Posters - Experimental

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TRANSROTATIONAL THIN-FILM CRYSTALS

V. Yu. Kolosov

Physics Department, Ural Federal University, Lenin Av.51, Ekaterinburg 620000, Russia
kolosov@urfu.ru

The paper accumulates our novel studies and main former data on novel microstructure with unexpected, dislocation independent, regular internal bending of the crystal lattice planes [1]. Usually it is revealed in thin films or layers after amorphous – crystalline transitions. Such *perfect crystals/grains with regularly curved lattice* (built up by simultaneous translation and small regular rotation of the unit cell) *demonstrate a new "transrotational" [2] type of solid state order realized in thin films*. It is primarily dislocation independent and takes place round an axis (or 2 axes, Fig. 1) lying in the film plane of the growing crystal. The maximal values correspond to essential lattice orientation gradients (up to 300 degrees per μm) resulting to several whole rotations for the crystal about 10 μm in length (in film plane).

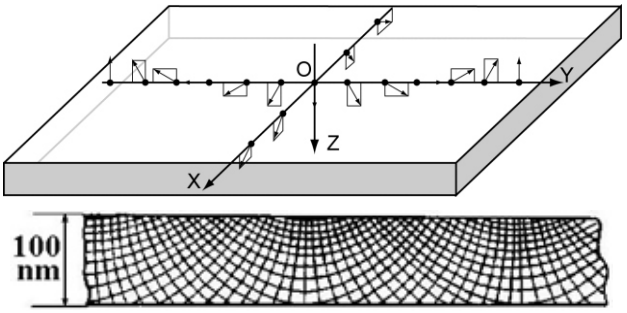

Figure 1. Regular changes of lattice orientation revealed by TEM in thin crystals with 2-axes lattice bending (left) and corresponding scheme of internal bending of lattice planes (right) shown in film cross section.

Thin (10 - 100 nm) crystallized areas with we study vary from small crystals (0.1 - 100 microns), ribbons, whiskers or spherulites to large-scaled polycrystalline areas with a complex texture. They can be grown with the help of heat treatment (or aging) and local annealing by focused electron (or laser beam) in amorphous films of substances of different chemical nature including oxides, chalcogen/ides, some metals and alloys (with or without amorphous sublayers and overlayers) and are stable with years. The films were prepared by laser, e-beam and thermal evaporation mostly with thickness or/and composition gradients across TEM grids (to study these factors directly), solid state amorphization, pyrolysis. The main data have been obtained by TEM, primarily bend-contour method [3], *in situ* studies, and HREM with EDX, EELS, CBED used in due cases. Comparative TEM-AFM studies were performed for definite transrotational microcrystals in amorphous matrix.

Opposite to other unusual regular nano aggregations of atoms widely recognized by the community in recent 30 years (quasi-crystals, fullerenes and nanotubes and other nano derivatives) our less known "transrotational" crystals/structures are less confined in dimensions. Bent atom layers in fine areas can be described as similar to that of hypothetical 2.5D halves (180°) of endless (continuous in film plane) multiwall nano- tubes/onions/tori. The geometry and the magnitude of transrotation depends upon the substance, film preparation and crystallization conditions, orientation of the crystal nucleus, presence of the sublayers, composition and film thickness. *In situ* studies in particular include HREM of amorphous-crystalline interface propagation during crystal growth and multiple reversible local transformations "amorphous – transrotational crystalline" inside the fingers in *Se*-based vacuum deposits, Fig. 2. Dynamic changes of TEM diffraction contrast (revealed by analysis of the video for the large Vg) fit the mechanism of transrotation formation based on the surface nucleation that we proposed earlier.

Most substantial are several examples of "transrotational single crystals" grown in the absence of grain boundaries and dislocations (See – Fig. 3, Te and chalcogenide whiskers/nanobelts, e.g. CuTe, right on Fig. 4) and also other perfect crystals with limited imperfection.

