline. Seminár uzatvoril spoločenský večer.

Tohoročný seminár, trinásty v poradí, sa podľa ohlasov zúčastnených vydal po všetkých stránkach. Je potešiteľné, že pokračoval v pozitívnej gradácii obsahovej a organizačnej stránky podujatia a potvrdil užitočnosť vzniknutej tradície týchto akcií. Pozitívne bol hodnotený i výber miesta konania seminára. Úspech 13. seminára je pre organizátorov zadosťučinením a zároveň výzvou na organizovanie podobných podujatí aj v budúcom období. Hlavným organizátorom nasledujúceho 14. seminára je Československá spoločnosť pre rast kryštálov. Pravdepodobné miesto konania seminára bude v Ostravici na Morave v septembri 2004.

K úspešnému priebehu seminára prispeli aj sponzori 13. seminára a to Slovenská spoločnosť priemyselnej chémie (predseda Ing. Miloš Révus) a ILABO s.r.o. Bratislava (majiteľ Ing. Miloslav Blecha).

Všetky informácie o činnosti OS CHFTL a o 13. seminári DMS-RE 2003 (vrátane bohatej fotografickej dokumentácie) je možné získať na webovej stránke OS <http://oschftl.bts.sk>.

Prof. Ing. Marian Koman, DrSc.
predseda

Structure Solution from Powder Diffraction Data SSPD'03

held on 14-19 September 2003 in Stará Lesná, Slovakia

The international meeting Structure Solution from Powder Diffraction Data (SSPD'03) was a logical continuation of a long series of local conferences on powder diffraction, organized in Slovakia since 1992. At the origin of SSPD'03 was an idea to get together the best specialist in the structure determination from powder diffraction data with those working on the field of structure prediction. The purpose of this conference was to assess the progress made in the theory and techniques of structure solution based on powder diffraction data and to point to areas where further work is needed. Special attention was paid to structure prediction done by energy minimization, because its results are frequently checked by Rietveld refinement. It is believed that a combination of these two methods will in a near future become a standard tool. As a conference venue the beautiful environment of High Tatra mountains in Slovakia was chosen. The idea seemed first to be quite risky in the view of uncertain whether in this region in September and also in the view of the accumulation of meetings in this time period.

Following topics were covered by invited lectures:

- *indexing* by Armel Le Bail (Le Mans),
- *structure modeling and prediction of extended solids* by J. Christian Schön (Stuttgart) and of *molecular solids* by Alexander Dzyabchenko (Moscow),
- *intensity extraction* by Jonathan P. Wright (ESRF),
- *direct methods* by Jordi Rius (Barcelona),
- *global optimization* by Peter W. Stephens (Stony Brook) and Radovan Černý (Geneva),
- *total pattern analysis* by Robert L. Snyder (Atlanta),
- *applications to physics and chemistry* by Daniel Louër (Rennes), Robert Von Dreele (Argonne), James A. Kaduk (Naperville) and Paolo Radaelli (ISIS).

These topics and others, like structure determination from neutron powder diffraction, real structure, were covered also by 18 oral and 21 poster presentations. Altogether 69 participants from Croatia, Russia, United Kingdom, Italy, Denmark, USA, Turkey, Austria, Sweden, Slovenia, Spain, France, Norway, Israel, Germany, Algeria, Switzerland, The Netherlands, Czech Republic and Slovakia attended this meeting. Commercial lectures were delivered by A.Coelho (Bruker), C.Reiss and S.Prugovecki (Philips/PANalytical), commercial exhibitions were organized by Philips/PANalytical, Stoe and Oxford Cryosystems. The meeting was also supported by Seifert company. Owing to generous support from the IUCr the Organizers we are able to offer a financial support to a limited number of students and young scientists from several countries.

The basic idea of the program committee of the meeting was to create an atmosphere where the participants felt free to present and exchange their ideas, even the craziest ones.



Lomnický peak



Radovan Černý, chairman of the programme committee



From the left: H. Gies, D. Louer, J. Rius



L. Smrčok, the head of organizing committee, E. Scholtzová



From the conference dinner



From the left: B. and P. Stephens, A. Coelho

No proceedings from the meeting were planned, and despite of busy conference program there was time available for informal discussions. According to the majority of participants the objective was met. Especially the exchange between the people working on structure prediction by energy landscape investigation and those developing the method of structure solution by global optimization of the structural model was stimulating. SSPD'03 showed that such type of creative meetings is very much appreciated in

the fields of science where the methodology is still under development, like is the case of powder diffraction.

Radovan Černý, Lubomír Smrčok