MS23-P12 Structural studies of MoS_2 intercalation compounds with aromatic molecules

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Molybdenum disulfide is an important graphene analog demonstrating semiconducting properties. The unique feature of the MoS_2 layers is the susceptibility of their atomic structure and properties to negative charge transferred onto layers. The crystalline MoS_2 can be exfoliated into single-layer dispersion of MoS_2 crystals by reduction of starting material to $LiMoS_2$ followed by detachment of its layers in aqueous solvents [1]. This dispersion reacts with organic salts in solution, producing precipitates of layered MoS_2 intercalated with their cations [2].

Recently [3], we have found that the powder X-ray diffraction patterns of $(R_4N)_xMoS_2$ (R= H, alkyl) can be modeled using the "supercell approach" [4,5] developed by C. Ufer for full-pattern modeling of turbostratically disordered clays. This method allowed direct refinement of both MoS_2 layer geometry and the cation positions.

In the current work, we investigate the applicability of this approach to intercalation compounds of MoS_2 with aromatic moieties. Initially, the difference between the calculated and experimental patterns was unacceptable due to intense symmetric peaks unexplained by purely turbostratic disorder. We found that these peaks correspond to short-range correlations between MoS_2 layer positions, and successfully modeled them assuming that the turbostratic disorder is actually exhibited by stable bilayer fragments (Fig. 1).

This new "bilayer-supercell" model allowed us to refine the powder patterns of new intercalation compounds. We obtained the preferred geometry and relative positions of MoS_2 layers, as well as the orientation of aromatic molecules in the interlayer space. The PW-DFT-d calculations based on this model confirm our results.

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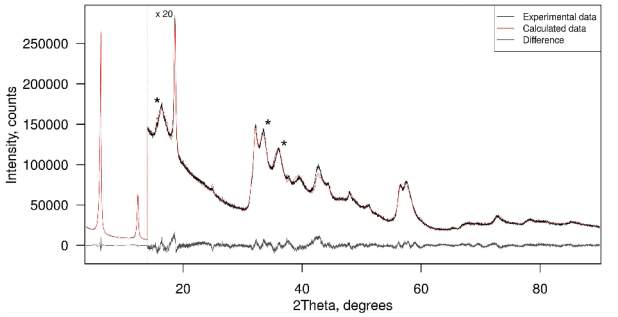

Figure 1. The powder pattern of intercalation compound of MoS_2 with 1,8-bis(dimethylamino)naphthalene. Asterisks (*) denote the peaks caused by correlation between the MoS_2 layers.

Keywords: powder diffraction, layered systems, molybdenum disulfide