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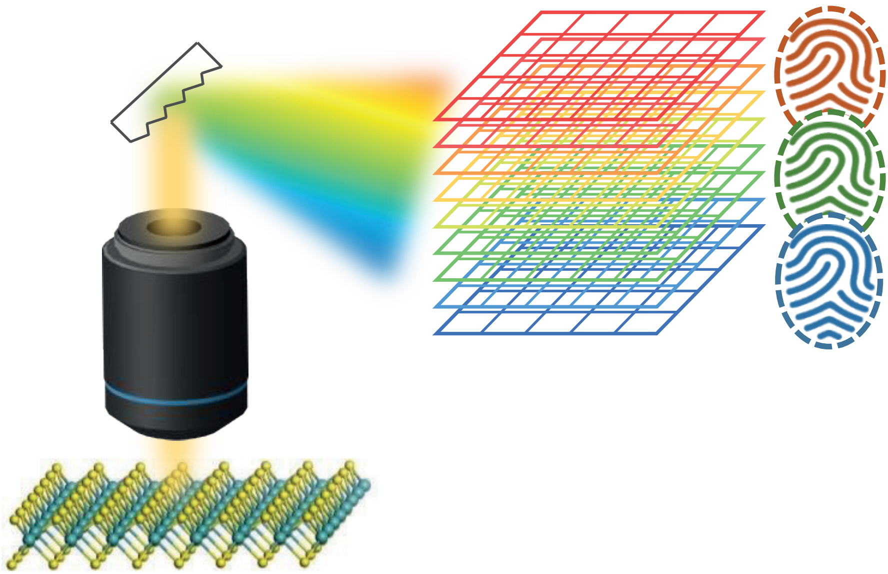
Hyperspectral Imaging Microscopy for Atomic Layer Mapping of Two-Dimensional Materials

Xingchen Dong



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Abstract

Two-dimensional (2D) materials including graphene, transition metal dichalcogenides (TMDs), and black phosphorus (BP) show unique physical properties when controlled to mono- and few-layer thickness, and therefore are promising for optic and photonic devices. The optical, electrical, and mechanical properties of 2D materials are largely dependent on their atomic layer numbers. Optical microscopy is widely implemented to distinguish 2D flakes but the lack of abundant spectral information makes it difficult to confirm the exact layer number. Spectroscopic techniques such as Raman and photoluminescence microscopy are time-consuming when applied for large-area flake searches due to the point-scan mode. Ellipsometry microscopy is an industrial-standard measurement technique, but modeling and interpretation of spectral ellipsometry data require previous knowledge of the properties and structures of the measured materials. Line-scan hyperspectral imaging microscopy which combines both spectroscopy and imaging techniques provides both spatial and spectral information, realizing a satisfying trade-off between the measurement speed and accuracy in layer number identification within a large-area sample. This work studies the suitability of hyperspectral imaging microscopy for rapid and accurate atomic layer mapping of 2D materials.

First, a hyperspectral imaging system including a line-scan hyperspectral imaging microscope, system control, data acquisition, and data processing was custom built. The control and image acquisition of the system worked in MATLAB. The image processing for reconstructing layer maps was developed from manual interpretation (MATLAB environment) to the machine-learning-based method (Python environment). The spatial and spectral parameters of the system were calibrated and the details of the system were introduced for rebuilding such a system.

Second, to interpret the multidimensional data set acquired by the hyperspectral system for 2D materials layer mapping, manual interpretation methods including spectral unmixing and peak position mapping were developed. A comparative study was conducted to process the multidimensional data set of multi-layer molybdenum disulfide (MoS_2), showing advantageous performances of the spectral unmixing method. A complete hy-

perspectral analysis, including single-band analysis, pixelwise spectral analysis, and image classification were conducted using MoS_2 and hexagonal boron nitride (hBN) with mono- and few-layer thickness. To test the identification limit of the system for layer mapping, the hyperspectral data set of MoS_2 flakes with monolayer, bilayer, trilayer, multi-layer, and bulk, was interpreted and spectral fingerprints of all flake categories were extracted to form a hyperspectral library. The reconstructed maps showed atomic layer maps with one-atomic-layer resolution.

Third, to further develop an intelligent system for fully automated large-area atomic layer mapping, a deep fusion neural network based on the U-Net architecture was proposed for imagery fusion of hyperspectral microscope data sets and RGB microscope images, with monolayer, bilayer, trilayer, and multi-layer MoS_2 employed as a demonstration. After multimodal information acquisition, data sets co-registration, network training and testing, the deep fusion neural network realized one-layer precision and accurate profile outputs. A quantitative comparison showed advantageous performances of the deep fusion network over the state-of-the-art single-stream U-Net model solely based on RGB microscope images. This deep-learning-supported technique with high speed, high spatial resolution, and high accuracy is prominent for fully automated 2D materials characterization.

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