**High-energy Spin-Density-Wave Correlated
Fluctuations in Paramagnetic Cr + 5 at.%V**

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ABSTRACT

Measurements of the magnetic fluctuations, termed spin-density-wave (SDW) paramagnons, in the nearly antiferromagnetic alloy Cr + 5 at.%V are extended up in energy to about 80 meV. These fluctuating spin-spin correlations occur at incommensurate positions, corresponding to the SDW wavevector Q . Their characteristic energy is at least an order of magnitude larger than that of the magnetic fluctuations seen in the paramagnetic phase of pure Cr, but their intensity is more than two orders of magnitude smaller. We find that the dynamic susceptibility decreases by about 50% between temperature $T = 10K$ and 300K.

PAPER FOR MMM 92

37th CONFERENCE ON MAGNETISM AND MAGNETIC MATERIALS

HOUSTON, TEXAS, DEC.1-4,1992

(PROCEEDINGS TO BE PUBLISHED IN JOURNAL OF APPLIED PHYSICS)

PACS Numbers 61.2.Ex, 64.70.Rh

The occurrence of a spin-density wave (SDW) in *Cr* corresponds to a singularity in the wavevector-dependent magnetic susceptibility $\chi(\mathbf{q})$, which results in part from nesting of the paramagnetic Fermi surface at a value of $\mathbf{q}$ close to the wavevector $\mathbf{Q}$ of the SDW.⁽¹⁾ Alloying *V* with *Cr* reduces the electron concentration, and thus increases the mismatch between the nesting electron and hole surfaces, which decreases the length of $\mathbf{Q}$.⁽²⁾ The observation of this effect by neutron diffraction,⁽³⁾ and conversely the increase of $\mathbf{Q}$ when *Mn* is allowed into *Cr* to increase the electron concentration, provides convincing evidence for the Overhauser SDW mechanism for magnetism in chromium metal.⁽¹⁾

The depression of the Néel temperature resulting from this increasing mismatch yields a phase diagram⁽⁴⁾ in which $Cr_{1-x}V_x$ alloys are paramagnetic beyond a critical concentration, $x_c \approx 4 \text{ at.}\%$. For a concentration close to but greater than the critical value, $x > x_c$, one might expect by analogy with the nearly-ferromagnetic case, that the dynamic susceptibility $\chi(\mathbf{q}, \hbar\omega)$ would show thermally-induced diffusive neutron scattering peaked at zero energy. In the SDW case however, the peak will occur near the nesting wave vector $\mathbf{Q}$, rather than at the origin of reciprocal space as in the ferromagnetic case. The corresponding excitation, the so-called spin-density-wave paramagnon was first observed⁽⁵⁾ by inelastic neutron scattering in a sample of *Cr* + *at.}\%V*. We report here measurements of the energy dependence of the scattering in this sample up to energy, $\Delta E \approx 80 \text{ meV}$, at temperature, $T = 300 \text{ K}$. We have previously reported data up to 42 meV at 150 K .⁽⁶⁾

The single crystal of nominal composition *Cr* + $5 \text{ at.}\%V$ was cut from a boule prepared by arc-zone-melting. The boule was supplied by F.A. Schmidt, Materials Research Center, Iowa State University, and was roughly cylindrical, of diameter about 1.5 cm , with its axis some 30° from the $[001]$ cubic axis. In the first series of experiments^(5,6), the sample was mounted in a Displex refrigerator with the $[001]$ axis vertical, for scattering in the $(hk0)$ reciprocal-lattice plane. In the present experiment, the sample cylinder axis was more nearly vertical, with the $[0\bar{1}1]$ axis perpendicular to the horizontal scattering plane. This geometry ensures better uniformity in scans along $[100]$ at constant energy transfer ΔE ,

while exposing roughly the same sample volume of about 10 cm^3 to the neutron beam. It also allows us to more easily close the scattering triangle by observing the magnetic excitations surrounding the (111) point in reciprocal space.

The neutron-scattering experiment was performed on the triple-axis spectrometer H7 at the Brookhaven National Laboratory Reactor, HFBR. In our earlier work, a pyrolytic graphite (002) monochromator and analyser were used, with collimation $40' - 40' - 80' - 80'$, according to the usual convention, and with fixed final neutron energies, $E_f = 14.7 \text{ meV}$ and 30.5 meV . In the present work, further data were taken for the energy dependence of the scattering at these same values of E_f , but also with a Be (002) monochromator. This allowed us to extend the measurements up to an energy transfer, $\Delta E \simeq 80 \text{ meV}$.

The scattering is weak, and despite the large volume of the sample and the broad collimation, which gives a relatively poor momentum space resolution of only about $0.02 \text{ \AA}^{-1}$, each data point in a representative q-scan at constant- ΔE shown in Fig.1 needs 2 to 7 minutes of counting time. The magnetic scattering cross-section is at least a factor of 100 less than in pure *Cr*. The absolute calibration of the scattered intensity is obtained by normalization to a transverse-acoustic phonon. We note that the large background is due to the incoherent scattering of both *V* and *Cr*, which corresponds to a cross-section of 2.04 barns/atom in this sample.

The double-peak form of the q-scan shown in Fig.1 at high energy transfer appears to be quite different from the single commensurate peak seen at high temperatures in the paramagnetic phase of pure *Cr*.^(7,8) Noakes et al.⁽⁹⁾ showed, however, that the expression for the dynamic susceptibility in the paramagnetic phase employed by Sato and Maki⁽¹⁰⁾, corresponding to the 6 magnetic satellites for SDW paramagnons having wavevector along each of the cube axes that surround the commensurate point, when folded with the resolution function for the spectrometer, can reproduce both forms in each system – a double, or even a triple peak structure at low energies and the single peak at high energies. The incommensurability parameter ($\delta = 0.084$) in *Cr* + 5 at.%*V* is about a factor two larger

than in pure *Cr*, so that a single commensurate peak is seen only at the highest energies. Conversely, in pure *Cr*, the incommensurate peaks with only a relatively weak incommensurate peak are seen at low energies close to the Néel temperature.

