

Abstract Submitted
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“Epi-nucleation” on Reconstructed Surface and a Model Study of Si(001) Homoepitaxy¹ RAJ GANESH PALA, FENG LIU, University of Utah — We introduce the concept of “epi-nucleation” to distinguish nucleation and growth on a reconstructed surface from that on a non-reconstructed surface. The ‘critical nucleus’ defined in the classical nucleation theory refers to a nucleus stable against dissociation, which is also implicitly assumed to have an epi-relation to the substrate. However, such assumption may fail on a reconstructed surface because although the “classical” nucleus is stable against dissociation, it may not yet establish the epi-relation with the substrate as the substrate surface underneath the nucleus remains reconstructed. Therefore, on a reconstructed surface, in addition to the stable “classical” nucleus, there must exist another “epi-nucleus” that is not only stable against dissociation but also has a epi-relation with the substrate (breaking the underlying substrate surface reconstruction). We illustrate the general concept of “epi-nucleus” using first-principles calculations of homoepitaxial nucleation on a reconstructed Si(001) surface and we find that here the epi-nucleus consists of six adatoms, in contrast to the classical nucleus of two adatoms.

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