Quantum phase transition in Cr-Ti alloys

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Abstract. In this work we present the results of electrical resistivity and Hall coefficient measurements for antiferromagnetic Cr$_{1-x}$-xat.Ti% alloys with 0 <x<5.0. Our results show an abrupt jump in in density of carriers as a function of concentration of Ti at 2K, characterizing a quantum phase transition, with quantum critical point in $x_c=1.2$at.Ti%.

1. Introduction
The antiferromagnetic phase of the pure chromium is described by spin-density waves (SDW) incommensurate with reciprocal lattice, characterized by wave vector $Q = 2\pi a(1+\delta)$, where $a$ is the lattice parameter and $\delta$ is the incommensurate parameter. For pure Cr, the Néel temperature ($T_N$) is $311$ K [1]. The persistence of this antiferromagnetic state in Cr alloys over a wide range of compositions, in particular with transition metals, opens interesting possibilities for magnetic studies in these alloys. The introduction of small amounts of transition metals in chromium such as V, Ti and Nb decreases the electron/atom ratio, causing an increase in the incommensurability parameter $\delta$ and decreasing of $T_N$. In particular, the introducing of Ti in Cr, causes a $T_N$ decreasing of -160 K/at.Ti% [2]. On the other hand, the introduction of elements such as Mn, Re and Fe, causes an increase in the electron/atom ratio, and as consequence, the increasing of $T_N$[2].

In the last decade new magnetic phenomena were observed in Cr alloys with transition metals. In Cr-V [4] and Cr-Nb [5] alloys were observed a Curie-Weiss like behavior in a certain temperature range above $T_N$, disappearing in characteristic temperature ($T_{LOC}$) and under high magnetic fields ($10 kOe$). In Cr-Mn alloys [6] was observed the spin-glass phase which present a small dependence with Mn concentration. More recently, quantum phase transition was reported in Cr-V [7] and Cr-Ru-V [8] alloys. These results stimulated the investigation of these phenomena in other Cr alloys. In Cr-Ti alloys, we observed that $T_N$ vanishes around 1.3 at.%Ti [2], and according to band rigid model, this transition should occurs at 1.9at.Ti%. In the same concentration we observed that the residual resistivity ($\rho^* = \rho(1.8K)/\rho(300K)$) measurements as a function of Ti concentration presents a crossover point of two regimes. This particular behavior could be an indication of quantum phase transition in Cr-Ti alloys.

In this work, we present the Hall coefficient and electrical resistivity measurements for Cr-Ti alloys, where the quantum critical point was determined when antiferromagnetic/paramagnetic phase transition occurs, associated with an abrupt jump in the density of carries observed close to concentration of 1.2 at.%Ti.
2. Experimental details
The polycrystalline samples of Cr–Ti were prepared in an arc-melting furnace, using high-purity Cr (99.9999%) and Ti (99.99%). Each sample was melted several times with a mixing procedure to ensure high-quality homogenous alloys with only a few grains. The AC electrical resistivity ($\rho_{AC}$) and the Hall coefficient measurements carried out with a PPMS (Physical Properties Measurement System), Quantum Design Corporation. AC electrical resistivity measurements ($\rho$) as a function of temperature were performed using the four-probe method, and for measurement of Hall coefficient was use five probe method for minimize the contacts effects. The carrier numbers were calculated as a function of applied magnetic field (0 to 90 kOe) at 2 K, and as function of temperature with applied magnetic field at 50 kOe perpendicular to electrical current of 200 mA.

3. Results and discussion
The Néel transition in Cr alloys is observed in electrical resistivity ($\rho$) measurements because of the itinerant characteristic of the antiferromagnetic phase. Around the $T_N$ $\rho$ increases when temperature decreases, exhibiting a local maximum. This behavior occurs because of the establishment of the SDW state which promotes the formation of new gaps in conduction band and promote a reduction in total energy, resulting in increased resistivity. In single crystal samples, these peaks are more pronounced, unlike what we observed here.

Figure 1. Electrical resistivity and carriers per Cr atom (obtained from inverse of the Hall coefficient) as a function of temperature for sample of Cr 0.7at.%Ti. The Néel temperature was obtained in inflection point in the first derivate of electrical resistivity curve. $T_N$=189.7K.

Figure 1 shows the electrical resistivity measurement, $\rho(T)$, without applied magnetic field, and carriers per Cr atom, $n_{Cr}(T)$, measured with an perpendicular applied magnetic field of 50 kOe, as a function of temperature for Cr- 0.7at.%Ti sample. The Néel temperature was determined, as usual [1,9], as the inflection point of the resistivity curve, that occurs just below its minimum. Immediately below $T_N$, $\rho(T)$ increases because the formation of the SDW state leads to a decrease in the number of...
carriers due to formation of new energy gaps in some of the directions of the Fermi surface. The antiferromagnetic/paramagnetic phase transition has a proportionately much larger effect on $n_{Cr}(T)$ than on $\rho(T)$ because the changes in Fermi surface manifests itself immediately as a change in the number of carriers. The local maximum exhibited in $\rho(T)$ occurs in the same temperature where the $n_{Cr}(T)$ decreases quickly. The decrease in $n_{\rho}$ is associated of establishing of the antiferromagnetic phase in the sample. Thus, the number of carriers would be an indication of paramagnetic/antiferromagnetic phase transition.

The Néel temperature as a function of Ti concentration is shown in Figure 2 (a). These critical temperatures were determined from electrical resistivity measurements. In previous work we are shown that the antiferromagnetic phase was suppressed for $x = 1.3$ at.% Ti [2]. However, the dependence of $T_N$ with Ti concentration is $-160$ K/at.%Ti, where expected that the SDW state disappears for $1.9$ at.%Ti.

For try understand this peculiar behavior we analyzed the number of carriers per Cr atom, obtained from Hall coefficient measurements ($n_{Cr}$). Figure 2 (b) shows the $n_{Cr}$ as a function of Ti concentration at 2 K. We observed an abrupt jump around the concentration of $x_c = 1.2$ at.%Ti, where $n_{Cr}$ increases approximately 80% in a narrow interval about $x_c$, jumping from one value weakly dependent on $x$ for $x < x_c$ to a linearly dependent value for $x > x_c$. The T=0 phase transition seems to involve the destruction of a fixed amount of Fermi surface, and the quantum critical point simply occurs when this destruction is no longer possible. This behavior was reported for other Cr alloys as Cr-V [7] and Cr-Ru-V [8]. Nevertheless, our results show that the Cr-Ti system exhibits the quantum phase transition in a critical concentration $x_c = 1.2$, when the expected value by band rigid model is $x_c = 1.9$ [2]. For Cr-V alloys, the critical concentration is agreements with this theory [1]. Other experiments, such as magnetic susceptibility and transport measurements will be performed for investigated this particular behavior exhibited by the Cr-Ti alloys.
4. Final remarks
The measurements of electrical resistivity and Hall coefficient show that a quantum phase transition for Cr-Ti alloys occurs around critical concentration $x_c = 1.2 \text{ at.}\% \text{Ti}$. However, new samples will be measured as a function of temperature and applied magnetic field. Other physical properties, as magnetic susceptibility, will be measured as a function of Ti concentration for understand completely this quantum critical transition.

Acknowledgments
This work was supported by Brazilians Agencies, FAPESP, CNPq and CAPES.

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