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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.*
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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

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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.*
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The relation of the reciprocal lattice between two complicated quasicrystal approximants ϵ_6 ($Pnma$, $a = 23.5 \text{ \AA}$, $b = 16.8 \text{ \AA}$, $c = 12.3 \text{ \AA}$) and ϵ_{16} ($B2mm$, $a = 23.5 \text{ \AA}$, $b = 16.8 \text{ \AA}$, $c = 32.4 \text{ \AA}$) 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 transmission electron microscopy (HRTEM). The simulated EDPs from the structure model are in good agreement with the experimental high-resolution precession electron diffraction (PED) patterns.

[1] Christensen, J., Oleynikov, P., Hovmöller, S. & Zou, X. D., *Ferroelectrics*, **2004**, 305, 273. [2] Zou, X. D., Hovmöller, S., *Acta Cryst. A*, **2008**, 64, 149. [3] Boudard, M., Klein, H., Boissieu, M. & Audier, M., *Philos. Mag. A*, **1996**, 74, 939.

Keywords: electron diffraction of crystals; HRTEM; quasicrystal

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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.*
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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

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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.*

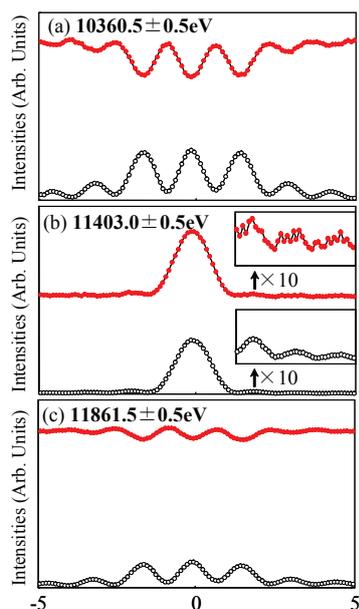
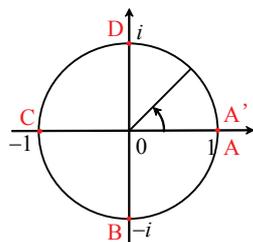
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For a crystal with a center of symmetry, the crystal structure factor is given by

$$F_h = F_h + F_{-h} = |F_h| (1+k^2)^{1/2} \cdot \exp[i\{\arg(F_h) + \theta\}]$$

Here, F_h and F_{-h} are the crystal structure factors due to the real and imaginary parts of the atomic scattering factor, respectively. $\theta = \tan^{-1}[k \cdot \cos\{\arg(F_h) - \arg(F_{-h})\}]$ and $k = |F_{-h}| / |F_h|$. In the two-beam approximation of the resonant X-ray dynamical theory of diffraction, the crystal structure factor must satisfy the condition:

$$F_h F_{-h} / (|F_h|^2 + |F_{-h}|^2) = e^{i2\theta}$$



This condition is satisfied on the unit circle in Fig.1[1].

To measure the scattered intensities by changing 2θ , the diffracted and transmitted rocking curves were measured for GaAs 200 reflection in Laue case as a function of X-ray energy. The experiment was carried out at BL-15C of KEK-PF using the crystal thickness $45\mu\text{m}$. Figs. 2 (a), (b) and (c) show the results of the diffracted I_h and the transmitted intensities I_t measured by changing incident X-ray energy as 10360.5 eV, 11403.0 eV, and 11861.5 eV [2]. The phase of interference fringes between I_h and I_t is anti-phase in Fig.2(a), in-phase in (b) and anti-phase in (c). The phase

change corresponds to the change of 2θ on the circle in Fig. 1 from 0 at point A to -2π at point A' through $-\pi$ at point C.

It is noted that the measured rocking curves as a function of 2θ are quite useful for the phase determination of the structure factor.

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Keywords: phase determination; resonant scattering; GaAs crystal