MS17-O4 Control of porosity through temperature and pressure

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Gaining control of phase transformations offers the possibility of tailoring the properties of polymorphic materials[1]. X-ray powder diffraction is ideally suited to studying such structural modifications, particularly since the bulk material is analysed, allowing the averaged structural features of the material to be correlated with its bulk physical properties, in this case the porosity. In addition, rapid X-ray diffraction data collection allows the determination of intermediate phases, onset points of reactions and information about the reversibility of processes involved.The material studied here exists in four distinct polymorphic forms, each porous to a differing extent. Control of the desired polymorph, and hence the desired porosity is achieved by manipulation of temperature and pressure. The X-ray diffractograms were modelled by Rietveld refinement using the HighScore Plus software[2] to study the structural processes during the phase transformations. The physical properties determined by sorption measurements were modelled using Partial Least Squares Regression (PLSR) analysis, and this data compared to the output from the Rietveld structural study.

[1] see for example Herbert, S.A. *et al. J. Am. Chem. Soc.*, **2013**, 17, 6411.

[2] Degen, T. *et al. Powder Diffr.*, **2014**, 29, S13.

Keywords: porosity, gas storage, polymorphism

MS18 Structures of minerals, planetary and carbon materials at Earth and planetary conditions

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MS18-O1 Discovering new materials, minerals and phenomena with evolutionary algorithms

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Thanks to powerful evolutionary algorithms, in particular the USPEX method, it is now possible to predict both the stable compounds and their crystal structures at arbitrary conditions, given just the set of chemical elements. Recent developments include major increases of efficiency and extensions to low-dimensional systems and molecular crystals and new techniques called evolutionary metadynamics and Mendelevian search.

Some of the results that I will discuss include:

1. Theoretical and experimental evidence for a new partially ionic phase of boron, γ-B and an insulating and optically transparent form of sodium.

2. Predicted stability of "impossible" chemical compounds that become stable under pressure – e.g. Na_3Cl, Na_2Cl, Na_3Cl_2, Na_4Cl_3, $NaCl_3$, $NaCl_7$, Mg_3O_2 and MgO_2.

3. New chemistry of planet-forming systems Mg-Si-O and N-H-O.

4. Fate of carbon inside the Earth.

5. Novel surface phases (e.g. boron surface reconstructions).

6. Prediction of new ultrahard materials and computational proof that diamond is the hardest possible material.

Keywords: crystal structure prediction, computational materials discovery, high-pressure geochemistry