One should distinguish clearly between the peak at the commensurate point, first seen by Mikke and Jankowska⁽¹¹⁾ in the ordered phase of *Cr* + 1.2 at.%*Al* and later in pure *Cr*^(7,8), and the superficially similar peak seen in the paramagnetic phase and in the paramagnetic alloy *Cr* + 5 at.%*V*. In the paramagnetic phase the peak at the commensurate point arises from the superposition of scattering at high energies from all 6 incommensurate satellites. In the ordered phase of pure *Cr*, on the other hand, the commensurate peak is seen clearly even at low energies in a single-*Q* sample, and is believed to have a microscopic origin (probably due to phase fluctuations) quite different from the spin waves responsible for the incommensurate scattering, thus warranting the term “commensurate-diffuse scattering” first employed by Fincher, Shirane and Werner.⁽⁷⁾

The dynamic susceptibility $\chi(\mathbf{q}, \hbar\omega)$ is obtained from the scattering intensity $S(\mathbf{q}, \hbar\omega)$ by removing the thermal factor corresponding to the population of magnon states,

$$\chi(\mathbf{q}, \hbar\omega) = S(\mathbf{q}, \hbar\omega) [1 - \exp(-\hbar\omega/kT)] \quad .$$

The energy dependence of χ appears to be rather different for the paramagnetic alloy *Cr* + 5 at.%*V* than for the paramagnetic phase of pure *Cr*, as seen in Fig.2. The energy dependence of the scattering in *Cr* is Lorentzian, with a characteristic energy varying from, $\Gamma \approx 3 \text{ meV}$, at the Néel temperature, (311 K), to, $\Gamma \approx 16 \text{ meV}$, at 500 K (see Fig. 2b). For *Cr* + 5at.%*V*. on the other hand, χ is linear in energy up to at least 40 meV, with some suggestion of levelling off beyond 80 meV (see Fig.2a).

Thus, the characteristic energy of the magnetic fluctuations in *Cr* + 5 at.%*V* at a temperature of 300 K is at least an order of magnitude larger than in pure *Cr*, even 200 K above its Néel temperature. This result is consistent with the severe reduction in the intensity of scattering by about two orders of magnitude in *Cr* + 5 at.%*V* at 300 K

relative to that in pure *Cr* at T_n . A similar trend is seen in dilute alloys, for which the scattering intensity is reduced relative to *Cr* by a factor four in *Cr* + 0.2at.%V⁽¹²⁾ and a factor ten in *Cr* + 0.5 at.%V.⁽⁹⁾ The temperature dependence of the dynamic susceptibility in the *Cr* + 5 at.%V is weak, as shown in Fig.3; χ decreases by only about 50% between 10 K and 300 K.

Magnetic fluctuations in both the paramagnetic phase and the ordered phase of pure *Cr* and *Cr* alloys have a pronounced effect on several bulk physical properties⁽⁴⁾. This is seen most clearly in the magnetoelastic properties, where the anomaly is greatly reduced in magnitude along with the inelastic scattering when *Cr* is doped with V. The apparent absence of any contribution to the magnetoelastic properties in *Cr* + 5 at.%V suggests that these small amplitude magnetic fluctuations extending to high energies do not couple to the lattice.

We plan to study in detail magnetic fluctuations in the paramagnetic phase as the Néel transition is approached in *Cr* alloys exhibiting a commensurate antiferromagnetic structure. It will be interesting to compare the dynamic susceptibility in the paramagnetic phase of pure incommensurate *Cr* with that in the commensurate *Cr*(*Mn*) SDW alloys.

ACKNOWLEDGEMENTS

Research at Brookhaven National Laboratory is supported by the Division of Materials Science, USDOE, under contract No. DE-AC02-76CH00016. E. Fawcett acknowledges support from the Natural Sciences and Engineering Research Council of Canada, and S.A. Werner acknowledges support from the NSF, grant number PHY-9024608.

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Figure Captions

Fig.1 (a) Constant energy scans at $\Delta E = 65 \text{ meV}$ along $[\zeta, 0, 0]$ in $\text{Cr} + 5 \text{ at.\%V}$ at temperature $T = 300 \text{ K}$, near (111), with Be(002) monochromator. (b) The $[0\bar{1}1]$ reciprocal lattice plane, with the magnetic satellites projected into the plane.

Fig.2 (a) Dynamic susceptibility $\chi(\Delta E)$ up to energy $\Delta E = \hbar\omega = 80 \text{ meV}$ in $\text{Cr} + 5 \text{ at.\%v}$ at $T = 300 \text{ K}$. The open squares ($\square$) are obtained from integrating the intensity in constant- ΔE scans using a PG monochromator. The triangles ($\triangle$) are obtained from peak heights normalized to the point at $\Delta E = 28 \text{ meV}$. The open circles ($\bigcirc$) are from data using a Be monochromator. Experimental difficulties occur in the region of 28 meV to 36 meV due to the longitudinal zone boundary phonon. (b) The dynamic susceptibility $\chi(\Delta E)$ for pure Cr at 500 K (from Grier, et al., ref. 8). The line is a guide to the eye. Note the difference in scale of about 200 between (a) and (b).

Fig.3 Temperature dependence of the dynamic susceptibility for *Cr + 5 at.%V*. Each point is the average of measurements of the integrated intensity for data taken at $\Delta E = 6\text{meV}$ and 9meV .

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Fig. 1

Fig. 2

Fig.3

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