Abstract

The dissertation presents a comprehensive approach to studying the physical properties of liquid phase exfoliated nanomaterials. The analysis covers structural, electronic, and optical properties, particularly particle size and morphology, lattice defects, interlayer interactions, and chemical bonding. The characterization of physical properties was carried out to optimize the production process's efficiency and determine the relationships between manufacturing parameters and the functional properties of nanomaterials. Given the considerable diversity of nanomaterials available, the materials produced were compared with commercial counterparts and with data reported in the literature. Research on the exfoliation of nanomaterials and their physical properties pertains to solid-state physics and forms the basis for designing materials with optimized performance characteristics.

The first part of the dissertation concerns the study of the physical properties of graphene flakes produced by exfoliation of graphite intercalated with SO₃ and H₂SO₄ molecules. This method enables efficient intercalation and exfoliation without the use of oxidizing agents. Predictions from density functional theory (DFT) calculations were referenced to explain the high efficiency of intercalation-assisted exfoliation in oleum. The interaction energies in graphite systems intercalated with such molecules were examined. The unique turbostratic structure of the obtained graphene flakes was characterized in detail using complementary research methods, which allowed verification of the effect of process parameters on the material's physical properties.

In the next part of the work, a method for assessing the quality of graphene flakes based on the analysis of Raman spectra, particularly changes in the shape of the 2D band, was proposed, complemented by X-ray diffraction analysis and surface imaging using scanning electron microscopy. Classification of graphene flakes based on the relationship between the coefficient of determination (R^2) and the full width at half maximum of the 2D band enables a statistical evaluation of material quality and categorization of flakes in terms of their structure. The method was validated on commercial carbon nanomaterials as well as produced under laboratory conditions.

The following section describes the properties of graphene flakes and MoS₂ produced in a high-pressure homogenizer using low-toxicity liquids. The applied research methods - including UV-Vis spectroscopy, Raman spectroscopy, and X-ray diffraction - allowed estimation of concentration, average number of layers, surface dimensions, crystal structure,

and structural defects of the materials, and subsequently correlated these parameters with the conditions of high-pressure homogenization and cascade centrifugation. Practical limitations of the homogenizer in exfoliation were identified and described, such as component wear and challenges in processing liquids containing layered materials.

In the final part of the study, the physical properties of various Ni(OH)₂ fractions obtained by the ultrasonic method were investigated. The starting material had a crystalline structure consisting of a mixture of phases, and significant differences in UV-Vis optical properties were demonstrated. The investigation of optical properties included an analysis of changes in extinction, absorption, and scattering coefficients, which allowed confirmation of structural changes in the obtained layers. The analysis of physical properties, in particular the crystalline structure of the examined material, was supplemented by Raman spectroscopy and X-ray diffraction. The obtained results provide a basis for interpreting the electrochemical study findings, including electrode capacitance in supercapacitors.

The work demonstrates the relationships between exfoliation process parameters and the physical properties of the obtained nanomaterials. In light of the wide variety of available nanomaterials, it is important to assess their quality and the correlation of properties with the manufacturing method. The results confirm the high effectiveness of the proposed exfoliation methods in producing nanomaterials with desirable physical properties.

Keywords: nanomaterials, graphene flakes, molybdenum disulfide, nickel hydroxide, layered materials, liquid exfoliation, Raman spectroscopy, UV-Vis spectroscopy, X-ray diffraction