

Oral Contributions

[MS26 - 04] The structure and ordering processes of MoS₂-based layered systems.

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The molybdenum disulfide MoS₂ is a naturally occurring layered solid that finds applications in industry both in its bulk and dispersed forms. The material consists of covalently bonded MoS₂ layers, which are linked together by van der Waals interactions [1]. The ability of these layers to move relatively easily against each other makes MoS₂ an important tribomaterial [2]. MoS₂-based composites are also used in petrochemical catalysis [3]. One of the important and mild methods for producing MoS₂ nanoparticles is single-layer dispersion of MoS₂ crystals, which implies the reduction of starting material to (Li)⁺(MoS₂)⁻ followed by detachment of its layers from each other in aqueous solvents [4].

The acidic treatment of the single-layer (Li)⁺(MoS₂)⁻ dispersed in polar solvent leads to exfoliated-restacked (E-R) MoS₂ differing significantly from initial crystalline MoS₂ due to irregularities of the stacking process and distortions of layers. We report extensive studies of this material and its thermal behavior using X-ray powder diffraction, TEM, TGA and DSC [5]. The E-R MoS₂ restacked in acidic conditions is a highly disordered metastable material with disorder-order transition at 98°C. Contrary to literature data, the ordering process does not stop after heating to 100 °C, and continues to the temperatures as high as 800°C. The resulting material, even after heating to 800 °C, cannot be described as hexagonal MoS₂ reported previously [6]: the uneven thermal-dependent broadening of diffraction peaks in the powder

pattern of this material shows significant amount of internal disorder, mostly stacking faults. The comparison with independent modeling results [7] supports our conclusion that this new material has equal probabilities of hexagonal- and rhombohedral-like stacking and thus should be considered a new MoS₂ polytype.

The (Li)⁺(MoS₂)⁻ dispersion also reacts with organic salts in solution, producing precipitates of layered MoS₂ intercalated with their cations. The structure and ordering degree of these compounds depends strongly on the nature of the organic moiety. Basing on powder diffraction data we demonstrate that intercalation of NMe₄⁺ and NEt₄⁺ leads to relative ordering of MoS₂ layers and formation of supercell in the *hk0* plane, while the less symmetric cations demonstrate no such behavior. For the long-chain Me₃N⁺R compounds the only ordered direction is *00l*, corresponding to the planes parallel to the MoS₂ layers. The latter compounds demonstrate a very strongly 2θ-dependent line broadening, which can be modeled by bimodal distribution of the interlayer distances, indicating simultaneous presence of layer structures with different relative positioning of fatty chains.

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