Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

***Ab-initio* study of early stages of III-V epitaxy on Si : direct *vs.* buffer deposition on vicinal surfaces** A.A. DEMKOV, ONISE SHARIA, HENDRIK BENTMANN, UT Austin — III-V materials, such as GaAs or InSb as well as other compound semiconductors with high carrier mobility are considered as potential candidates for a channel material in future CMOS-type devices. The most promising route to incorporate these advanced materials into CMOS is by growing epitaxial thin films on Si, either directly or *via* a buffer layer. Direct deposition suffers from a large lattice mismatch, and domain formation caused by the presence of steps on the Si surface. Perovskite oxides such as $SrTiO_3$ (STO) offer a possibility to reduce the lattice mismatch between Si and, e.g. GaAs in a step-wise fashion, however, the steps on the semiconductor surface present a somewhat unusual challenge. On the other hand, the use of vicinal surfaces for the direct deposition of GaAs on Si may eliminate the problem of orthogonal domains. Thus understanding the role of steps during the crystal growth is key to both approaches. In this talk we report a theoretical study of STO epitaxy on the vicinal Si(001) surface. In particular, we find that at the early stages of growth, Sr adatoms segregate to the step edges. We also consider the direct epitaxy of III-V compound semiconductors on high index Si surfaces, specifically, the silicon (112) surface. We consider In adsorption on this surface and identify a stable 7x1 substitutional reconstruction which is fundamentally different from a 6x1 reported for Ga.

Alex Demkov
UT Austin

Date submitted: 10 Jan 2008 Electronic form version 1.4