

Research Group for Nanoscale Structure and Function of Advanced Materials

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Nanoscale structures including nanoclusters, two-dimensional materials, surfaces, interfaces, and defects reveal particular features different from bulk materials. Our group fabricates novel nanoscale materials with synthesis techniques of chemical vapor deposition and molecular beam epitaxy. We also elucidate the underlying mechanisms behind the phenomena such as Dirac states, nuclear-spin conversion, and cation- π interaction by making full use of quantum beams, such as muons, positrons, neutrons, IR-THz photons, and ions. In close collaboration between the members and theoreticians, we aim to explore novel functions in advanced nanoscale structures.

Nuclear-spin conversion analysis of $\nu_2 + \nu_4$ combination band of crystalline methane in phase II

A methane molecule (CH_4) has four normal vibrational modes named ν_1 , ν_2 , ν_3 , and ν_4 . In accordance with the total nuclear spin I , CH_4 is classified into three kinds of isomers: ortho ($I = 1$), meta ($I = 2$), and para ($I = 0$). Since each isomer occupies specific rotational states, infrared absorption spectroscopy can be applied to the detection of interconversion between the isomers. In this work [1], we conducted reflection-absorption infrared spectroscopy in an ultrahigh vacuum and observed the $\nu_2 + \nu_4$ combination band of crystalline CH_4 in phase II, where the rotating and librating species coexist. We analyzed the time dependence of the spectrum (see Fig. 1) due to the nuclear-spin conversion of CH_4 to update the assignment of the rotational and librational structure of this band observed. For instance, the absorption signals observed at 2806 and 2824 cm^{-1} had been assigned to the Q(1) and R(1) branches in a previous work [2], but were found to be due to P(1) and R(0), respectively. The conversion analysis performed in our work will also be applicable to the detailed assignments of overtones and other combination bands.

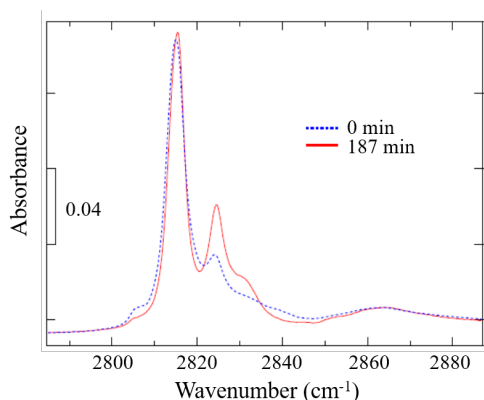


Fig. 1 Infrared spectra of crystalline CH_4 in phase II at 5.3K. The range of the $\nu_2 + \nu_4$ combination band is shown. The blue dashed and red solid lines indicate the spectra just after and 187 minutes after annealing at 38 K, respectively [1].

Atomic configuration of quasicrystal bilayer graphene revealed by positron diffraction

Geometrical consideration suggested that two hexagonal lattices superimposed with the twisted angle of 30° forms a dodecagonal quasicrystal that has 12-fold rotational symmetry without translational symmetry. Graphene, a hexagonal lattice sheet of carbon, is a good candidate material for dodecagonal quasicrystal. Recently, the successful fabrication of quasicrystal bilayer graphene has been reported by using chemical vapor deposition technique. Quasicrystal bilayer graphene has attracted increasing attention as a two-dimensional quasicrystal having relativistic Dirac fermions. However, the fundamental information on atomic configurations remained unknown. In this study [3], we have investigated the atomic configuration of quasicrystal bilayer graphene on a silicon carbide substrate using positron diffraction method. By means of the structure analysis based on dynamical diffraction theory, we determined the interlayer spacing of quasicrystal bilayer graphene as 3.46 Å, while the normal stacked bilayer graphene 3.29 Å (see Fig. 2). We found that the twisted angle of 30° gives rise to the expansion of the interlayer spacing. The origin of Dirac cone replica is one of the unresolved issues in quasicrystal bilayer graphene [4]. Our results will pave the way to understand such peculiar electronic properties.

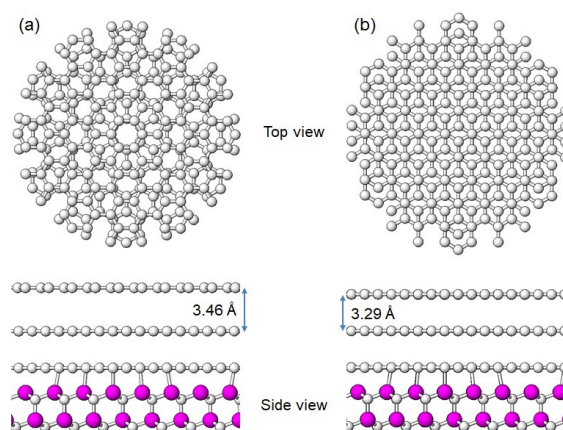


Fig. 2 Structure models of (a) quasicrystal bilayer graphene and (b) normal (Bernal-type) stacked bilayer graphene on silicon carbide substrate. Grey and magenta circles denote C and Si atoms, respectively [3].

References

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