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Elastic neutron scattering in Quantum Critical Antiferromagnet $Cr_{0.963}V_{0.037}$

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Abstract

We have performed elastic neutron scattering studies of the quantum critical antiferromagnet $Cr_{0.963}V_{0.037}$. We have found that unlike pure Cr, which orders at two incommensurate wavevectors, $Cr_{0.963}V_{0.037}$ orders at four incommensurate and one commensurate wavevectors. We have found strong temperature dependent scattering at the commensurate and incommensurate wavevectors below 250 K. Results indicate that the primary effect of V doping on Cr is the modification of the nesting conditions of the Fermi surface and not the decreasing of the Neel temperature.

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Keywords: Chromium; Neutron scattering; QCP

Pure Cr is a body centered cubic itinerant antiferromagnet, which orders at 311 K via spin-density wave (SDW) instability. The electron and hole octahedra, which compose the Fermi surface of Cr are nested by the $q = (1 \pm \delta 00)2\pi/a$ wavevectors, where a is a lattice constant of Cr [1]. In the elastic neutron scattering experiment the antiferromagnetism in Cr is marked by resolution limited superlattice peaks at the nesting wavevectors $q = (1 \pm \delta 00)2\pi/a$, which appear at the Neel temperature (T_N). It has been reported that doping Cr with V reduces T_N, and at V concentrations close to 4% $T_N \to 0$ [2]. The Neel temperature in CrV alloys is usually determined by the minimum in the temperature dependence of the electrical resistivity, usually attributed to removal of the parts of the Fermi surface due to nesting. The possibility of generating a quantum critical point (QCP) in a simple metal motivated a number of experimental and theoretical studies of quantum criticality in Cr [3–5]. The main evidence for a QCP in CrV in addition to $T_N \to 0$ is the increase of the number of carriers when doping into the paramagnetic state, determined from the Hall effect measurements [3]. In this work we report the results of the first neutron scattering measurements performed on a high quality single crystal of nominally quantum critical $Cr_{0.963}V_{0.037}$.

Single crystals of $Cr_{1-x}V_x$, $x = 0.0$, 0.02, 0.037 were grown by the arc zone melting method at the Materials Preparation Center at Ames National Lab. Electron microscopy measurements confirmed that the V concentration remains uniform on length scales from 1 to 50 nm. Electrical resistivity ρ of $Cr_{1-x}V_x$, $x = 0.0$, 0.02, 0.037 was measured by a conventional four probe method using a PPMS by quantum design. Neutron scattering experiments were carried out at the NIST Center for Neutron Research on 40 g single crystal of $Cr_{0.963}V_{0.037}$ and 30 g single crystal of pure Cr using BT9 triple-axis spectrometer with a fixed incident energy $E_i = 14.7$ meV. The measurements were done using a 40′-44′-44′-open collimation configuration. Data were collected near the (1 0 0) reciprocal lattice

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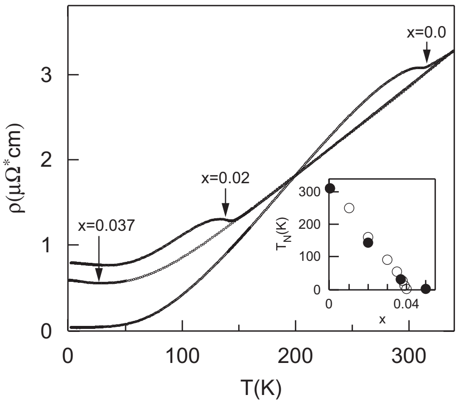

Fig. 1. The temperature dependence of the electrical resistivity of $Cr_{1-x}V_x$, $x = 0.00$, 0.02, 0.037. Arrows indicate the Neel temperature. Inset shows T_N for $Cr_{1-x}V_x$ alloys, determined from the electrical resistivity measurements reported in Ref. [2] (○), and in the current studies (●).

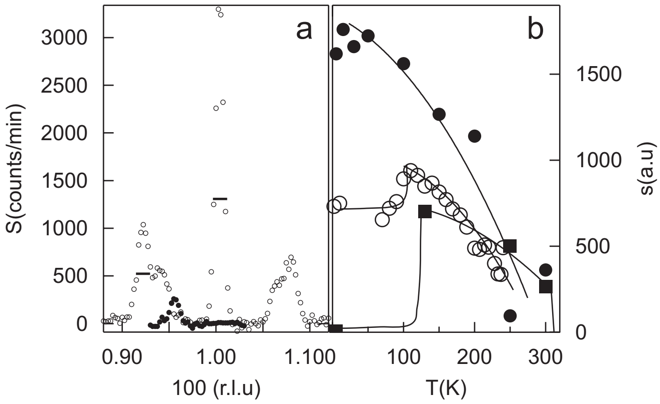

Fig. 2. (a) Elastic longitudinal scans [(1 0 0) direction] in $Cr_{0.963}V_{0.037}$ (○) and in pure Cr (●) at 5 K. Solid horizontal lines indicate spectrometer resolution at the corresponding wavevectors. (b) Temperature dependence of commensurate elastic scattering in $Cr_{0.963}V_{0.037}$ (●), incommensurate scattering in $Cr_{0.963}V_{0.037}$ (○), and incommensurate scattering in pure Cr (■). Solid lines are a guide for the eye.