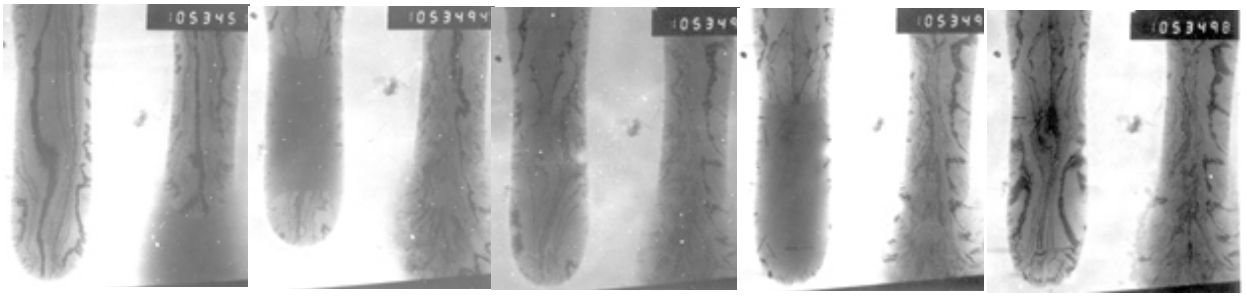

Figure 2. Some of TEM images of multiple reversible local transformations "amorphous – transrotational crystalline" (see drastic change of contrast in left finger) in Se-based vacuum deposits. Initial magnification 10K.

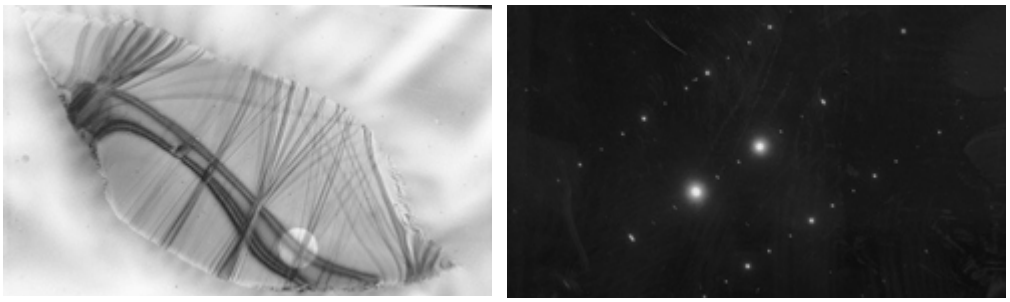

Figure 3. TEM image of transrotational Se single crystal (left) with one of the sequential SAED patterns (right) from the zone-axis pattern marked by selected area 1 μm aperture.

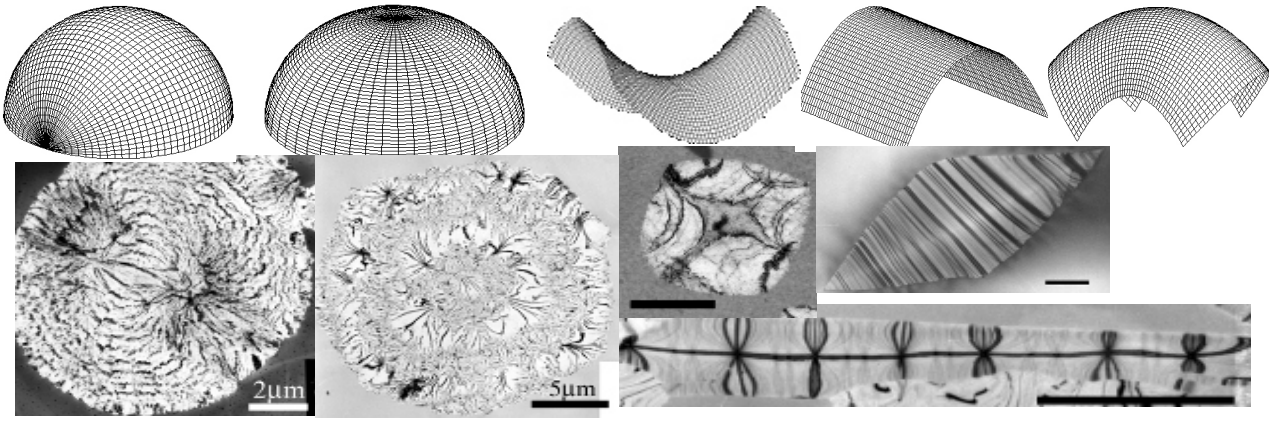

Figure 4. Schemes of transrotation geometry with the TEM images below: Se, Fe_2O_3, Ta_2O_5, C+Se+C, Cu-Te. Bar = 1 μm (where not specified).

Atomistic mathematical model (based on conformal transformations) for the atom positions in "transrotational" single microcrystal and the probable physical reasons are discussed. Transrotational microstructure can be considered as an intermediate between amorphous and crystalline (likewise the structure of liquid crystals, intermediate between crystalline structure and liquid one). We reflect it as one of the reasons of easy phase changes in chalcogen-based films which tend to crystallize in such manner. Transrotational crystals during last years have been eventually recognized/studied in a large variety of thin film systems: Se-C, Se-Te, Sb_2Se_3, Sb_2S_3, Ge-Sb_2Se_3, Ge-Te, Tl-Se, Cu-Te, -Fe_2O_3, Cr_2O_3, Co-Pd, Re, W, carbides, amorphous metals, ferroelectrics, etc., including well-known chalcogenide compositions [4, 5] used for optical memory (CD-RW, DVD RW disks) and prospective for other memories.

