

**MS41 P11**

**Pressure induced deformations and elastic behaviour of wairakite.** [Silvia Ori](#)<sup>a</sup>, [Giovanna Vezzalini](#)<sup>a</sup>, [Simona Quartieri](#)<sup>b</sup>, [Vladimir Dmitriev](#)<sup>c</sup>. <sup>a</sup> *Dipartimento di Scienze della Terra, Università di Modena e Reggio Emilia, Italy.* <sup>b</sup> *Dipartimento di Scienze della Terra, Università di Messina, Italy.* <sup>c</sup> *Swiss-Norwegian Beam Lines at ESRF, France.* E-mail: [ori.silvia@unimore.it](mailto:ori.silvia@unimore.it)

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The elastic behaviour and the HP-structural evolution of the zeolite wairakite ( $\text{Ca}[\text{Al}_2\text{Si}_4\text{O}_{12}]\cdot 2\text{H}_2\text{O}$ , s.g. I2/a), the Ca-analogue of analcime, were investigated by means of in-situ synchrotron X-ray powder diffraction from Pamb to 7.8 GPa, and upon decompression [1]. No complete X-ray amorphization is observed up to the highest investigated pressure and the original unit cell parameters are completely recovered upon decompression. The Rietveld structural refinements converged successfully up to 2.5 GPa; above this pressure, a transition to a triclinic phase is observed and consequently only the unit cell parameters were refined. An overall reduction of about 14% of the unit cell volume is observed, demonstrating that wairakite is much more flexible upon compression than upon heating. The cell parameters  $-P$  dependence is strongly anisotropic and larger after the transition to the triclinic s.g. The elastic parameters are  $V_0 = 23\,2533(4)\text{ \AA}^3$ ,  $K_0 = 40(2)\text{ GPa}$ ,  $K_p=4$  (fixed) and  $V_0 = 2660(30)\text{ \AA}^3$ ,  $K_0 = 22(2)\text{ GPa}$ ,  $K_p = 4.5(1.0)$  for the monoclinic and triclinic phase, respectively. The structure distortion of monoclinic to triclinic in the 4-, 6- and 8-membered rings and the increase in wairakite, proceeding via tetrahedral tilting, induces deformation of the extra-framework Ca coordination number. A comparison between wairakite and analcime HP structural evolution [2] shows for both phases 1) analogous deformation mechanisms, 2) the increasing of the extraframework cation coordination number from 6 to 7 and 3) reversible HP-induced cell parameter variations. Conversely, the following differences can be evidenced: 1) wairakite transition from monoclinic to triclinic phase occurs at higher P than that from cubic to triclinic analcime, probably due to the higher capacity of the monoclinic structure to adsorb the HP-induced strains; 2) in the low pressure regime wairakite is more compressible than analcime, due to the different extra-framework content and distribution; 3) different anisotropic behaviour of the cell parameters under HP.

[1] Ori S., Quartieri S., Vezzalini G., Dmitriev V. (2007) *American Mineralogist*, submitted.

[2] Gatta G. D., Nestola, F., Boffa Ballaran, T. (2006) *American Mineralogist*, 91, 568-578.

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**Three-dimensional Birefringence Imaging of Optically Anisotropic Materials** [L. A. Pajdzik](#), [A. M. Glazer](#), *Physics Department, University of Oxford, Parks Road, Oxford OX1 3PU, UK.* E-mail: [pajdzik@physics.ox.ac.uk](mailto:pajdzik@physics.ox.ac.uk)

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We have developed a new optical technique that combines the Metripol<sup>TM</sup> imaging system (see [www.metripol.com](http://www.metripol.com)) with a two-axis tilting-stage that allows us to obtain precise birefringence information on anisotropic materials. The Metripol<sup>TM</sup> microscope employs a combination of a

rotating polarizer and a circular analyzer to separate out three quantities. The first one represents the light transmission  $I_0$ , the second corresponds to the angular orientation  $\varphi$  of a section of the optical indicatrix and the third provides quantitative information on  $|\sin \delta|$  at any point within the image captured by a CCD camera, where  $\delta$  is the phase difference introduced by the birefringent sample.

The addition of a two-axis tilting-stage enables three-dimensional data for  $|\sin \delta|$ ,  $\varphi$  and  $I_0$  to be measured as a function of the two perpendicular tilt angles of the tilting-stage. Examination of optically anisotropic materials using the new approach reveals the three-dimensional character of their anisotropic properties and provides a versatile optical technique. With this system it is possible to obtain information about the principal birefringence, the optical orientation and also to determine other optical characteristics of uniaxial and biaxial samples in any general orientation. This also provides a comprehensive approach for the determination of preferred orientation of uniaxial and biaxial crystallites when the technique is applied to the study of polycrystalline materials. In addition to this, the optical information obtained from a crystalline sample may enable an unknown crystalline material to be identified, or at least classified within a specific group of crystalline materials. This becomes possible by performing computer analysis of the three-dimensional data according to specially designed algorithms using equations derived for the uniaxial and biaxial cases.

We are currently developing new computer software which will enable the process of analysis to be significantly less time-consuming and to be carried out more efficiently. The new program will employ digital image processing to find the crystallite boundaries in order to analyze all the crystallites of the measured data images virtually simultaneously. In order to reduce the time needed for the polarizer rotation and data collection, the rotating polarizer has been replaced with a liquid crystal polarization rotator. This enables the polarization state to be changed in milliseconds which is significantly shorter than that for the mechanical rotation of the polarizer. Furthermore, the quarter wave-plate has been replaced by a liquid crystal variable retarder. This enables the calibration process of the system to be carried out in a more convenient manner and also makes it possible to determine the linear dichroism for samples exhibiting this phenomenon. Further work will also include the development of an environmental tilting-stage to carry out measurements involving temperature changes, electric fields application, etc.

[1] Pajdzik L.A. and Glazer A.M., *J. Appl. Cryst.*, 2006, 39, 326-337.

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[3] Glazer A.M., Lewis J.G. and Kaminsky W., *Proc. Roy. Soc. London*, 1996, A452, 2751-2765.