position in the (0 1 1) plane. Some of our results were obtained on the HB3 triple-axis spectrometer at HFIR, ORNL.

Fig. 1 shows the temperature dependence of the electrical resistivity ρ of single crystals of $Cr_{1-x}V_x$, $x = 0.0$, 0.02, 0.037. ρ for $x = 0.0$ and $x = 0.02$ were normalized to yield the same value as ρ for $x = 0.037$ at 340 K. $Cr_{1-x}V_x$ alloys are good metals with residual resistivity $<1\,\mu\Omega\,$cm. The Neel temperature (T_N) is marked by a minimum in ρ(T), which becomes broader and shifts to lower temperature as the V concentration increases. The inset in Fig. 1 shows T_N of $Cr_{1-x}V_x$ as a function of V concentration of single crystals reported in this work and in previously reported studies of polycrystalline $Cr_{1-x}V_x$ [2]. The results of this work and [2] are in a good agreement. Results of transport measurements indicate that doping Cr with V reduces T_N and make the antiferromagnetism disappear at $x \geqslant 0.037$.

While the minimum in the temperature dependence of ρ in pure Cr occurs at T_N, neutron scattering experiments have not yet confirmed the absence of the antiferromagnetism in $Cr_{0.963}V_{0.037}$. Fig. 2a shows elastic longitudinal scans along (1 0 0) direction in $Cr_{0.963}V_{0.037}$ and in pure Cr collected at 5 K. The striking feature of Fig. 2a is the strong scattering at the commensurate wavevector (1 0 0), absent in pure Cr. Incommensurate scattering in $Cr_{0.963}V_{0.037}$ occurs at four wavevectors $q = (1 \pm \delta_{1,2}00)2\pi/a$, where $\delta_1 = 0.078$, $\delta_2 = 0.058$, which are all larger than the wavevectors corresponding to antiferromagnetic ordering in pure Cr. Both commensurate and incommensurate scattering in $Cr_{0.963}V_{0.037}$ are resolution limited, which corresponds to long range order in the crystal. Fig. 2b shows the temperature dependence of the commensurate and incommensurate scattering in $Cr_{0.963}V_{0.037}$ and the incommensurate scattering in pure Cr. The commensurate scattering in $Cr_{0.963}V_{0.037}$ increases monotonically upon cooling to 5 K. The incommensurate scattering increases on cooling to ~120 K, where it decreases and remains finite upon further cooling to 5 K. The temperature dependence of the incommensurate scattering in pure Cr is well understood. Below 311 K the SDW is transversely polarized and the scattering increases on cooling. At ~120 K, the SDW changes polarization to longitudinal, which results in the loss of the component of the magnetic moment perpendicular to (1 0 0) in a single magnetic domain sample. We observed a qualitatively similar temperature dependence of incommensurate scattering in $Cr_{0.963}V_{0.037}$, though the scattering remains finite below ~120 K. We conclude that contrary to the results of the transport measurements, $Cr_{0.963}V_{0.037}$ orders antiferromagnetically between 250 and 300 K. Our findings indicate that the temperature and wavevector dependence of elastic scattering in $Cr_{0.963}V_{0.037}$ is very different from the one in pure Cr and is likely to originate from the different nesting between the hole and electron octahedra of the Fermi surface of $Cr_{0.963}V_{0.037}$. Such mechanism was suggested previously to account for observed commensurate and incommensurate scattering in $Cr_{1-x}Mn_x$ alloys [6].

We have found strong temperature dependent elastic scattering at the commensurate and incommensurate wavevectors in nominally quantum critical $Cr_{0.963}V_{0.037}$. Although the results of transport measurements reported in this work and other measurements reported elsewhere indicate that $Cr_{0.963}V_{0.037}$ is a quantum critical antiferromagnet, the neutron scattering unambiguously establishes that the composition orders antiferromagnetically at high temperature ($T > 250$ K). The main effect of V doping on Cr is not the reduction of the Neel temperature but rather the change in nesting conditions of the Fermi surface and, perhaps the restructuring of the Fermi surface itself.

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