1. I E Bolotov, V Y Kolosov and A V Kozhyn, *Phys. Stat. Sol.* **72**a (1982), p. 645.
2. V Y Kolosov and A R Thölen, *Acta Mat.* **48**, (2000), p. 1829.
3. I E Bolotov and V Y Kolosov, *Phys. Stat. Sol.* **69**a (1982), p. 85.
4. B J Kooi and J T M De Hosson, *J. App. Phys*. **95** (2004), p. 4714.
5. E Rimini *et al*, *J. App. Phys.* **105** (2009), p.123502.

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PARTIAL ISOTHERMAL SECTION AT 850 °C OF Al-Pd-Co PHASE DIAGRAM

Ivona Černičková, Pavol Priputen, Marián Drienovský, Dušan Janičkovič, Jozef Janovec

Slovak University of Technology, Faculty of Materials Science, Paulínska 16, Trnava, Slovakia

In Al–Pd–Co alloys investigated recently [1-2], more structurally complex phases were observed, e.g. the ternary monoclinic U-phase, the ternary cubic F-phase, and orthorhombic phases of the -family. This is reflected in isothermal sections of the Al-Pd-Co ternary diagram at 700, 790, 940, 1000 and 1050 °C published earlier [3-5].

In the present work, more Al-Pd-Co alloys with various metal compositions annealed at 850 °C for 500 h were studied by scanning electron microscopy including energy dispersive X-ray spectroscopy, differential thermal analysis and X-ray diffraction. The near-equilibrium phases formed after long-term annealing were identified and transitions between phases on continuous heating/cooling were also determined. The obtained experimental results were used to propose the partial isothermal section of the Al–Pd–Co phase diagram at 850 °C not published till now.

1. Yurechko M, Grushko B (2000) A study of the Al–Pd–Co alloy system. *Mater Sci Eng* **A294**:139–142.
2. Matsuo Y, Hiraga K (1994) The structure of Al_3Pd—close relationship to decagonal quasicrystals. *Philos Mag Lett* **70**:155–161.
3. Yurechko M, Grushko B, Velikanova T, Urban K (2002) Isothermal sections of the Al–Pd–Co alloy system for 50–100 at% Al. *J Alloys Compd* **337**:172–181.
4. Raghavan V (2008) Al–Pd–Co. J Phase Equilib 29:54–56.
5. Černičková I, Čička R, Švec P, Janičkovič D, Priputen P, Janovec J (2013) Study of Phase Equilibria in the Al–Pd–Co System at 700°C. In Springer. Cairns: 133–139.

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ISOTHERMAL SECTION AT 1000 °C OF Al-Mn-Fe PHASE DIAGRAM IN VICINITY OF TAYLOR PHASE

P. Priputen[1], I. Černičková[1], D. Janičkovič[2], J. Janovec[1]

[1]Slovak University of Technology in Bratislava, Faculty of Materials Science and Technology in Trnava, Paulínska 16, 917 24 Trnava, Slovak Republic
[2]Institute of Physics, Slovak Academy of Science, Dúbravská 9, 845 11 Bratislava, Slovak Republic
pavol.priputen@stuba.sk

Taylor phase in Al-Mn-Fe system is a complex intermetallic compound useful for the construction of thermal memory cells. The thermal memory cell is a new concept of information storage, where a byte of digital information can be stored into the storage medium by a pure thermal manipulation [1]. For this purpose a thermodynamical description of Taylor phase in Al-Mn-Fe system is required. Isothermal sections of the Al-Mn-Fe phase diagram at selected temperatures were recently published by Balanetskyy *et. al.* [2].

This contribution is focused on the study of isothermal section of Al-Mn-Fe phase diagram at 1000 °C. At this temperature the Taylor phase is still stable in binary Al-Mn system. Therefore, several alloys with different chemical composition were prepared by arc melting, annealed at 1000 °C for 330 h, and investigated by X-ray diffraction as well as scanning electron microscopy including both energy dispersive X-ray spectroscopy and electron backscatter diffraction. The obtained results were used to construct the partial isothermal section of Al-Mn-Fe phase diagram at 1000 °C.

1. J. Dolinšek, M. Feuerbacher, M. Jagodič, Z. Jagličić, M. Heggen, and K. Urban, *J. Appl. Phys*., **106**, (2009), 043917.
2. S. Balanetskyy, D. Pavlyuchkov, T. Velikanova, B. Grushko, *J. Alloy. Compd.,* **619**, (2015), 211.

