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Strain fields and electronic structure of CrN[1] TOMAS ROJAS , SERGIO E. ULLOA, Ohio University — Chromium nitride (CrN) has a promising future for its resistance to corrosion and hardness, and very interesting magnetic and electronic properties. CrN presents a phase transition in which the crystal structure, magnetic ordering and electronic properties change at a (Nel) temperature $\sim 280K$. Thin films from different labs exhibit different conductance behavior at low temperature. We study the unusual electronic and magnetic properties of thin layers. For that purpose we develop a tight binding Hamiltonian based on the Slater-Koster approach, and estimate the interaction between the Cr-3d and N-2p orbitals, by analyzing the band structure and comparing it with ab initio calculations performed using the LSDA+U method [1]. These calculations show the system to behave as a semiconductor below the Nel temperature. Based on our model we calculate the effective masses and analyze the effect of strain fields in the electronic structure in order to understand the electronic behavior near the phase transition. [1] A. Herwadkar and W. Lambrecht, Phys. Rev. B 79(3), 035125 (2009).

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Tomas Rojas
Ohio University

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