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Phase Transition Sequence in Ferroelectric Aurivillius Compounds

J. Manuel Perez-Mato^a, J. Tellier^b, Ph. Boullay^b, D. Mercurio^b, F.J. Zuniga^a, ^a*Dept. de Fisica de la Materia Condensada, Facultad de Ciencia y Tecnologia, Universidad del Pais Vasco, Apdo. 644, 48080 Bilbao, Spain.* ^b*SPCTS UMR6638 CNRS/Univ. Limoges, 123 av. Albert Thomas, 87060 Limoges, France.* E-mail: wmpemam@lg.ehu.es

The high-temperature paraelectric-ferroelectric transformation in Aurivillius materials is not yet well characterized. They are known to be non-polar tetragonal at high temperature and ferroelectric at room temperature, but an intermediate phase has been reported in some cases and explained using ab-initio calculations [1]. This intermediate phase is related with the existence of an additional non-polar anti-ferrodistortive instability. Its independent freezing in this intermediate phase seems a necessary condition for a subsequent continuous or quasi-continuous phase transition into the ferroelectric phase [1]. We present a single-crystal X-ray diffraction investigation of the transition sequence in some representative members of the family as SrBi₂Ta₂O₉ (SBT) and SrBi₂Nb₂O₉ (SBN). By monitoring specific reflections as a function of temperature, sensitive either to the superstructure formation or to polar displacements, it was possible to check the existence or not of an intermediate phase. This latter was confirmed in SBT, but within experimental accuracy could not be detected in SBN, confirming previous reports [2]. The reason for this different behaviour is unclear and requires further theoretical investigations.

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Keywords: aurivillius, ferroelectric, phase transitions

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New Graphical User Interface for Calculating Structural Distortions Using the ISOTROPY Software

Harold T. Stokes, Branton Campbell, Dorian M. Hatch, *Brigham Young University, Provo, Utah, USA.* E-mail: stokesh@byu.edu

ISOTROPY (<http://stokes.byu.edu/isotropy.html>) is a set of computer programs which use group-theoretical methods for solving a variety of crystallographic problems dealing with structural phase transitions in crystalline materials. One of the most useful features is the association of distortions (patterns of atomic displacements) with the reduction of space-group symmetry in a transition. We have designed a new interface for ISOTROPY which guides the user through the process of choosing a distortion mode based on considerations such as initial and final space group symmetry, distortion k-vector, irreducible irrep, etc., and subsequently returns the distorted structure which the user can import into a 3rd-party package for analysis or visualization.

Keywords: structural change associated with phase transitions, group theory, graphical interfaces

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General Method for Determining Atomic Pathways in Reconstructive Phase Transitions: SiC and GaN

Dorian M. Hatch^a, Harold T. Stokes^a, Jesse Gunter^a, J. J. Dong^b, James P. Lewis^a, ^a*Brigham Young University, Provo Utah, USA.* ^b*Auburn University, Auburn, Alabama, USA.* E-mail: hatchd@byu.edu

We have developed a general method for determining atomic pathways in reconstructive phase transitions in crystalline materials.

Using a computer program COMSUBS, we first collect a large number of possible pathways under a set of constraints determined by the user. Second, we estimate the enthalpy barrier for each pathway by finding the barrier along pathways which are linear in the structural parameters. Third, we use the bow-function method to calculate the enthalpy barrier for the pathways with the lowest estimated barriers. Fourth, we search for possible ways to lower the barrier even further along each pathway by lowering the symmetry and increasing the number of structural parameters. We have successfully applied this method to the zincblende-rocksalt transition in SiC and the wurtzite-zincblende transition in GaN.

Keywords: structural change associated with phase transitions, group theory, ab-initio calculations

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Phase Transition and Structures of the Phosphate Zn_{0.50}Ti₂(PO₄)₃

Jean-Pierre Chaminade^a, Abdelsam El Bouari^b, Abdelaziz El Jazouli^b, Stanislas Péchev^a, Eric Lebraud^a, Pierre Gravereau^a, ^a*ICMCB-CNRS, University of Bordeaux1, Pessac, France.* ^b*LCMS, Faculté des Sciences Ben M'Sik, Casablanca, Maroc.* E-mail: chamin@icmcb-bordeaux.cnrs.fr

Compounds of general formula M^{II}_{0.5}M^{IV}(PO₄)₃ with M^{II} = Mg, Mn, Fe, Co, Cu, Cd, Ca, Sr, Pb and M^{IV} = Ti, Zr crystallize with either a Nasicon-type structure or a Sc₂(WO₄)₃-type structure, depending on the size of the M^{II} element [1]. Temperature dependent XRD study of Zn_{0.5}Ti₂(PO₄)₃ reveals a reversible α→β phase transition around ~400°C.

Single crystals of the α phase have been obtained with cell parameters, a=14.652(2)Å, b=8.602(1)Å, c=16.930(2)Å, β=125.89(1)° and V=1728.7(1)Å³. The single crystal structure was solved in the non standard space group P2₁/a (referring to the Fe₂(MoO₄)₃ study [2]) with R₁=0.059 and wR₂=0.090.

Diffraction data of the β phase were collected at 500°C on a Philips PW 1050 equipped with an Anton Paar furnace. X-ray diffraction pattern of this powder can be indexed in the P2₁/n monoclinic cell: a=11.918(5)Å; b=8.610(4)Å, c=8.506(4)Å; β=90.37(3)°; V=873.8(1)Å³ referring to the Sc₂(WO₄)₃ study [1]. This structure type was confirmed by Rietveld refinement (R_B=0.043, R_{wp}=0.076, R_p=0.053). The α phase can be considered as a superstructure of the β one with an ordering of zinc atoms and vacancies along b direction.

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Two Phase Transitions in the Low-dimensional Quantum Spin System TiOBr

Jun Akimitsu^a, T. Sasaki^a, M. Mizumaki^b, K. Kato^{b,c}, M. Takata^{b,c}, T. Nagai^d, T. Asaka^d, Y. Matsui^d, ^a*Dept. of physics and mathematics, Aoyama-Gakuin University.* ^b*JASRI/Spring-8.* ^c*CREST, JST* ^d*HVEM/NIMS.* E-mail: jun@phys.aoyama.ac.jp

Recently, Seidel *et al.* [1] suggested from the susceptibility measurements and LDA(+U) calculation that the new inorganic compound TiOX (X=Cl, Br) is a possible candidate for the new spin-Peierls system. However, nobody can observe the new superlattice reflection originated from the spin-Peierls transition.

We report here on the lattice distortion in the new quasi-dimensional spin system TiOBr by x-ray [2] and electron diffractions. Superlattice reflections were observed mainly at around (h, k+1/2, 0) which implies the dimerization along b-axis. The temperature dependence of superlattice reflections shows the two successive phase transitions, a second order transition at T_{c2}=47K and a first order transition at T_{c1}=27K. We will discuss on the key roles of the two successive phase transition of this system.