PHONON DISPERSION AND SPECIFIC HEAT IN TWISTED BILAYER GRAPHENE

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We theoretically investigated phonon dispersion and specific heat in twisted bilayer graphene with various rotation angles. It was found that rotation affects the out-of-plane acoustic phonon modes the most. It was established, that the relative difference between specific heat in bilayer graphene without twisting and twisted bilayer graphene constitutes 10—15% at 1 K and 3—6% at 5 K in dependence on rotational angle. Obtained theoretical results contribute to a better understanding of the phonon processes in graphene and are important for the design of novel heat management applications.

Keywords: twisted graphene, phonons, specific heat.

In recent years the interest of the physics community has been shifting toward investigation of the twisted few-layer graphene systems. When two graphene layers are placed on top of each other they can form a Moiré pattern [1, 2]. In this case, one layer is rotated relative to another layer by a specific angle. Phonon properties of twisted graphene are of fundamental scientific interest. Phonon spectrum determines a series of important physical quantities, such as sound velocities, phonon density of states, specific heat and thermal conductivity.

Here, in the framework of the lattice dynamics approach, we investigate phonon properties of twisted bilayer graphene (T-BLG) with different angles of rotation θ. Schematic view of considered structure is presented in Fig. 1 (R denotes rotation axis, Γ and K denote two high-symmetry points).

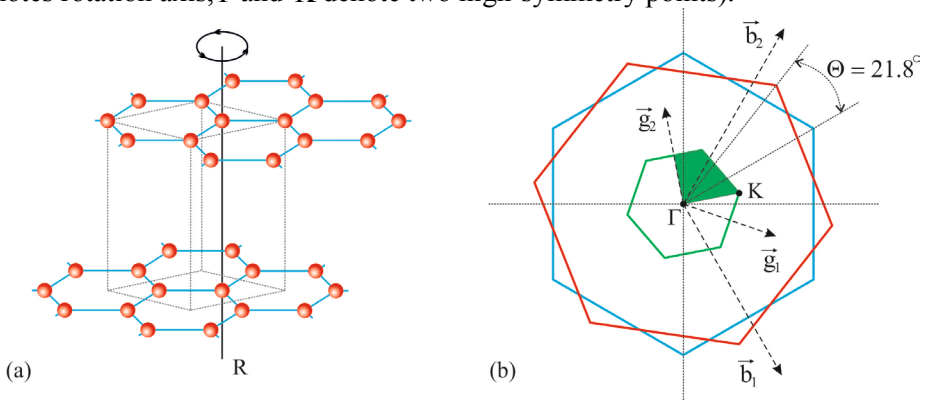

Fig. 1. Rotational scheme (*a*) and Brillouin zone of T-BLG with $\theta = 21.8°$ (*b*)

In the case of the intralayer coupling the hexagonal symmetry of the interatomic interaction is preserved for different θ, while in the interlayer coupling, the atomic configuration and force constant matrices are dependent on the rotational angle. For intralayer interaction we used Born – von Karman lattice dynamics approach [3] taking into consideration 4 nearest-neighbor atomic spheres. For the interlayer interactions we used the centrally-symmetric Lennard-Jones potential $V(r) = 4\varepsilon\left(\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right)$. The parameters $\varepsilon = 4.6$ meV and $\sigma = 0.3276$ nm reproduce the experimental values of the interlayer space and phonon dispersion along the $\Gamma - A$ direction (perpendicular to the graphene planes) of bulk graphite.

The frequencies of the shear (LA_2, TA_2) and flexural (ZA_2) phonons are affected stronger by the twisting. The specific properties of these modes in T-BLG with $\theta = 21.8°$ (gray solid curves) and T-BLG with

$\theta = 13.2°$ (black dashed curves) as well as in AA-stacked bilayer graphene (AA–BLG; black solid curves) are presented in Fig. 2, *a*. In AA-BLG, the phonon branches LA_1 and TA_2 intersect at $q \sim 0.7$ nm^{-1}. Twisting changes the interaction between these phonons in T-BLG and leads to anti-crossing of LA_1 and TA_2 hybrid folded phonon branches (see dashed circle in Fig. 2, *a*).

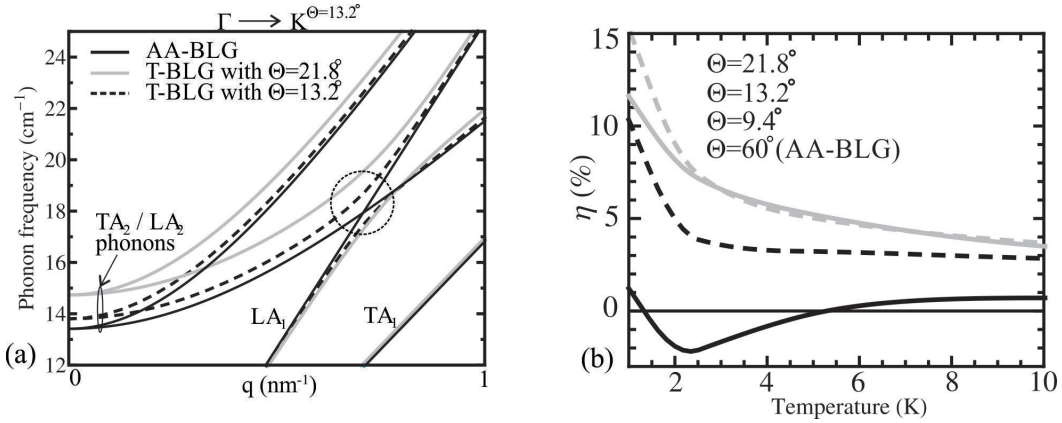

Fig. 2. Zone-center dispersions of in-plane acoustic modes in AA-BLG, T-BLG with 21.8° and 13.2° (*a*) and the relative difference between AA-BLG and T-BLG specific heats as a function of temperature (*b*)

At low temperatures the relative difference between specific heat c_V in AA-BLG ($\theta = 0°$) and T-BLG: $\eta = (1 - c_V(\theta)/c_V(0)) \times 100\%$ constitutes substantial 10—15% at T = 1 K and 3—6% at T = 5 K in dependence on θ (see Fig. 2, *b*). The low temperatures specific heat depends stronger on the twist angle because twisting affects the low-frequency ZA phonon modes the most [4].

In conclusion, we found that the phonon specific heat reveals an intriguing dependence on the twist angle in T-BLG, which is particularly pronounced at low temperature. The results suggest a possibility of phonon engineering of thermal properties of layered materials by twisting the atomic planes.

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А. Кочемасов

Дисперсия фононов и теплоемкость в двухслойном твистед-графене

Теоретически исследованы дисперсия фононов и теплоемкость двухслойного твистед-графена с различными углами поворота. Было установлено, что поворот графеновых слоев больше всего влияет на акустические колебания, перпендикулярные плоскости слоев. Было установлено, что относительная разница между теплоемкостью двухслойного графена без поворота и двухслойного твистед-графена составляет 10—15% при 1 К и 3—6% при 5 К в зависимости от угла поворота. Полученные теоретические результаты способствуют более глубокому пониманию фононных процессов в графене и могут быть важными для новых применений в области управления тепловыми свойствами.

Ключевые слова: твистед-графен, фононы, теплоемкость.