surface increases up to value of the film thickness. Considering the DCV6T-Bu$_4$ films of the same thickness, use of heated substrates gives rise to the film relaxation, resulting in reducing the interplane DCV6T-Bu$_4$ distances, d, (from d = 11.29(5) Å to d = 10.78(5) Å, resp., for 50 nm-thick films deposited on Si wafers) closer to the bulk value (10.14(1) Å) observed for bulk powder material. Similarly, with increasing thickness of the films deposited on heated up to 90 °C substrates, the interplane DCV6T-Bu$_4$ distances are reduced (on an example of 10 nm- and 50 nm-thick films on Si substrate, from d = 10.92(5) Å to d = 10.78(5) Å, resp.) accompanied by a decrease of the microstrain, s, (from s = 1.6(2) % to s = 0.6 %). For the same substrate temperature and film thickness, the contraction of the DCV6T-Bu$_4$ films is reducing for growth on Si to BPAPF to C$_{60}$ (compare d = 10.92(5) Å, 10.88(5) Å and 10.78(5) Å for 10 nm-thick films deposited on corresponding 90 °C-heated substrates).

An attempt was performed to index the DCV6T-Bu$_4$ powder XRD pattern recorded at room temperature. Best results confirmed by comparable rather good quality of the Whole-X-ray-Powder-Pattern-Fitting of the experimental XRD powder pattern using the Pawley approach were obtained in frames of space groups $P\bar{1}$ (triclinic; unit cell parameters a = 11.988(5) Å, b = 13.645(12) Å, c = 17.458(9) Å, α = 125.13(4)°, β = 57.88(3)°, γ = 110.58(5)°; number of independent molecules Z = 2; calculated density ρ = 1.466(3) g/cm^3) and $P2_1/n$ (monoclinic; a = 15.1586(6) Å, b = 17.2220(5) Å, c = 14.5872(7) Å, β = 93.845(4)°; Z = 4; ρ = 1.5228(1) g/cm^3). According to XRR investigations, the thicker films are characterized by smaller density and higher roughness independent on the substrate kind. An up to 6 nm-thick intermediate layer with linear density-gradient is formed at the DCV6T-Bu$_4$/C$_{60}$ interface for the films with buffer C$_{60}$ underlayer.

Keywords: organic thin films, X-ray reflectometry, X-ray diffraction

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Theory of phonons in 2D, 3D crystals and multilayers of hexagonal boron nitride. K.H. Michel, B. Verberck. *Department of Physics, University of Antwerp, Belgium.*
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Starting from an empirical force constant model of valence and van der Waals interactions and calculating by Ewald's method the ion-ion force constants, we derive the dynamical matrices for two-dimensional (2D), three-dimensional (3D) and multilayer crystals of hexagonal boron nitride (h-BN). The phonon dispersion relations in h-BN are calculated and the evolution of the spectra from 2D to multilayer and 3D crystals is studied. The interplay between valence and Coulomb forces is discussed. It is shown by analytical and numerical methods that in the 2D crystal the longitudinal and transverse optical (LO and TO) phonon frequencies for in-plane motion are degenerate at the Γ-point of the Brillouin zone. Away from Γ, the LO branch exhibits pronounced overbending. It is found [1] that the nonanalytic Coulomb contribution of the dynamical matrix causes a linear increase of the slope of the LO branch with increasing wave vector q starting at Γ. In the multilayer case, the LO and TO branches are still degenerate at Γ, away from Γ we obtain a phonon band where the number of LO branches is equal to the number

of layers. The slope of the highest LO branch increases steeply with q. In 3D h-BN the highest LO and TO modes are split, in agreement with the Lyddane-Sachs-Teller theory for ionic crystals. The splitting at Γ is found to be 61 cm^{-1}. Away from the Γ-point the LO branch in 3D h-BN can be considered as the envelope limit of the highest mode of the multilayer band for a large number of layers. Since 2D and 3D h-BN are ionic crystals where the lattice points are not centers of symmetry, the mechanical and electrical properties are coupled. The phonon spectra calculated by the present theory for 3D h-BN are reasonably close to the results of inelastic X-ray scattering experiments [2]. Piezoelectric effects are found to be important in two ($e_{1,11}$ = -1.19 × 10^{-12} C/cm) [1] and in three ($e_{1,11}$ = -0.357 × 10^{-4} C/cm^2) dimensions.

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Investigation of the Water-Pyrite-(100)-Interface with GIXRD. Sandrina Meis, Uta Magdans. *Department of Geology, Mineralogy and Geophysics, Ruhr-University Bochum, Germany.*
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Pyrite surface reactions play an important role in many geological, biological and environmental processes, e.g. acid mine drainage, heterogeneous catalysis. Pyrite could also serve as a template for complex reactions and the formation of amino acids in the iron-sulphur-world scenario under prebiotic conditions [1]. The knowledge about the adsorption processes of H$_2$O under ambient conditions is essential to understand the surface reactions and template properties of the pyrite surface. The three-dimensional pyrite surface and the interface structure of the (100) pyrite surface and water were investigated using grazing incidence X-ray diffraction (GIXRD) under ambient conditions. The measurement of non-specular crystal truncation rods (CTR) provided information about the periodic order of the vertical and lateral surface and the interface structure on atomic scale, using integrated and corrected intensities in a least square fit.
A general structure model for H$_2$O adsorption was found by refining models with different start parameters for the site occupation factors of the surface cell of FeS$_2$, the occupancy of O-atoms mimicking water molecules and their positions. The pyrite surface is terminated by the bulk structure, it shows no reconstruction and only small relaxations of <0.1Å for the bottom FeS$_2$-layers and up to 0.5Å for the topmost layer. The cubic surface cell with the dimensions a$_1$=a$_2$=5.417Å is extended in z-direction to a$_3$=8.748Å. We found a defect structure resulting from an increasing amount of S and Fe vacancies for the topmost layers.
In good agreement with results from molecular dynamic simulations of a water film on the pyrite surface [2], three layers of H$_2$O molecules adsorbing on the pyrite surface were found at distances of 1.9(1)Å, 3.0(3)Å and 5.4(4)Å from the topmost Fe-layer. Additionally, part of O-atoms occupies the Fe-vacancies of the topmost layers, so that we found another O position in 3Å distance above the 2nd Fe layer of the pyrite surface. Between the adsorbate structure and the bulk structure of H$_2$O, a transitional zone of up to 8Å above the topmost Fe