Interfacial property measurement of van der Waals heterostructures

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Abstract

By combining two-dimensional materials, such as molybdenum disulphide (MoS_2), graphene, black phosphorus (BPs), and MXene materials, van der Waals heterostructures can be fabricated and are widely used in various electrical and optical devices due to their unique properties. In the heterogeneous structures, the interfacial interactions are mainly weak van der Waals interactions, which dominate the main behavior of van der Waals heterostructures. Therefore, a well understanding of interfacial properties is of great significance for their synthesis and applications. So far, many pioneers have explored the interfacial properties of vdW heterostructures. However, there is still a lack of experimental protocols that can be used to accurately measure the interface strength of van der Waals heterostructures.

In this paper, two methods of measuring the cohesive energy of van der Waals heterostructure, i.e., shaft loaded blister method and nanoparticle intercalation method, are introduced and analyzed by using molecular dynamics simulation and theoretical analyses. It is found that both methods can accurately measure cohesive energies of van der Waals heterostructure. The results provide a reliable basis for the measurement of the interface energy of van der Waals heterostructures.

Keywords: Molecular dynamics simulation; Cohesive energy; Bilayer heterostructure;

Shaft loaded blister test; Nanoparticle intercalation