FA4-MS11-P01

Ab-initio Calculations on Complex Rare Earth Transition Metal Borides. Heinrich Orsini-Rosenberg[a], Daniel Jung[a], Walter Steurer[a]. [a]*Laboratory of Crystallography, ETH Zurich, Switzerland.*
E-mail: orsini@mat.ethz.ch

The interest in rare earth transition metal boride structures has recently grown, since Jun Akimitsu discovered high-T_C superconductivity in MgB_2 with a critical temperature of 39 K [1] (the highest in conventional superconductors so far). Several structure types are known, which combine a variety of transition metals and rare earth elements. Up to now, mostly cubic or tetragonal metal rich systems have been tested for superconductivity. From the theoretical point of view, testing for superconductivity means exploring the structures of the band gaps. This important feature has proved to be highly correlated with superconducting properties. The yet uninvestigated $YCrB_4$ structure type [2] features over 100 representatives and is therefore an excellent testing system.
We have performed extensive systematic total energy calculations by means of density functional theory, using VASP [3]. We focused on band gap tuning by doping the ternary $YCrB_4$ type structures with other transition metals or rare earth elements. Band structures, electronic density of states and reaction enthalpies for the resulting quaternary systems were calculated. It will be discussed how the structures relate to each other, to what extent they are stable and how we can derive reasonable candidates for high-T_C superconductors.

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Keywords: borides; superconductor; band gap

FA4-MS11-P02

Structure ε_{16} Solved by the Strong Reflections Approach. Mingrun Li[a], Junliang Sun,[a] Sven Hovmöller[a], Xiaodong Zou[a], Grushko Benjamin[b]. [a]*Structural Chemistry, Stockholm University, SE-106 91 Stockholm, Sweden.* [b]*IFF, Forschungszentrum Jülich GmbH, D-52425 Jülich, Germany.*
E-mail: mingrunl@struc.su.se

The relation of the reciprocal lattice between two complicated quasicrystal approximants ε_6 (*Pnma*, a = 23.5 Å, b = 16.8 Å, c = 12.3 Å) and ε_{16} (*B*2*mm*, a = 23.5 Å, b = 16.8 Å, c = 32.4 Å) is studied by comparing their precession electron diffraction (PED) patterns, as seen in Fig. 1. In reciprocal space, the positions of the strongest reflections and their intensity distributions are similar for both structures. For the indexed corresponding reflections, they have the same h and k, but l of ε_{16} is about τ^2 times that of ε_6, such that the very strong reflection 006 in ε_6 corresponds to 0016 in of ε_{16}. By applying the strong reflection approach [1, 2], the structure factors (phases and amplitudes) of ε_{16} can be deduced from the corresponding ones of the known ε_6 structure [3]. Although their symmetry-related structure-factor phases are not identical due to the different space groups, the phases of ε_{16} can be obtained by shifting the phase origin. An electron density map of ε_{16} is calculated. Similar to that of ε_6, the structure of ε_{16} contains 8 layers, stacked along the b-axis in each unit cell. Common features of ε_6 and ε_{16} in Fig. 2 are described as the packing of two typical columns, the decagonal column (Dc) and the pentagonal column (Pc). In that of ε_{16}, eleven Dcs form a banana shaped cluster attached with a pentagon (BP) packed along the a-axis. They are observed by high-resolution transimission electron microscopy (HRTEM). The simulated EDPs from the structure model are in good agreement with the experimental high-resolution precession electron diffraction (PED) patterns.

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Keywords: electron diffraction of crystals; HRTEM; quasicrystal

FA4-MS11-P03

The Crystallographic Structure Modeling of AsSJ and GeAsS by X-Ray Spectroscopy. A. A. Lavrentyev[a], B. V. Gabrelian[a], I. Ya. Nikiforov[a], L. E. Kosarenko[a], J. J. Rehr[b]. [a]*Department of Physics, Don State Technical University, Gagarin Sq.1, Rostov-on-Don, Russia.* [b]*Department of Physics, University of Washington, Seattle, WA 98195-1560, USA.*
E-mail: alavrentyev@dstu.edu.ru

The semiconductive compounds AsSJ and GeAsS have unsufficiently studied because of their complicated crystallographic and electron structures. For these compounds we have obtained X-ray, K-and $L_{2,3}$-emission and K-absorption spectra of sulfur. We performed ab initio calculations using FEFF8 code [1] of electron structure for these compounds of supposed various model crystallographic structures and their X-Ray spectra of S. The most appropriate crystallographic structures were found by comparison of the calculated curves with experiment.

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Keywords: crystallographic structure; X-ray spectroscopy

FA4-MS11-P04

Phase Observation of Crystal Structure Factor by using Rocking-curves. Riichirou Negishi[a], Tomoe Fukamachi[a], Masami Yoshizawa[a], Kenji Hirano[a], Keiichi Hirano[b], Takaaki Kawamura[c]. [a]*Saitama Institute of Technology.* [b]*KEK-PF.* [c]*University of Yamanashi.*