The authors wish to thank to the European Regional Development Fund (ERDF) for financial support of the project ITMS:26220120014 "Center for development and application of advanced diagnostic methods in processing of metallic and non-metallic materials" funded within the Research & Development Operational Programme, to the Slovak Acad. Sci. for the support in the frame of the "Center of Excellence for functional multiphase materials" (FUN-MAT, I/2/2011), as well as to the Grant Agency VEGA for the financial support under contract 1/0018/15, and to the Slovak Research and Development Agency for the financial support under contract APVV-0076-11.

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FLUX GROWTH OF PURE AND Mn-MODIFIED ALKALI BASED $Bi_{0.5}(Na_{1-y}K_y)_{0.5}TiO_3$ SINGLE CRYSTALS FOR OPTOELECTRONIC APPLICATIONS

Sonia Bhandari and Binay Kumar

Crystal Lab, Department of Physics and Astrophysics, University of Delhi, Delhi-110007, India
bhandarisonia14@yahoo.in

Single crystals of alkali based ferroelectric $Bi_{0.5}(Na_{1-y}K_y)_{0.5}TiO_3$ (BNKT) and $Bi_{0.5}(Na_{1-y}K_y)_{0.5}Mn_xTi_{1-x}O_3$ (i.e Mn-modified BNKT) were grown via flux method. Crystal sizes varied from 5-8 mm across in case of BNKT and were yellow in colour. Large single crystals of 1-1.5 cm across and brownish black in colour were obtained as a result of Mn-doping. The crystals were found to show maximum absorbance with a broad peak in the UV-region of electromagnetic spectrum. Dielectric studies showed a diffused phase transition for both crystals with phase transition maxima at 310 °C for Mn-modified crystals at 10kHz. A wide direct energy band gap of 2.23 eV was calculated for BNKT single crystal that increased to 2.61 eV in case of Mn-modified BNKT crystal. Photoluminescence spectroscopy was used to study the translational symmetry and nature of associated defects or impurities that break the periodicity of the lattice, perturbing the band structure locally. A broad spectrum with blue- green emissions has been observed in photoluminescence study of BNKT and Mn-modified crystals. Pure BNKT crystals showed a high piezo-response with piezoelectric charge coefficient d_{33} of 216 pC/N while in Mn-modified crystal it was found as high as 202 pC/N. Mechanical strength was tested on flat and smooth surfaces of BNKT and Mn-modified crystals using micro-indentation tester with varied loads and dwelling time. Meyer's index (n) describing the relation between indentation size and load has been used to establish the nature of as grown crystals. Meyer's index *n* was found to be 1.17 for BNKT and 1.15 for Mn-modified crystals establishing hard nature of grown crystals experimentally. This set of material characterization suggests the usefulness of ferroelectric BNKT and Mn-modified BNKT single crystals in several optoelectronic applications.

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KUBO CONDUCTIVITY IN ONE AND TWO DIMENSIONAL SYSTEMS WITH APERIODICALLY PLACED FANO DEFECTS

C. Ramírez[1], V. Sánchez[1], C. Wang[2]

[1]*Departamento de Física, Facultad de Ciencias, Universidad Nacional Autónoma de México, Apartado Postal 70-542, 04510 México D.F., México*
[2]*Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México, Apartado Postal 70-360, 04510 México D.F., México*
carlos@ciencias.unam.mx

Defects in crystals make richer their properties, as occurred in microelectronic devices. There are many kinds of defects such as point, line, planar ones. Among these, the Fano defect consists in an atomic chain attached to the system, producing rich wave interferences in conductivity spectra [1]. Their presence in crystals avoids the use of the reciprocal space and then, we have developed a real-space renormalization method [2] for the Kubo-Greenwood formula within the tight-binding formalism including Fano defects. We have analytically proved the existence of null and ballistic conduction states in one-dimensional (1D) periodic systems with a Fano defect attached [3] as well as a novel ballistic conduction state in a two-dimensional (2D) system with aperiodic arrangements in the cross section and along the Fano plane defect [4]. In this work, we study electric conductivity spectra generated by the inclusion of Fano defects attached at positions following aperiodic sequences. In particular, ballistic conduction states are observed for several values of the chemical potential. Finally, this study is extended to 2D systems with multiple Fano plane defects attached.

