layers [2], selective broadening of the reflections was observed and occurrence of stacking faults was suggested.

An expression for intensity distribution in powder diffraction from a sample containing stacking faults [3] has been modified in consideration the misfit between two-dimensional lattices of the subsystems, and applied to stacking disorder in composite crystals. The analyses have been made for neutron and X-ray powder patterns of faulted $(Ca_2CoO_3)_{0.62}CoO_2$, and X-ray powder patterns of faulted $(PbS)_{1.12}VS_2$. The experimental results have been interpreted satisfactorily on the basis of stacking disorder model.

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Keywords: composite crystals, stacking faults, diffuse scattering

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5-D Modeling of the Co-rich decagonal Al-Co-Ni Quasicrystal

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Even twenty years after the discovery of quasicrystals, not a single structure is known with the accuracy and reliability commonly expected for regular periodic structures [1]. One way leading towards understanding the structure of quasicrystals, is given by the examination of approximants.

The main interest of this work is to investigate the complete stability field of decagonal Al-Co-Ni by 5-D modeling, starting from the W-phase [2]. The latter is of particular interest, as it is the only known approximant in this system, containing the complete atomic cluster [3]. The focus will be on order, disorder and phase transformations of the decagonal Al-Co-Ni.

First 5-D modeling results of the Co-rich decagonal phase will be discussed. Via embedding the W-phase, models of the decagonal phase are rendered and phasonic modes are being applied.

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Keywords: quasicrystal, 5-D modeling, W-phase

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Modulated Structure of $[FeCl(DMPE)_2(NCC_6H_4NO_2)][PF_6]$ a Material for Use in NLO

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It is well known the recent interest in the nonlinear optical (NLO) properties of organometallic complexes [1,2]. Most efficient NLO-active complexes have a dipolar composition, with an electron-donating group linked by a π-conjugated bridge to an electron-accepting group. Our studies on complexes with this composition have been focused on metal σ-nitriles, for which the second-order NLO responses have been determined [3,4]. Since, it is also of interest to assess the importance of co-ligands in the donor metal coordination sphere, our attention has turned to an alternative coordinated Fe(II) system, namely trans-chloro(diphosphine)iron nitriles. In the solid state our main interest is to align the molecules and avoid centrosymetric space groups. When trying to solve the structure of the title complex we had several difficulties and the structure proved to be modulated. Refinements are being done using JANA and final results will be presented in this work.

[1] Whittall I.R., et al, *Adv. Organomet. Chem.*,1999, **43**, 349. [2] Goovaerts E., et al, *Handbook of Advanced Electronic and Photonic Materials*, Ed. H.S. Nalwa, 2001, **9**, Ch. 3, 127. [3] Wenseleers W. et al, *J. Mater.Chem.*, 1998, **8**, 925. [4] Garcia M.H., Robalo M.P., Teixeira A.P.S., Piedade M.F.M., Duarte M.T., Dias A.R., *J. Organomet. Chem.*, 2001, **632**, 145.

Keywords: NLO, organometallic compound, modulated structure

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Dislocation Dynamics in a Dodecagonal Quasiperiodic System

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We have developed a set of numerical tools for the quantitative analysis of defect dynamics in quasiperiodic structures, with the intention of addressing some of the open questions regarding the dynamics of dislocations in quasicrystals. We are applying these tools to study dislocation motion in the dynamical equation of Lifshitz and Petrich [1] whose steady state solutions are quasiperiodic, exhibiting dodecagonal symmetry.

Here we demonstrate - by showing real-time computer simulations - our ability to inject an arbitrary set of dislocations, parameterized by the homotopy group of the D-torus, and quantitatively follow the positions of these dislocations as the equation evolves in real time. We measure and analyze the dislocation velocity as a function of applied stress and shear, as well as the phonon and phason strains that accompany this motion as the system evolves in time. These results display intriguing differences with respect to the behavior of dislocations in periodic solutions of the dynamical equation.

[1] Lifshitz R., Petrich D.M., *Phys. Rev. Lett.*, 1997, **79**, 1261.

Keywords: dislocation dynamics, quasicrystals, computer simulation

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Ab initio Simulations on the W-phase of the Al-Co-Ni System

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The W-phase [1] is the highest stable approximant of the decagonal quasicrystal known in the system Al-Co-Ni. Its structure contains the so-called “20 Å-cluster", which is a characteristic building unit of decagonal Al-Co-Ni.

The Co/Ni ratio determines which modification of decagonal $Al_{72}Co_{28-x}Ni_x$ ($8 \leq x \leq 20$) is formed. Therefore, we studied the influence of the Co/Ni ratio on the structure of the W-phase, starting from binary compositions Al-Co and Al-Ni with idealized positions. From these results a realistic ternary model was derived.

The structure models were optimized using the VASP code [2,3]. Our calculations are based on the generalized gradient approximation and utilized PAW potentials [4] supplied with VASP. The band structure, electron density districution and electron localization function were calculated.

These calculations help to get insight into the factors governing formation and stability of this kind of complex intermetallic alloy. They also corroborate the results of the single-crystal X-ray structure analysis, from which a significantly distorted and disordered structure model was obtained.

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Keywords: quasicrystals, ab initio calculations, clusters

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Interaction and Phase Transitions in a Pototype Self-assemblied Supramolecular Aperiodic Crystal

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This contribution reports on very new structural and physical