MS22-O4 **Structure analysis of decagonal ZnMgDy quasicrystal.** Taylan Örs, Walter Steurer, *Laboratory of Crystallography, Department of Materials, ETH Zurich, Switzerland*
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In this study, the first structure analysis of the ZnMgRE (Rare Earth) family of decagonal quasicrystals (d-ZnMgDy) based on single crystal X-ray diffraction data is performed. Crystals were grown in samples having the nominal composition $Zn_{57.6}Mg_{40.8}Dy_{1.6}$. These samples were prepared by induction melting followed by annealing at 375°C for 10 months and quenching to room temperature. X-ray diffraction experiments were carried out both in-house (Oxford Xcalibur PX diffractometer, CCD detector, Mo Ká radiation) and at the Synchrotron facility in Swiss-Norwegian Beam Line, ESRF, Grenoble (λ=0.6980 Å). The Laue group is determined as 10/mmm and no systematic extinctions were observed. The direct space quasilattice parameters are a_{1-4} = 4.626(8) Å and a_5 = 5.214(5) Å. SUPERFLIP program package [1] (based on charge flipping and low density elimination algorithms) was used for structure solution. Reconstructed electron density shows structural motifs similar to previous HRTEM studies [2]. Initial modeling based on Penrose tiling shows that the structure differs significantly from the well-studied Al-TM (transition metal) type of decagonal phases. One important difference is that the structure exhibits additional occupation domains (OD), which create edge centering positions for a regular rhomb or pentagonal tiling. The modeling of this new type of OD by using the higher dimensional approach will be discussed. The results obtained with a cluster covering model will also be presented.

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MS22-O5 **Multi-shell nanoclusters with the γ-brass polyhedral core in intermetallics** Arina A. Pankova,[a] Vladislav A. Blatov,[a] Gregory D. Ilyushin,[b] Davide M. Proserpio,[c] [a]*Inorganic Chemistry Department, Samara State University, Russia,* [b]*Shubnikov Institute of Crystallography, Russian Academy of Sciences, Russia,* [c]*Dipartimento di Chimica Strutturale e Stereochimica Inorganica (DCSSI), Università di Milano, Italy*
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We discuss the nanocluster models of the 2309 crystal structures of cubic intermetallics with a 26-atom core (0@4@22) of the γ-brass type (γ-*configurations*) as well as centered nanoclusters with a similar 27-atom core (1@14@12). Crystal data has been taken from ICSD (release 2011/2) and Pearson's Crystal Data (version 2010/2011). For all the intermetallics we have performed the nanocluster modeling using a recently developed algorithm [1] that unambiguously separates connected structural units assembling the whole structure; the algorithm is implemented into the program package TOPOS [2].

We found complex multi-shell nanoclusters with the 0@4@22 core and additional outer atomic shells. The results obtained establish that topological relationships between the crystal structures of intermetallics containing 26-atom ă-configuration occur thanks to migration of atoms between nanocluster shells resulting in shell transformations. This fact allows one to suppose that these structures are genetically related, although they differ by symmetry and composition.

Using the TOPOS procedure for detecting finite subgraphs of any complexity in infinite periodic graphs, we have found 32 distinct topological nanocluster configurations containing 26-atom γ-configuration in more than 23,000 intermetallics. The results of the analysis suggest that the nanoclusters can be considered as typical building blocks whose combinations can produce the whole variety of intermetallic architectures.

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