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1. A. E. Miroshnichenko, S. Flach, and Y. S. Kivshar, *Rev. Mod. Phys.* **82**, (2010), 2257.
2. V. Sánchez, C. Wang, *Physical Review B*, **70**, (2004), 144207.
3. C. Ramírez and V. Sánchez, *Phys. Status Solidi A*, **210**, (2013) 2431.
4. C. Wang, C. Ramírez, F. Sánchez, V. Sánchez, *Phys. Status Solidi B*, (2015) DOI: 10.1002/pssb.201451516.

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SPIN WAVE EXCITATION IN APERIODIC Co/Au MULTILAYERS

J. Quispe-Marcatoma[1], H, Tarazona[1], M. A. Sousa[2], C. Landauro[1], F. Pelegrini[3], and E. Baggio-Saitovitch[2]

[1]Facultad de Ciencias Físicas, Universidad Nacional Mayor de San Marcos, 14-0149, Lima 14, Perú
[2]Centro Brasileiro de Pesquisas Físicas, Rio de Janeiro, 22290-180, Brazil
[3]Instituto de Física, Universidade Federal de Goiás, Goiânia, 74001-970, Brazil jquispem@unmsm.edu.pe

Ferromagnetic Resonance (FMR) of aperiodic Co/Au multilayers reveals that spin wave and uniform resonance modes are excited by the oscillating microwave field. The four samples studied, with Co layer thickness equal to 0.8 nm, were produced by magnetron sputtering at a pressure of 2 mTorr of Ar atmosphere. The aperiodic structures were generated obeying the Fibonacci sequence $S_n = S_{n-2}S_{n-1}$, (n 2), using S_0 = Au(3ML)/Co and S_1 = Au(7ML)/Co as building blocks. In this work we report the study of the aperiodic S_3, S_5, S_6 and S_7 structures. FMR experiments at microwave frequency of 9.5 GHz were done at room temperature using a commercial electron magnetic resonance spectrometer, standard resonant cavity, swept static magnetic field, and the usual modulation and phase sensitive detection techniques. The perpendicular FMR spectra reveal that the number of volume spin wave resonance modes increase with the number of repetitions of the S_1 building block, up to seven modes for the S_7 structure. In this structure, in particular, a surface spin wave resonance mode is also excited by the microwave field. This behavior, to the best of our knowledge, was not revealed before in FMR experiments of aperiodic multilayers.

1. E. L. ALBUQUERQUE and M. G. COTTAM, *Phys. Rep*. **376**, 225-337 (2003).

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PHOTONIC LOCALIZATION AND TRANSMITTANCE IN MACROSCOPIC APERIODIC MULTILAYERS

J. G. Munguía[1], C. Ramírez[1], V. Sánchez[1], C. Wang[2]

[1]Departamento de Física, Facultad de Ciencias, Universidad Nacional Autónoma de México, D.F., México
[2]Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México, D.F., México
juanguillermo@ciencias.unam.mx

The propagation of a wave through a medium could be very sensitive to the structure if its scale is around half the wavelength of the incident one. In consequence, dielectric materials with periodic, quasiperiodic, or aperiodically ordered structures are considered excellent candidates for making optical components capable of reflecting, confining or guiding light, just as electrons and holes in electronic devices [1]. These materials are called photonic crystals. In this work, we study the optical properties of quasiperiodic and aperiodic multilayers [2], whose layers are ordered following the generalized Fibonacci sequence defined by the substitution rules of A $A^m B^n$ y B A [3]. To carry out this study, we developed a new unified renormalization method for the quasiperiodic and aperiodic transfer matrixes in order to analyse the transmittance for a macroscopic number of layers. In particular, we calculate the transmittance in quasiperiodic or aperiodic multilayers for transverse electric (TE) and magnetic (TM) polarizations by varying parameters such as the angle of incidence, refractive index, layer thickness and wave length. We find an analytical expression for the transmittance, when the layers follow a generalized Fibonacci sequence for several generations. In addition, we find the self-similarity in transmittance spectra when the arrangement of layers follows a quasiperiodic sequence (n = 1) and a zone where the spectrum presents an oscillating behaviour if the order is aperiodic (n > 1), when the incidence angle is null. Finally, the photonic localization is investigated by looking at the Lyapunov coefficient and its results are compared with the transmmitance ones for different incident angles.

This work has been partially supported by CONACyT 131596, UNAM IN113813 and IN113714. Computations were performed at Miztli of DGTIC-UNAM

1. J. D. Joannopoulos, S. G. Johnson, J. N. Winn, R. D. Meade, *Photonic Crystals: Molding The Flow of Light*, 2nd Ed., Princeton University Press, 2008.
2. A. Palavicini, C. Wang, *Optics and Photonics J.* **3** (2013) 20.
3. E. Maciá, *Rep. Prog. Phys.* **75** (2012) 036502.