Quantifying the thickness of WTe_2 using atomic-resolution STEM simulations and supervised machine learning

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In the realm of two-dimensional (2D) materials, the thickness of the material greatly influences their physical and chemical properties. WTe_2, a 2D quantum material, exhibits intriguing properties as it transitions from a single layer to multiple van der Waals layers. However, due to its distorted crystal structure, determining thicknesses in atomic-resolution images is challenging. Additionally, its susceptibility to air and electron beam-induced damage underscores the importance of direct measurements. Here, we present an efficient method to determine the thickness of T_d-WTe_2, up to ten van der Waals layers, utilizing atomic-resolution high-angle annular dark-field scanning transmission electron microscopy image simulation. Our method involves analyzing intensity line profiles of overlapping atomic columns and constructing a standard neural network model from the line profile features. We demonstrate the capability to distinguish even and odd thicknesses (up to seven layers) without employing a machine learning model, by just comparing deconvoluted peak intensity ratios or area ratios. Furthermore, the trained neural network model achieves a high accuracy of up to 94% with variable amounts of Gaussian and Poisson noise, enabling the identification of thicknesses up to ten layers. This approach not only quantifies T_d-WTe_2 thicknesses accurately but also gives insights in characterizing atomic structures and defects in related 2D materials with partially overlapping atomic columns.