Flower Defect of Epitaxial Graphene on 6H-SiC(0001)

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Introduction ***Graphene, a zero-gap semiconductor with single atomic sheet of sp^2-bonded carbon atoms arranged in a honeycomb lattice, exhibits extraordinary electrical and mechanical properties. The symmetrical honeycomb lattice is a key element for determining many of its unique electronic properties. The sublattice symmetry gives rise to its linear energy-momentum dispersion. To realize technologically feasible graphene-based electronic devices, progress is needed in the large-scale production of high quality graphene thin film and the modification of their electronic properties. Of all the growth methods, epitaxial graphene (EG) via the thermal decomposition of SiC substrate has the advantage of being a simple and direct approach in forming graphene layers on a supported substrate. During the graphene growth, the defects are inevitable. Defects have profound effects on the chemical, mechanical and electronic properties of graphene in unexpected ways. In this work, flower defects have been observed on the EG in the STM experiments and analyzed via DFT, ARPES, etc. Flower defects came out under specific growth condition, and showed regular structure. Sometiime bud-like defect could be observed near the flower defect. The gap of EG opened by flower defects can be seen in DFT simulation, but can't be observed in ARPES experiment.***

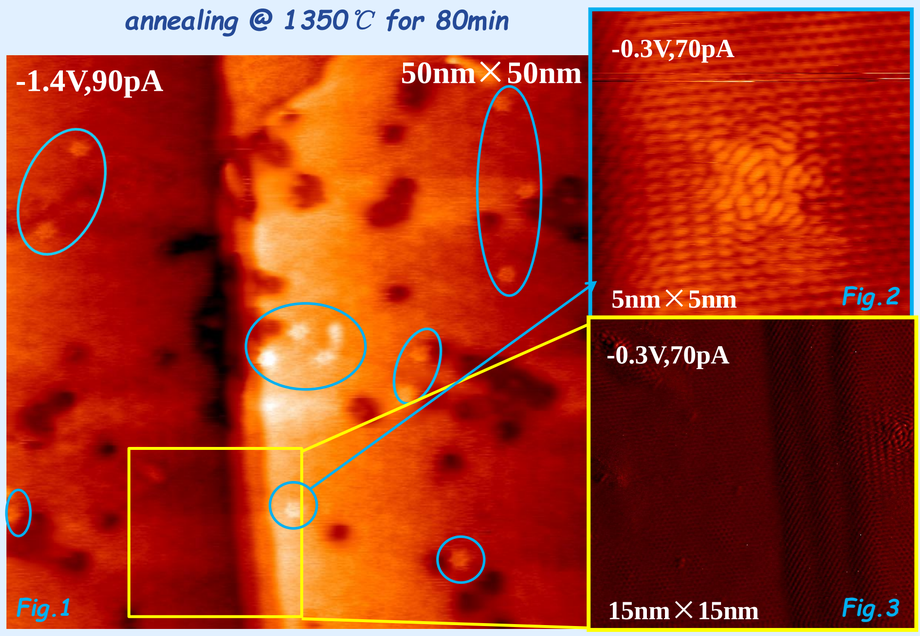
Experimental ***Omicron RT UHV-STM system (base pressure < 2.0×10^{-10} mbar) 6H-SiC(0001) 10×5×0.3 mm^3 miscut ≤0.5° , $\rho = 0.076\Omega cm$***

Experiment Process ***a) Degassing < 600℃ with resistive heating for 2 hours. b) Annealing @ 1350℃ for several hours for EG growth. c) STM observations in situ, Raman measurements (632.8 nm) ex situ, ARPES in BSRF 4B9B PES experimental establishment. (21.2 eV, 0.5mm VGR4000, 7meV)***

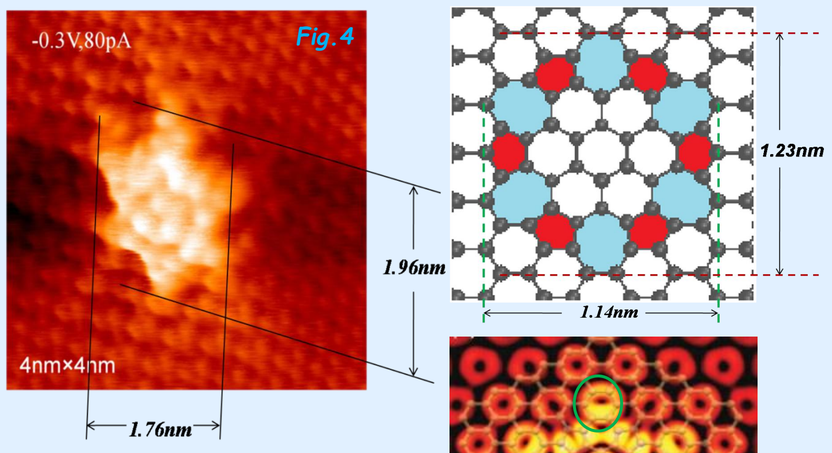
Observation and Analysis of Flower Defect

