Mikito Koshino
Department of Physics, Osaka University, Toyonaka, 560-0043, Japan

koshino@phys.sci.osaka-u.ac.jp

Lattice relaxation and moiré phonons in the twisted bilayer graphene

We study the lattice relaxation and the acoustic phonons in the twisted bilayer graphene using the continuum approach. The twisted bilayer graphene (TBG), or a pair of graphene layers rotationally stacked on top of each other, exhibits a variety of physical properties depending on its twist angle θ. While the early theoretical studies on TBG simply assumed a stack of rigid graphene layers, the actual TBG spontaneously relaxes to the energetically favorable lattice structure, where the in-plane distortion maximizes the area of AB stacking (graphite's Bernal stacking) to form a triangular domain pattern. The electronic band structure is also significantly affected by the lattice relaxation. [1]
It is naturally expected the lattice deformation of the moiré superlattice significantly influence the phonon properties. We study the in-plane acoustic phonons in TBG and investigate the effects of the moiré superlattice structure on the phonon spectrum.[2] The calculation is based on the continuum approach using the elastic theory and the registry-dependent interlayer potential. We find that the moiré interlayer potential only affects the in-plane asymmetric modes (i.e., the top and bottom layers slide in the opposite directions parallel to graphene layers), where the original linear dispersion is broken down into mini phonon bands separated by gaps. The phonon wave functions are regarded as collective vibrations of the domain wall network, and the low-energy phonon band structure can be qualitatively described by an effective moiré-scale lattice model. We expect that these effects should affect the thermal conductivity directly and also phonon-related thermal phenomena.

References

[1] Nguyen N. T. Nam and Mikito Koshino, Phys. Rev. B 96, 075311 (2017).
[2] Mikito Koshino and Young-Woo Son, arXiv:1905.09660 (2019).

Figures

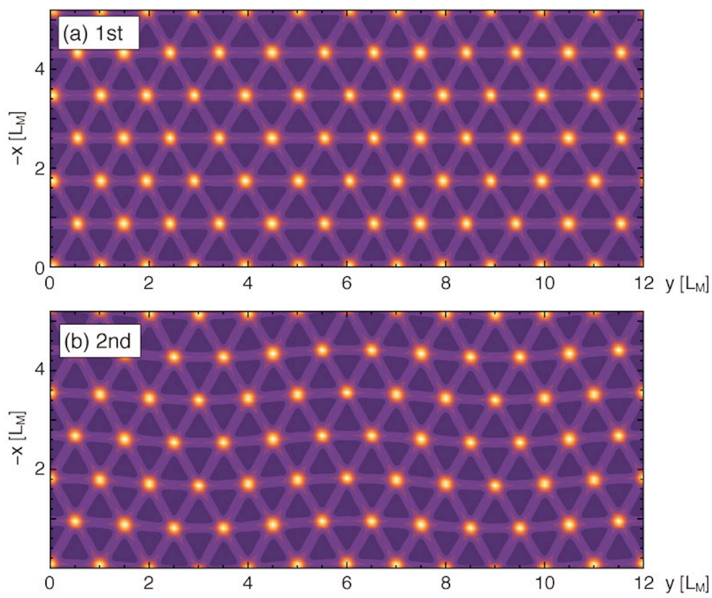

Figure 1: Examples of phonon wave function in TBG of θ = 1.05 deg.