

instead 264. The minimal energy surface was accordingly mapped by changing the values of those none (twelve) factors. Consequently, atoms are allowed to move in particular directions dictated by the symmetry relations between groups.

[1] R. Caputo, A. Tekin, W. Sikora, A. Zuttel, *Chemical Physics Letters* **2009**, 480, 203-209. [2] W. Sikora, L. Pytlik, Copyright @ 2010 by Nova Science Publishers, NY in *Group Theory: Classes, Representations and Connections, and Applications*. **2010**, 1, 1-40.

Keywords: complex borohydrides, symmetry analysis, first-principles crystal structure prediction

MS20.P06

Acta Cryst. (2011) **A67**, C334

Local instability above t_c in ab_2O_6 perovskites with discontinuous phase transitions

K. Roleder,^a K. Szot,^{a, b} M. Górný,^a Z. Ujma,^a D. Kajewski,^a I. Jankowska-Sumara,^c A. Majchrowski,^d ^a*Institute of Physics, University of Silesia, ul. Uniwersytecka 4, Katowice, (Poland)*. ^b*Forschungszentrum Jülich, D-52425 Jülich, (Germany)*. ^c*Institute of Physics, Pedagogical University, ul. Podchorążych 2, Kraków, (Poland)*. ^d*Institute of Applied Physics, Military University of Technology, ul. Kaliskiego 2, Warszawa, (Poland)*. E-mail: Krystian.Roleder@us.edu.pl

One of the direct proofs for local lattice instability above T_C in ferroelectric perovskites ABO_3 is a weak birefringence [1]. Its temperature dependence characterizes local maximum on $\Delta n(T)$ run, with large thermal hysteresis. This is due to a specific co-existence above T_C of the local lattice instability and non-polar matrix. Bussmann-Holder *et al* [2] have theoretically considered temperature range of this co-existence as polar micro/nano-regions. However, such instability has not been verified yet for antiferroelectric phase transition. That is why for model antiferroelectric material lead zirconate $PbZrO_3$, in which transition from the paraelectric to antiferroelectric phase is realized directly or through an intermediate ferroelectric phase, the investigations of the optical, dielectric, electrostrictive properties and local electric conductivity measured in nano-scale by means of LC-AFM method have been carried out. The goal of these experiments was to check if locally breaking symmetry is a common feature for discontinuous phase transitions regardless of whether transition is realized as the transition to a polar (ferroelectric) phase or to a non-polar (antiferroelectric) phase. Similar experiments have been performed for solid solutions based on the antiferroelectric $PbZrO_3$. The temperature range of the pre-translational local instability has been verified for different phase transformations appearing in these solutions.

[1] A. Ziębińska, D. Rytz, K. Szot, M. Górný, K. Roleder, *J. Phys.: Condens. Matter* **2009**, 20, 142202. [2] A. Bussmann-Holder, H. Beige, G. Völkel, *Phys. Rev. B* **2009**, 79, 184111. [3] J.H. Ko, S. Kojima, T.Y. Koo, J.H. Jung, C.J. Won, N.J. Hur, *Appl. Phys. Lett.* **2008**, 93, 102905.

Keyword: perovskites, phase transitions, local breaking symmetry

MS21.P01

Acta Cryst. (2011) **A67**, C334

A quinquethiophene based self-assembled monolayer for organic electronic applications

R. Resel,^a H.-G. Flesch,^a A. Moser,^a O. Werzer,^a E.C.P. Smits,^{b, c, d} S.G.J. Mathijssen,^c F. Gholamrezaei,^{b, c} H.J. Wondergem,^c S.A. Ponomarenko,^e D.-M. Smilgies,^f G. Hlawacek,^g Q. Shen,^g C. Teichert,^g P. Puschnig,^h D.M. de Leeuw,^{b, c} ^a*Institute of Solid State Physics, Graz University of Technology, Petersgasse 16, 8010 Graz, (Austria)*. ^b*Molecular Electronics, Zernike Institute for Advanced Materials, University of Groningen, Nijenborgh 4, 9747 AG Groningen, (The Netherlands)*. ^c*Philips Research Laboratories, High Tech Campus 4, 5656 AE Eindhoven, (The Netherlands)*. ^d*Dutch Polymer Institute, PO Box 902, 5600 AX Eindhoven, (The Netherlands)*. ^e*Enikolopov Institute of Synthetic Polymer Materials, Russian Academy of Sciences, Profsoyuznaya 70, 117393 Moscow, (Russia)*. ^f*CHESS Centre, Cornell University, 14850 Ithaca, New York, (USA)*. ^g*Institute of Physics, University of Leoben, Franz Josef Strasse 18, 8700 Leoben, (Austria)*. ^h*Chair of Atomistic Modelling and Design of Materials, University of Leoben, Franz Josef Strasse 18, 8700 Leoben, (Austria)*.

In organic electronics the use of self-assembly is one promising approach to high yield and reproducibility in device fabrication. Thin film transistors have been built from a quinquethiophene self assembled monolayer with a yield of one and accordingly integrated circuits like bit generators could be realized [E.C.P. Smits *et al.*, "Bottom-up organic integrated circuits", *Nature* 455, 956-959 (2008)]. Three elements of the molecule are crucial for the monolayer formation and the electronic properties. First the monofunctional anchoring group which avoids uncontrolled polymerization, second the flexible dodecyl part and third the rod-like quinquethiophene units. The flexible spacer groups allow the semiconducting quinquethiophene units to form two-dimensional crystallographic order. It is the first system reported with a long range ordered self-assembled monolayer formed on silicon oxide. The formation of monolayers has been followed by atomic force microscopy and x-ray reflectivity. The in-plane order of the monolayer has been investigated by grazing incidence in-plane diffraction which reveals three nicely pronounced Bragg rods already in the submonolayer state. Two-dimensional crystals with a rectangular unit cell are deduced with up-right standing molecules which are packed in a herringbone pattern. Several irreversible effects are observed by heat treatment: i) a phase transition where the molecules are tilted 13° towards the b-axis of the unit cell is found after a heat treatment at 400K and ii) a gradual increase of the tilt angle with increasing temperature of heat treatment. In-situ experiments reveal that the expansion of the unit cell is not fully reversible, that the crystallographic order is lost above 520K and that the monolayer remains in an amorphous state until 620K. Above that temperature, desorption of the self-assembled monolayer is clearly detectable by a reduction of the monolayer thickness. No detectable monolayer is present above 880K.

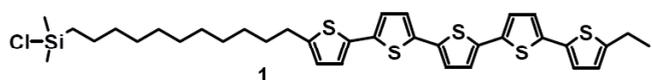


Figure: Chemical structure of the quinquethiophene based molecule used to prepare self-assembled monolayers on silicon oxide surfaces

Keyword: monolayer, organic semiconductor

MS21.P02

Acta Cryst. (2011) **A67**, C334-C335

Quick measurement of crystal truncation rod in multi-wavelength dispersive mode

Tetsuroh Shirasawa,^a Toshio Takahashi,^a Etsuo Arakawa,^b Hiroo Tajiri,^c Hidenori Toyokawa,^c Tadashi Matsushita,^d ^a*Institute for Solid State Physics, University of Tokyo, Kashiwa, Chiba, (Japan)*. ^b*Department of Physics, Tokyo Gakugei University, Koganei, Tokyo,*