Growth condition of flower defects on EG

annealing @ 1350℃ for 80min



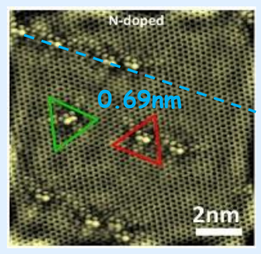
Size and structure of flower defect



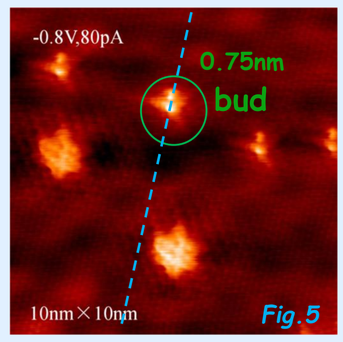
N. Khosravian et al, Computational Materials Science 79 (2013) 132-135

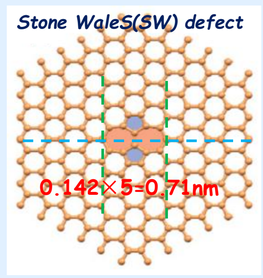
Physical Review B 83, 195425 (2011)

Bud-like defects



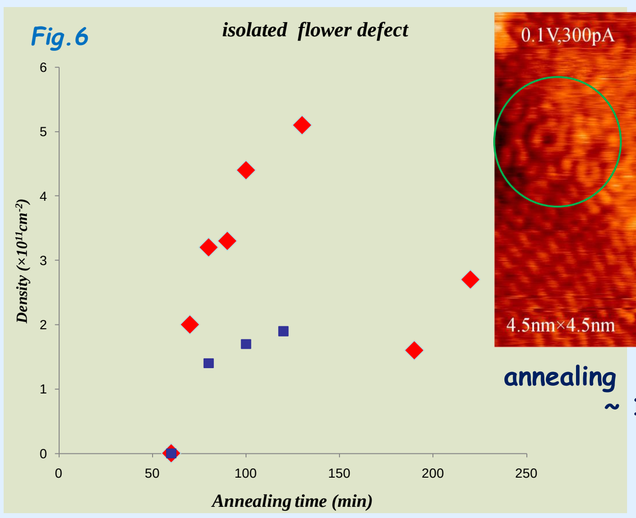
Liuyan Zhao et al, Nano letter,10.1021,2013





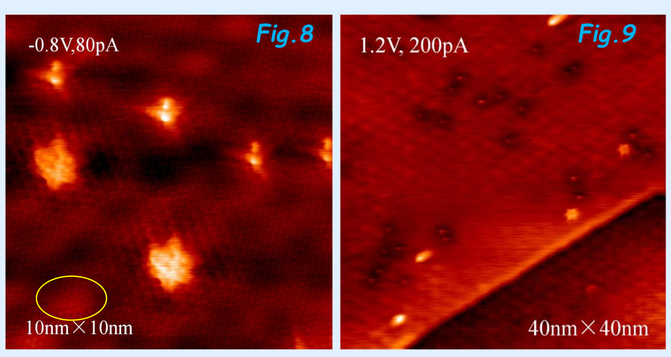
① The size of bud-like defect is similar to the SW defect.
② Structure of EG near the bud-like is changed.
③ The trend of morphology structure is invariant shown in blue dashed.

Density with annealing time



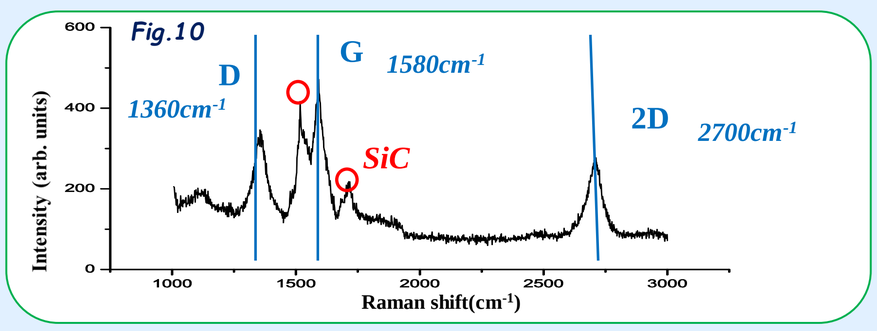
annealing @ 1350℃ ~ 190min

Distribution with layer number



①The structure in yellow circle is induced by Bernal stacking.
② Flowers defect distribute on bilayer Graphene mainly.

