MS15-P3 A topological method for classification of entanglements in crystal networks Eugeny V. Alexandrov,[a] Vladislav A. Blatov,[a] and Davide M. Proserpio,[b] [a]*Inorganic Chemistry Department, Samara State University, Russia*, [b]*Dipartimento di Chimica Strutturale e Stereochimica Inorganica, Università di Milano, Italy*
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A rigorous method is proposed to describe and classify topology of entanglements between periodic networks. We consider the entanglements caused by Hopf links and/or multiple crossing links [1] between *strong rings*, *i.e.* cycles that cannot be represented as sums of smaller cycles [2]. If then each ring is represented by its barycenter and the barycenters of catenating rings are interconnected we obtain a *Hopf ring net* (*HRN)*. The *HRN* directly characterizes the *catenation pattern*, *i.e.* the method of catenation of the rings, if the kind of network and the degree of interpenetration are fixed. Thus, the topological type of *HRN* can be considered as the basic taxon for classification of entanglements. Before comparing two *HRNs* (*i.e.* two catenation patterns), they should be simplified, *i.e.* pruned of *collisions* [2] and the nodes corresponding to *inessential* rings (*i.e.* the rings that do not belong to the ring basis) [3]. We have algorithmized the method and implemented it into the program package TOPOS [4]. The Hopf ring net approach is compared with other methods of characterizing entanglements; a number of applications of this approach to various kinds of entanglement (interpenetration, polycatenation, and self-catenation) both in modeled network arrays and in coordination polymers are considered. In particular, we found that all interpenetration patterns in 149 three-periodic sphere packings [5] are matched to 18 simplified *HRNs.* We showed that the approach can easily be extended to other types of links between rings, such as the Borromean entanglement or, more general, the Brunnian interlocking. The comprehensive taxonomy of entanglements in coordination polymers should help us to develop design methods for new interlocking motifs.

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Keywords: crystal chemistry, topological aspects of structure, structural motifs

MS15-P4 3D mapping of reciprocal space and structural complexity of $A_xFe_{2-y}Se_2$ superconductor (A = Rb, Cs). Alexei Bosak[a], Volodymir Svitlyk[b], Alexander Popov[a], Daniele de Sanctis[a], Ekaterina Pomjakushina[c], Vladimir Pomjakushin[d], Anna Krzton-Maziopa[c], Kazimierz Conder[c], and Dmitry Chernyshov[b]. [a]*European Synchrotron Radiation Facility, Grenoble, France,* [b]*Swiss-Norwegian Beamlines at ESRF, Grenoble, France,* [c] *Laboratory for Developments and Methods, PSI, CH-5232 Villigen PSI, Switzerland,* [d] *Laboratory for Neutron Scattering, Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland*
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3D mapping of reciprocal space reveals that a "single crystal" form of $A_xFe_{2-y}Se_2$ (A = Rb, Cs) superconductors is a complex mixture of phases. The diffraction pattern is a sum of several components. The main contribution to the Bragg scattering comes from the phase with ordered Fe vacanses [1]. Pronounced diffuse scattering, the elastic nature of which has been confirmed by the complementary inelastic X-ray scattering experiment, is commensurate to the main phase. The diffuse scattering forms 3D objects topologically similar to a Fermi surface nesting construction [2]. While the main phase used to be described as tetragonal in previous diffraction experiments, thorough treatment of 3D reciprocal space maps has revealed its orthorombic distortion and rotational twinning (4-fold).

Additional diffraction spots together with a set of modulated Bragg rods indicate a presence of a second phase with apparent planar disorder, subject to the rotational twinning (4-fold). A third phase is ordered with the same motif as the main one but possesses much higher orthorhombic distortion, 8-fold rotational twinning has practically the same tilt angle as the second disordered phase. Most probably it separates the regions of the first two phases. Such a complex multiscale structure is apparently stabilized by a stress induced by the phase separation process taking place at elevated temperatures [3].

The results are illustrated by metrical analysis of reciprocal layers and local 3D distributiuons of diffraction intensity near reciprocal nodes, compared to the model patterns; both local maps and sections of the large volume of reciprocal space are measured within one experiment with PILATUS 6M detector at ID29 ESRF beamline (~15 min per 3600 patterns for entire volume). Further develpment of the approach explored would allow following *in situ* evolution of complex diffraction patterns as a function of external stimuli.

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Keywords: twinning; superconductivity; phase separation