can take several directions including comparison of the actual geometry to either theoretical models or experimental structures from the PDB or small molecular databases. In this contribution we will present integration of search and validation tools from the Cambridge Crystallographic Data Centre, in particular Mogul, into an automated structure solution and refinement workflow. Apart from a post-refinement assessment of structure quality, we explore the use of Mogul to compare programs applied to generate ligand parameter dictionaries for crystallographic refinement. Finally, trends in the quality of ligand geometry as function of structure determination parameters will be discussed based on kinase structures from the PDB as well as those solved in-house. Systematic errors in ligand structures will be highlighted along with potential pitfalls of this validation approach.

Keywords: structure validation, statistical analysis CSD PDB, kinases

P24.09.11

Acta Cryst. (2008). A**64**, C629

Nucleation of heat storage materials - search algorithms for similarities of crystal surfaces

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The demand for e・ciant use of energy leads to an increasing interest in energy storage. For the storage of thermal energy latent heat storage materials are most convenient. These materials use a phase transition solid - liquid in order to store heat. Because of large melting enthalpies and low melting points salt hydrates are of particular relevance for the storage of heat at moderate temperatures. Latent heat storage materials based on salt hydrates show a strong undercooling of the melt. This inhibits the technical development of latent heat storage as an economic useful product. The controled release of the stored energy is possible by triggering the crystallisation using nucleators. Heterogenous nucleators are found empirically or by comparing geometric crystal properties like lattice parameters. The disadvantage of these methods is, that the nucleating agents known for di・erant materials so far are unreliable. Heterogeneous nucleation is expected if the melt gets in contact with epitactic and che-mical similar surfaces. Search algorithms for similar crystal surfaces were developed in order to improve the developement of nucleators for latent heat storage materials and to gain a de-eper insight to the mechanism of nucleation. This approach provides an extension of existing search routines in crystal structure databases and enables more specific search results. The program ATBEL performs a morphology prediction based on the BFDH-method. For all predicted faces ATBEL creates entries in two di・erant databases. These database are used by the program EPITAX for the search of lattice match and chemical similarity of crystal surfaces. New algorithms for automatic handling of crystal structure data are introduced.

Keywords: nucleation, heat storage, morphology

P25.01.01

Acta Cryst. (2008). A**64**, C629

Hydration of activated belite cements studied by synchrotron X-ray powder diffraction

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In spite of its universal use in contemporary construction, ordinary Portland cement is one of the most environmentally contentious materials. On average, for every tone of cement produced, 0.97 tons of CO_2 are released into the atmosphere. So, cement industry contributes around 6% of all CO_2 anthropogenic emissions. Hence, cement chemists are making great efforts to find ways to reduce the environmental impact of the cement-production process. Belite cements may reduce 10% de CO_2 emissions but belite reactivity with water is slow and thus these cements develop low mechanical strengths at early stages. The reactivity of these materials may be increased by two complementary ways: i) stabilize high temperature belite polymorphs and ii) produce calcium sulfoaluminate (CSA) belite cements. CSA clinkers contain $Ca_4Al_6O_{12}SO_4$, which reacts rapidly with water forming ettringite, AFt or $Ca_6Al_2(SO_4)_3(OH)_{12.26}H_2O$, and enhancing development of early age mechanical strengths. CSA clinker manufacture may reduce CO_2 emissions up to 35%. Here, we report an in-situ synchrotron powder diffraction hydration study of these cements. Both alkaline oxides activated belite and CSA cements have been analysed. The patterns were collected in transmission in BM08 beamline of ESRF using the translating image-plate detector. This methodology minimise powder averaging errors which are critical for obtaining accurate analyses. All patterns have been treated by the Rietveld method in order to extract the quantitative phase contents. The water/cement weight ratio was kept fixed to 0.5 and the gypsum role has been investigated by adding different amounts. The starting crystalline phase assemblage and the evolution of the hydrate phases will be reported and related to the calorimetric studies.

Keywords: cement hydration, synchrotron powder diffraction, quantitative Rietveld cement phase analysis

P25.03.02

Acta Cryst. (2008). A**64**, C629–630

Bath quantitative XRD control at Russia aluminum smelters

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The electrolysis cell used in the production of aluminum is a dynamic system. The concentration of main components in the electrolyte must be rigidly controlled in order to maintain optimum conditions during the production process. Key parameters for control include cryolite ratio (CR) or bath ratio (NaF/AlF_3) and additions of calcium, magnesium or lithium fluorides The bath analysis must be done during about 2 to 3 minutes because there are often several hundred or even thousands of cells to measure. The XRD quantitative phase