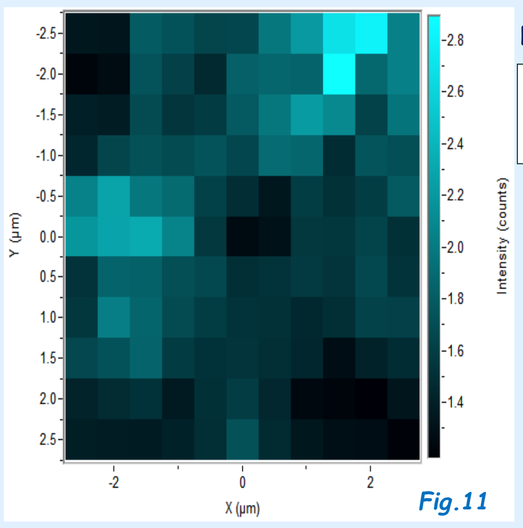
Raman shift



2D peak for bilayer graphene can be decomposed into four Lorentzian peaks. One peak is used to fit the Raman data for monolayer graphene. There is no fitted result in this experiment.

Ni,Z.H.et al, PRB 2008, 77, 115416
Wang, Y. Y. et al, J.Phys.Chem.C 2008, 112, 10637

Raman mapping of I_D/I_G



Density of Defects:

$$n_D\ (\mathrm{cm}^{-2}) = \frac{(1.8 \pm 0.5)\times 10^{22}}{\lambda_L^4}\left(\frac{I_D}{I_G}\right)$$

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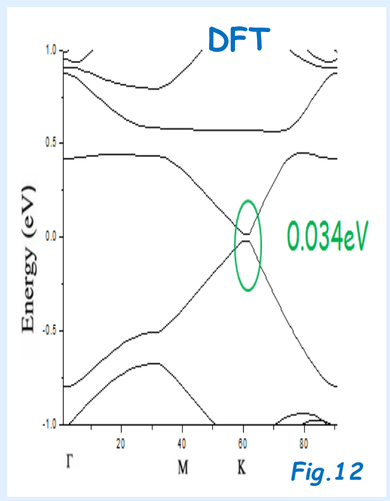
I_D/I_G = (1.2~2.9)

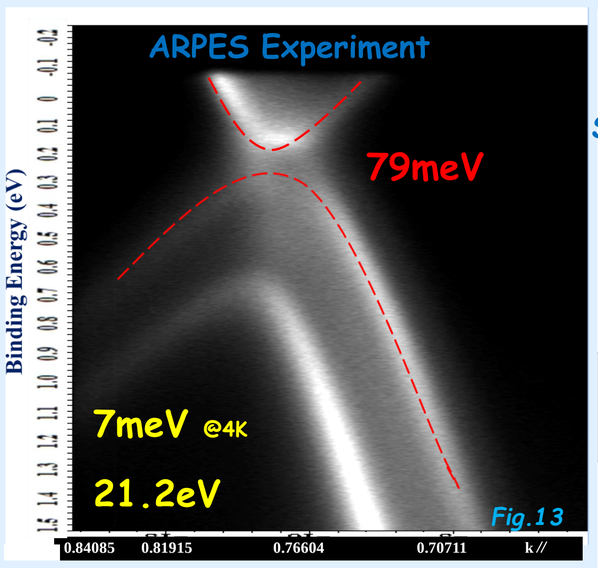
n_D = (1.0~4.2)×$10^{11}cm^{-2}$

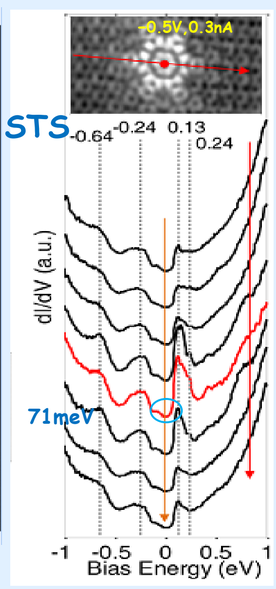
n_D (exp.) = 1.9×$10^{11}cm^{-2}$

Electronic structure of EG with flower defects



198 C atomic → 23/100nm²
STM Exp → 0.23/100nm²





① The gap of EG opened by flower defects is 34meV in DFT simulation.
② The gap of EG with flower defects and SiC substract is 79meV in ARPES experiment .
③ STS of flower defect shows a 71meV gap, as well as VHS.
④ The result of ARPES approches observation of STS in reference

Zhao et al.Nano letter,10.1021,2013

Conclusions ***Flower defect begin to come out when annealing at 1350℃ longer than 80min, and its total density rise with annealing time. The flower defect with diameter less than 2nm distributes on bilayer Graphene mainly. The bud-like defect is similar as the SW defect extremely.The Gap of EG opened by flower defects can be seen in DFT simulation, but can't be observed in ARPES experiment.The origin and evolution of flower defects are unknown, and the research for them is a challenge in experiment currently.***