# Microscopic Origin of the Structural Phase Transitions at the $Cr_2O_3$ (0001) Surface

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The surface of a $Cr_3O_3$ (0001) film epitaxially grown on Cr undergoes an unusual reentrant sequence of structural phase transitions ($1 \times 1 \rightarrow \sqrt{3} \times \sqrt{3} \rightarrow 1 \times 1$). In order to understand the underlying microscopic mechanisms, the structural and magnetic properties of the $Cr_3O_3$ (0001) surface are here studied using first-principles electronic structure calculations. Two competing surface Cr sites are identified. The energetics of the surface is described by a configurational Hamiltonian with parameters determined using total energy calculations for several surface supercells. Effects of epitaxial strain and magnetic ordering on configurational interaction are also included. The thermodynamics of the system is studied using Monte Carlo simulations. At zero strain the surface undergoes a $1 \times 1 \rightarrow \sqrt{3} \times \sqrt{3}$ ordering phase transition at $T_C \sim 165K$. Tensile epitaxial strain together with antiferromagnetic ordering drive the system toward strong configurational frustration, suggesting the mechanism for the disordering phase transition at lower temperatures.

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