Abstract Submitted
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The role of structural ordering in the semiconducting behavior of Cr_3Al[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_3Al 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_3Al occupy the sites of a bcc lattice, like Cr. Calculations comparing possible structures show that the proposed chemically ordered, rhombohedrally distorted Cr_3Al 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_2Al) structure have metallic resistivity. References: [1] D. J. Chakrabarti and P. A. Beck, J. Phys. Chem. Solids 32, 1609 (1971) [2] F. J. A. den Broeder et al, Phys. Status Solidi A, 67, 233 (1981)

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