surface increases up to value of the film thickness. Considering the DCV6T-Bu4 films of the same thickness, use of heated substrates gives rise to the film relaxation, resulting in reducing the interplane DCV6T-Bu4 distances, \(d\), (from \(d = 11.29(5) \text{ Å} \) to \(d = 10.78(5) \text{ Å} \), 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-Bu4 distances are reduced (on an example of 10 nm- and 50 nm-thick films on Si substrate, from \(d = 10.92(5) \text{ Å} \) to \(d = 10.78(5) \text{ Å} \), 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-Bu4 films is reducing for growth on Si to BPAPF to C60 (compare matrices for two-dimensional (2D), three-dimensional (3D) and van der Waals interactions and calculating by Ewald’s theory of phonons in 2D, 3D crystals and calculating by Ewald’s approach 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 \((e_{11} = -1.19 \times 10^{-12} \text{ C/cm})\) [1] and in three \((e_{33} = -0.357 \times 10^{-4} \text{ C/cm})\) dimensions.


Keywords: 2D crystals, multilayers, piezoelectricity

FA5-MS39-T05

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 \(\text{H}_2\text{O}\) 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-symmetric 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 \(\text{H}_2\text{O}\) adsorption was found by refining models with different start parameters for the site occupation factors of the surface cell of FeS2, 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 FeS2-layers and up to 0.5Å for the topmost layer. The cubic surface cell with the dimensions \(a_{0} = a_{0} = 5.417 Å\) is extended in z-direction to \(a_{0} = 8.748Å\). 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 \(\text{H}_2\text{O}\) 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 3rd Fe-layer of the pyrite surface. Between the adsorbate structure and the bulk structure of \(\text{H}_2\text{O}\), a transitional zone of up to 8Å above the topmost Fe

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FA5-MS39-T04

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 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].

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26th European Crystallographic Meeting, ECM 26, Darmstadt, 2010