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First-principles studies of quantum growth of PbBi alloy films[1]
YU JIA, Zhengzhou University, M. M. OZER, JAMES R THOMPSON, H. H. WEITERING, The University of Tennessee, ZHENYU ZHANG, ORNL — Quantum growth of $Pb_{0.89}Bi_{0.11}$ alloy films freestanding or grown on Si(111) and Ge(111) substrates has been studied using first-principles calculations within density functional theory. Our studies show that the surface energy, work function, and lattice relaxation of the quantum alloy films all oscillate strongly with the film thickness. Similar to the case of pure Pb(111) films, the oscillation pattern is bilayer, interrupted with even-odd crossovers. However, the positions of the crossovers and the beating periodicity can be tuned by the contents of Bi in the alloys, with the beating periodicity given by 13ML, 15ML and 17ML for $Pb_{0.89}Bi_{0.11}$, $Pb_{0.86}Bi_{0.14}$ and $Pb_{0.75}Bi_{0.25,}$respectively. These results are in quantitative agreement with experiment.

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