# 博士論文公聴会の公示 (物理学専攻)

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(モアレ超格子におけるフォノン及び熱伝導の理論)
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## 論文要旨

In this thesis, we investigate the in-plane acoustic phonons and thermal transport properties in moiré superlattices, focusing on twisted bilayer systems. Moiré pattern holds an important role in the physical properties of van der Waals materials. A well-known example is twisted bilayer graphene (TBG), where the long-wavelength moiré potential modulates the original Dirac fermions of graphene and various correlated phases were observed due to the emergence of nearly flat bands at some specific twist angles. Novel electronic phenomena were also observed in other twisted bilayer materials such as graphene/hexagonal boron nitride or twisted bilayer transition metal dichalcogenides (TMD).

The interlayer moiré potential in twisted bilayer systems also induces a structural change which is expected to strongly renormalize of the vibrational properties. In TBG, the in-plane acoustic phonons were shown to be reconstructed into superlattice mini bands with a notable flattening of some particular bands. These phonons behave as a vibration of the effective triangular structure of the moiré superlattice with a different mechanical characteristic to the original graphene honeycomb lattice. However, the moiré effect on the in-plane acoustic phonons of twisted bilayer materials beyond TBG was not understood. Furthermore, changes in the band structure of the acoustic phonons would have an immediate impact on thermal transport properties, particularly at low temperature.

In the first part of this thesis, we investigate the in-plane acoustic phonons in twisted bilayer systems beyond TBG, which includes twisted graphene/hexagonal boron nitride (t-G/hBN), and twisted bilayer molybdenum disulfide (t-$MoS_2$) as a representative of TMD systems. We utilize the continuum approach, where the interlayer potential is a continuous function of the local stacking configurations which changes smoothly across the moiré superlattice unit cell. We show that there is a strong correspondence between the relaxed lattice structure and the phonon band structure which leads to the appearance of universal features across different twisted bilayer systems. To elucidate this correspondence, we develop an effective mass-spring model that can perfectly reproduce the original phonon bands at low-frequency. One particular characteristic of the band structures is the presence of multiple flat bands that can be understood as independent oscillations of a collection of isolated strings. Furthermore, we also show that the moiré phonons can also exhibit chiral properties for systems with no inversion symmetry in the moiré potential, such as t-G/hBN.

In the second part of this thesis, we calculate the thermal conductivity of the twisted bilayer systems using the semiclassical transport equation. We focus on the low-temperature regime, where the mean free path of phonons is roughly constant, and the energy of the reconstructed phonons are the most relevant. We demonstrate that the significant flattening of phonon bands leads to a reduction in thermal conductivity for up to 40% at a particular temperature. Furthermore, we show that these changes are also manifested in the temperature dependence of thermal conductivity, where a characteristic deviation from the usual $T^2$ of in-plane acoustic phonons are found for every twisted bilayer systems with notable moiré effect.

Our results hold an important role in the study of moiré materials. We expect that the electron-phonon interactions are enhanced by the moiré effect which could help explaining the mechanism behind various transport phenomena observed in twisted bilayer systems. The flat phonon bands are also expected to entail interesting physics, such as localized excitations that was previously realized in photonic lattices. Lastly, the characteristic changes introduced by the moiré effect in the thermal conductivity should be useful for the definitive verification of the presence of moiré phonons as well as the future of thermal device engineering.