Editors' Suggestion

Topological nature of dislocation networks in two-dimensional moiré materials

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(Received 12 July 2022; revised 21 February 2023; accepted 23 February 2023; published 16 March 2023)

Moiré superlattice patterns at the interface of two-dimensional (2D) van der Waals (vdW) materials, arising from a small displacement between similar lattices, have been extensively studied over the past decade for their dramatic ability to tune material properties. However, previous work to understand the structure of these interfaces has largely focused on some special cases, particularly honeycomb lattices displaced by twist or isotropic scaling. In this work, we develop practical and analytical tools for understanding the moiré structure that can be generalized to other lattice distortions and lattice types. At large enough moiré lengths, all moiré systems relax into commensurated 2D domains separated by networks of dislocation lines. The nodes of the 2D dislocation line network can be considered as vortexlike topological defects. However, we find these topological defects to exist on a punctured torus, requiring different mathematical formalism than the topological defects in a superconductor or planar ferromagnet. In the case of twisted bilayer graphene, the defects are characterized by the free group on two generators. We find that antivortices occur in the presence of anisotropic heterostrain, such as a shear or anisotropic displacement, while arrays of vortices appear under a twist or isotropic displacement between vdW materials. Utilizing the dark field imaging capability of transmission electron microscopy (TEM), we experimentally demonstrate the existence of vortex and antivortex pair formation in a moiré system, caused by competition between different types of heterostrains in the vdW interfaces. We also present a methodology for mapping the underlying heterostrain of a moiré structure from experimental TEM data, which provides a quantitative relation between the various components of heterostrain and vortex-antivortex density in moiré systems.

DOI: 10.1103/PhysRevB.107.125413

I. INTRODUCTION

Moiré patterns are quasiperiodic in-plane projections of two similar stacked two-dimensional (2D) periodic lattices. Atomic scale moiré superlattices can be formed by stacking atomically thin van der Waals (vdW) materials; one such example is twisted bilayer graphene. Moiré patterns formed by incommensurately stacking 2D materials have been used to manipulate a system's electronic structure, from Hofstadter's butterfly [1–3] to the valley Hall effect [4,5] to magic angle strongly correlated physics [6,7]. As the number and type of layers in experimentally relevant systems proliferates, including twisted double bilayer [8–10], twisted monobilayer [11–13], twisted trilayer [14–16], and twisted quadrilayer graphene [17,18], as well as hexagonal boron nitride [19] and transition metal dichacolgenides (TMDs) [20–22], it is important to be able to predict the structure in vdW stacked combinations of atomic layers.

Increasing attention has been paid to the effects of strain disorder on the structure and properties of such systems [23]. The effect and extent of twist angle disorder in magic angle graphene is an active area of research [24,25]. Strained moiré patterns in excitonic systems have been proposed as a way to create 1D quantum wires [26]. In this paper, we present a generalizable topological interpretation of the structure of moiré interfaces that allows for the characterization of arbitrary strain and the proposition of new types of moiré patterns.

A topological description of the moiré structure is appealing in part because some of the major features of the structure seem to be fixed once certain boundary conditions, such as total twist angle and strain, are pinned. For large enough moiré length, moiré systems are known to relax into domains of nearly commensurate alignment, separated by domain walls which can be characterized as dislocation lines [27]. The topological connectivity of the network of dislocation lines remains fixed even as the domain lengths become distorted by local strain fields.

The nodes of the network where dislocation lines meet in the relaxed moiré system (sometimes known as AA points in graphene or TMD moiré) have been referred to as topological

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