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Surface Structure of $L1_0$-MnGa(111) Ultra-Thin Films Studied Using Scanning Tunneling Microscopy and First Principles Calculations[1] REYES GARCIA DIAZ, KANGKANG WANG, Ohio University Nanoscale and Quantum Phenomena Institute, NOBORU TAKEUCHI, Centro de Nanociencias y Nanotecnologia, Universidad Nacional Autonoma de Mexico, ARTHUR SMITH, Ohio University Nanoscale and Quantum Phenomena Institute — Manganese gallium alloys have drawn lots of attention recently for their many desirable properties such as high spin polarization and low damping terms. Furthermore, the magnetic properties depend sensitively on the Mn:Ga stoichiometry, ranging from ferromagnetic for MnGa, to ferrimagnetic for $Mn_{2-3}Ga$, and antiferromagnetic for Mn_3Ga, giving this material great magnetic tune-ability. In this talk, we will focus on the stoichiometric $L1_0$-structured MnGa(111) surface and study its atomic, electronic, and magnetic properties. Ultra-thin MnGa films ($<$ 10 nm) are grown on GaN(0001) substrates using molecular beam epitaxy, and transferred *in-situ* to the analysis chamber for room-temperature scanning tunneling microcopy studies. Atomic resolution images reveal the existence of both 1×1 and 2×2 surface structures. We investigate these structures using periodic, spin-polarized density functional theory with the generalized gradient approximation (GGA), Vanderbilt ultra-soft pseudo-potentials, and a repeated slab geometry. The parameters are optimized to achieve the lowest-energy configuration. Results from these calculations and their comparison with the STM images will be reported.

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[X] Prefer Oral Session
[ ] Prefer Poster Session

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