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Autonomous robotic assembly of two-dimensional crystals to build van der Waals superlattices

Van der Waals heterostructures are comprised of stacked atomically thin two-dimensional crystals and serve as novel materials providing unprecedented properties. However, the random natures in positions and shapes of exfoliated two-dimensional crystals have required the repetitive manual tasks of optical microscopy-based searching and mechanical transferring, thereby severely limiting the complexity of heterostructures.

To solve the problem, we develop a robotic system that automatically searches exfoliated 2D crystals and assembles them into vdW superlattices inside glovebox [1]. The system can automatically scan the surface of silicon substrates, analyze optical microscope images, and detect 400 monolayer graphene flakes per hour. The stacking order, positions, and crystallographic orientations of the 2D crystals are designed using the customized CAD software. The robotic assembly system of two-dimensional crystals enabled stacking four cycles of the designated two-dimensional crystals per hour with few minutes of human intervention for each stack cycle.

The system enabled fabrication of the vdW superlattice structures consisting of 29 alternating layers of the graphite and the hexagonal boron nitride (hBN) flakes. Encapsulated graphene devices exhibited high charge carrier mobilities (>1,000,000 cm^2/Vs), demonstrating the applicability of the system for prototyping variety of high quality vdW superlattices.

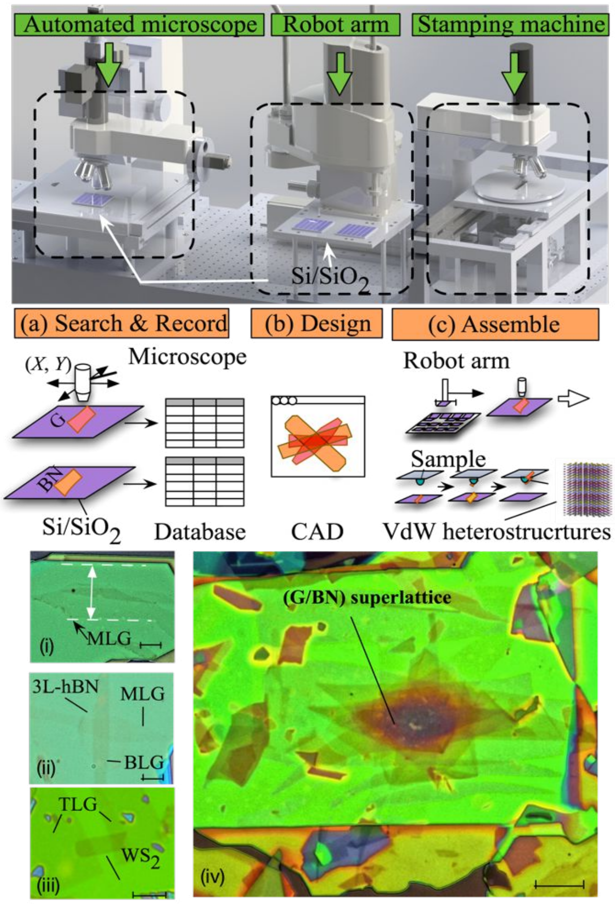

Fig1. (top) The computer-assisted design schematics of automated assembly system. (middle) Fabrication process of van der Waals heterostructures. (a) 2D crystals on Si substrates are searched by automated optical microscopy. (b) vdW heterostructures are designed. (c) The heterostructures are assembled by robots. (bottom) vdW heterostructures fabricated by the system. Scale bar corresponds to 5 μm.

The level of automation can be further enhanced by building machine-learning algorithms[2]. We develop a clustering analysis to automatically identify the position, shape, and thickness of graphene flakes. Application of the feature extraction algorithm to optical images of exfoliated graphene on SiO_2/Si yielded optical and morphology feature values for the regions surrounded by the flake edges. The feature values formed discrete clusters in the optical feature space, which were derived from 1-, 2-, 3-, and 4-layer graphene. The cluster centers are detected in unsupervised manner by the machine-learning algorithm, enabling highly accurate classification of monolayer, bilayer, and trilayer graphene. The analysis can be applied to a range of substrates with differing SiO_2 thicknesses. We demonstrate the deep-learning based image analysis for semantic segmentation of two-dimensional crystals in the optical microscopy images.

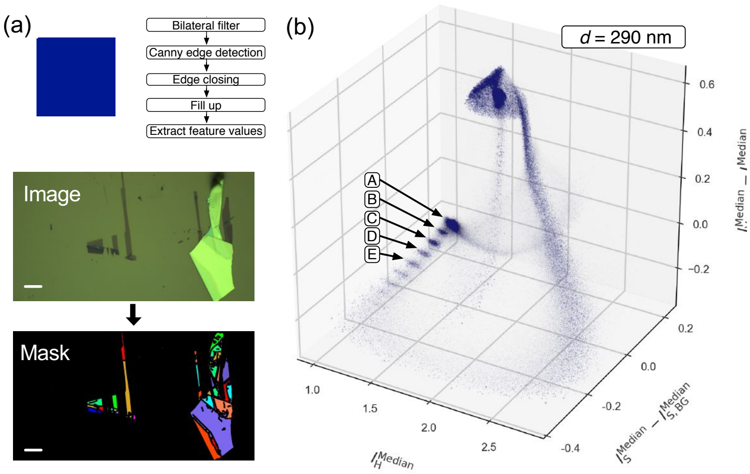

Fig2. (a) The schematics of feature extraction. (b) Three-dimensional scatter plot of optical feature values. The clusters deriving from mono-, bi-, tri- layer graphene are marked by B–D.

The wider material design freedom enabled by our system offers unprecedented opportunities for exploring the potential of vdW heterostructures. By this development, we can reduce the human intervention involved in the vdW heterostructure fabrication by orders. We believe that this work free up researchers from repetitive tasks and letting them to focus on more intellectually creative tasks.

References

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[2] S. Masubuchi et al., npj 2D Materials and Applications 3, 4 (2019).