

Abstract Submitted
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Quantum size effect on the diffusion barriers and growth morphology of Pb/Si(111) TZU-LIANG CHAN, CAI-ZHUANG WANG, MYRON HUPALO, MICHAEL TRINGIDES, KAI-MING HO, Ames Laboratory-U.S. DOE. and Department of Physics and Astronomy, Iowa State University — Using first-principles total energy calculations, we have studied the diffusion barriers of Pb adatoms on a free-standing Pb(111) film as a function of film thickness. We found that diffusion of an adatom on the Pb film has very low barriers (less than 60 meV). A bi-layer oscillation in the diffusion barriers due to quantum size effect(QSE) is observed, with lower barrier on the odd-layered,relatively unstable Pb films. The diffusion barrier difference between the odd-and even-layered film is found to be as large as 40 meV. This big difference in the diffusion barriers due to QSE is the origin of the intriguing growth morphology of Pb islands on Si(111) surface observed in the STM experiments: the growth of a Pb layer on Pb islands with unstable heights starts from the periphery and moves towards the center, while the nucleation of the next layer on stable Pb islands starts away from the periphery.

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