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Semiconducting behavior in $Cr_{1-x}Al_x$ thin films

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Abstract – $Cr_{1-x}Al_x$ in the range x = 0.15 to 0.25 behaves like a small band gap semiconductor and could be a candidate for a thermoelectric material. The semiconducting behavior has never been explained theoretically. We have used thin film growth techniques to study the link between the electronic properties and the structural properties, finding that the semiconducting behavior seems to be related to a long-range ordered structure. Polycrystalline films have lower resistivity than epitaxial films due to disorder eroding the hybridization gap, while annealing at a temperature higher than the long range ordering temperature reduces the resistivity by favoring the bcc phase over the long range ordered phase. In addition, density functional theoretical calculations show that $Cr_{1-x}Al_x$ without any long range order should be metallic. Further calculations of $Cr_{1-x}Al_x$ in an ordered structure may reveal the source of the semiconducting behavior.

$Cr_{1-x}Al_x$ in the range x = 0.15 - 0.25 behaves like a small band gap semiconductor and could be a candidate for a thermoelectric material[1,2]. The semiconducting behavior, likely due to a hybridization band gap, has never been adequately explained by theory. It has been suggested that long range order exists in this material[3]; in addition, the system is a known antiferromagnet[2]. The combination of hybridization, structural ordering, and magnetism is reminiscent of the Heusler alloys and promises a wealth of interesting behavior. Unlike the Heusler alloys, the relationship between structural ordering, antiferromagnetism, and semiconducting behavior in $Cr_{1-x}Al_x$ has not been established. We are using thin film growth and characterization techniques along with density functional theoretical (DFT) calculations to study this tripart relationship and have found that the semiconducting behavior is intimately tied to the structure.

We have synthesized a series of $Cr_{1-x}Al_x$ thin films, varying Al concentration and substrate, and measured the resistivity, obtaining a maximum of 2000 μΩ-cm at x = 0.20. We have found that the resistivity of the films strongly depends on the substrate. $Cr_{1-x}Al_x$ films grown on MgO, epitaxial for x = 0 - 35 at. %, have the highest resistivity, while films grown on sapphire, which are polycrystalline, have up to 40% lower resistivity. This shows that disorder in the polycrystalline films erodes the hybridization gap. Annealing studies show that for a high resistivity, epitaxial film, annealed at 1000 °C and rapidly cooled, the resistivity is decreased from the unannealed state by 50%. The annealing process favors the non-equilibrium bcc phase over the long-range ordered phase due to rapidly cooling through the proposed ordering temperature of 410 °C[3]. These studies suggest that the semiconducting behavior in $Cr_{1-x}Al_x$ is strongly tied to its structure.

We have also performed DFT calculations within the coherent potential approximation showing that a bcc $Cr_{1-x}Al_x$ alloy without long range order does not have the semiconducting gap observed experimentally. Further DFT studies on ordered structures should predict what type of ordering leads to the hybridization gap.

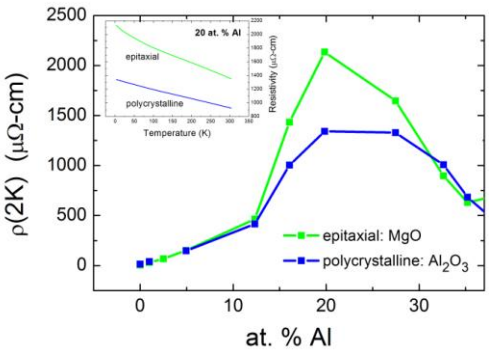

Figure 1: Resistivity vs. x for $Cr_{1-x}Al_x$ thin films grown on MgO substrates (epitaxial) and sapphire (polycrystalline). Inset: Resistivity vs. temperature for an epitaxial and polycrystalline sample of $Cr_{0.8}Al_{0.2}$

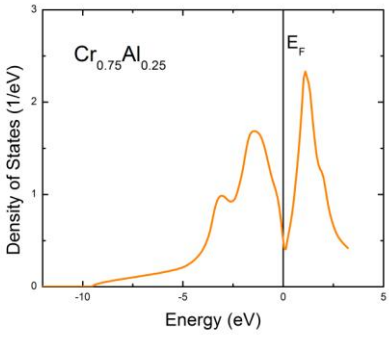

Figure 2: Densiy functional calculation of the density of states of $Cr_{0.75}Al_{0.25}$ alloy with no long range order shows significant density of states at the Fermi level suggesting that semiconducting behavior is not possible without long range order.

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