The role of structural ordering in the semiconducting behavior of Cr$_3$Al$^1$ ZOE BOEKELHEIDE, UC-Berkeley, D.A. STEWART, Cornell, F.J. WONG, Y. SUZUKI, F. HELLMAN, UC-Berkeley — Cr$_{1-x}$Al$_x$ displays unexpected semiconducting behavior for $x \sim 0.25$; an ordered Cr$_3$Al structure has been proposed to explain it.[1, 2] In this work, density functional theory calculations and nonequilibrium thin film growth were used to study the role of ordering on the transport properties. The atoms in Cr$_3$Al occupy the sites of a bcc lattice, like Cr. Calculations comparing possible structures show that the proposed chemically ordered, rhombohedrally distorted Cr$_3$Al structure, with ordering along the $<111>$ direction, is the lowest energy of those considered. In addition, the band structure shows a pseudogap, consistent with experimentally observed transport properties. Thin films of Cr$_{1-x}$Al$_x$ were grown with various growth and annealing temperatures to vary the properties. Samples with the most rhombohedral ordering are semiconducting. Decreased rhombohedral ordering leads to lower resistivity. Samples with a tetragonal distortion due to the C11$_b$ (Cr$_2$Al) structure have metallic resistivity.


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