s8.m27.p22 **Collaborative Computational Project Number 14 for Single Crystallography and Powder Diffraction (CCP14).** Richard Stephenson[a], Jeremy Cockcroft[a], Bob Cernik[b], David Watkin[c] and Lachlan M.D. Cranswick[d]. *Department of Crystallography, Birkbeck College, Malet Street, London, WC1E 7HX[a], UK, Synchrotron Radiation Daresbury Laboratory, Warrington, WA4 4AD U.K[b], Chemical Crystallography Laboratory Oxford University, 9 Parks Road, Oxford, OX1 3PD, U.K[c], NRC, Chalk River Laboratories, Chalk River, Ontario Canada K0J 1J0[d]. E-mail: r.stephenson@mail.cryst.bbk.ac.uk*

Keywords: CCP14; Crystallography; Diffraction

From June 2004 Richard Stephenson was appointed the new CCP14 PDRA, replacing Lachlan Cranswick, who left in March 2003 to take up a permanent position at NRC, Chalk River.

The CCP14 is continuing in its efforts to provide freely available crystallographic resources and workshops to academics. Presented here is a snapshot of the continually expanding catalogue of the new and updated crystallographic software archives available for download from the website.

Present CCP14 initiatives include:

Auto-mirroring of crystallographic software, information and resources.

Auto-mirroring of source code, algorithms, free C and Fortran compilers and GUI development kits.

Growing list of tutorials, run throughs and help files for people who make use of single crystal and powder diffraction.

New CCP14 initiatives include:

With the sponsorship and support of the IUCr, an updated edition of the Crystallographic Nexus Virtual Internet/Virtual World Wide Web on CD-ROM will be released this autumn.

Joint BCA/PCG and CCP14 workshop on Rietveld methods held in April 2004. Further workshops to be organized after topic feedback.

[1] www.ccp14.ac.uk

s8.m27.p23 **Thermal expansion of chromium doped mullite.** E. Tkalcec[a], B. Grzeta[b], H. Ivankovic[a], [a]*Faculty of Chemical Engineering and Technology, University of Zagreb, Marulicev trg 20, HR-10000 Zagreb, Croatia,* [b]*Rudjer Boskovic Institute, P.O. Box 180, HR-10002 Zagreb, Croatia. E-mail: etkalcec@fkit.hr*

Keywords: Cr-doped mullite; Thermal expansion; X-ray diffraction

Mullite (nominally $3Al_2O_3{\cdot}2SiO_2$) is an important engineering ceramic material due to its excellent thermomechanical properties like high thermal shock resistance, high temperature shape stability and low thermal expansion. It possesses an orthorhombic structure in the space group *Pbam*. Incorporation of Cr^{3+} ion in mullite is of great interest because the low thermal expansion of mullite can be further reduced in this way [1]. A major goal of this work is to understand dependence of the thermal expansion of Cr-doped mullite on the Cr content. The samples of pure mullite and of mullite with 2, 4, 6 and 8 mol% Cr_2O_3 were derived from single-phase precursors and sintered at 1673 K for two hours. Prepared powder samples were examined by in-situ high temperature X-ray powder diffraction up to 1213 K. Unit-cell parameters of the samples were determined using Si as an internal standard, and refined by the whole-powder-pattern fitting method [2]. It was noticed that the unit-cell parameters of as-prepared samples linearly increased with chromium incorporation up to 6 mol% Cr_2O_3, and nonlinearly above this content. The samples generally displayed strongest thermal expansion parallel to the *b* axis, followed by *c* and *a*. Linear thermal expansion coefficients along *a*, *b*, and *c* axes were determined in the temperature range between 753 and 1213 K. The thermal expansion coefficients decreased with Cr content up to 6 mol% Cr_2O_3, and then pronouncedly increased at 8 mol% Cr_2O_3 [$\alpha(a)$=2.5 × 10^{-6}/K to 1.8 × 10^{-6}/K, and 4.5 × 10^{-6}/K; $\alpha(b)$=4.0 × 10^{-6}/K to 2.3 × 10^{-6}/K, and 6.0 × 10^{-6}/K; $\alpha(c)$=3.9 × 10^{-6}/K to 2.1 × 10^{-6}/K, and 4.9 × 10^{-6}/K]. Such behaviour could be attributed to the change of chromium incorporation mode into mullite structure at higher Cr content.

[1] Schneider, H. & Eberhard, E. (1990). *J. Am. Ceram. Soc*. **73**, 2073-2076.
[2] Toraya, H. (1986). *J. Appl. Cryst*. **19**, 440-447.