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**Surface states control and thermoelectric properties of CrN films**

ANTIA S. BOTANA, ALBERTO PIÑEIRO, University Santiago de Compostela, VICTOR PARDO, University of California Davis, DANIEL BALDOMIR, University Santiago de Compostela — The manipulation of the electronic structure of a material by quantum confinement has attracted much attention recently, e.g. the appearance of conducting surface states or the novel phenomena at the interface between oxides being the most notorious. CrN is a degenerate semiconductor with large thermoelectric power in the bulk[1]. We have performed electronic structure calculations in thin CrN films and studied the evolution of the electronic structure and conduction properties (calculated using Boltzmann formalism) with thickness, focussing on the evolution of the Seebeck coefficient and electrical conductivity. We have utilized a density functional theory (LDA+U) formalism for our calculations with the U value (4 eV) that reproduces the experimental gap for the material as a bulk. When nanostructured, (almost conducting) surface states arise due to the dangling bonds at the surface that reduce the symmetry of the octahedral crystal field around Cr. When the film is relaxed, a gap opens and the material remains semiconducting. In addition, we have analyzed the role of these surface states in a possible improvement of the CrN thermoelectric properties by studying the figure of merit dependence with thickness.

[1] C. X. Quintela et al., Appl. Phys. Lett. 94, 152103 (2009).

Victor Pardo  
University of California Davi

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