

Abstract Submitted
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Epitaxial graphene on SiC(0001): It takes a Si jump G.F. SUN, Y. LIU, S.H. RHIM, University of Wisconsin, Milwaukee, WI 53211, J.F. JIA, Q.K. XUE, Tsinghua University, Beijing 100084, P. R. China, M. WEINERT, L. LI, University of Wisconsin, Milwaukee, WI 53211 — Using scanning tunneling microscopy with transition metal (Fe, Cr)-coated W tips and first-principles calculations, we have recently shown that interface of epitaxial graphene/SiC(0001) is a warped graphene layer with periodic inclusions of hexagon-pentagon-heptagon ($H_{5,6,7}$) defects that break the six-fold honeycomb symmetry [1]. Here we show that this unique structure facilitate a novel pathway for the disposal of Si during growth: the diffusion of Si vertically through the warped interfacial layer via a series of configurations that involve the dissociation and formation of C-C and Si-C bonds within the pentagon and heptagon of the $H_{5,6,7}$ complex. The calculated energy barrier for this diffusion path is 4.7 eV. These results and their implications on the self-limiting growth of epitaxial graphene on SiC(0001) will be presented at the meeting.

[1] Qi et al., Phys. Rev. Lett. **105**, 085502 (2010).

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