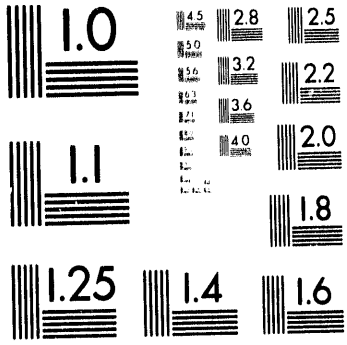
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1.1
1.25
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1.8
2.0
2.2
2.5
2.8
3.2
3.6
4.0
4.5
5.0
5.6
6.3
7.1

1 of 1

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Title: MAGNETIC PHASES IN UNiGe

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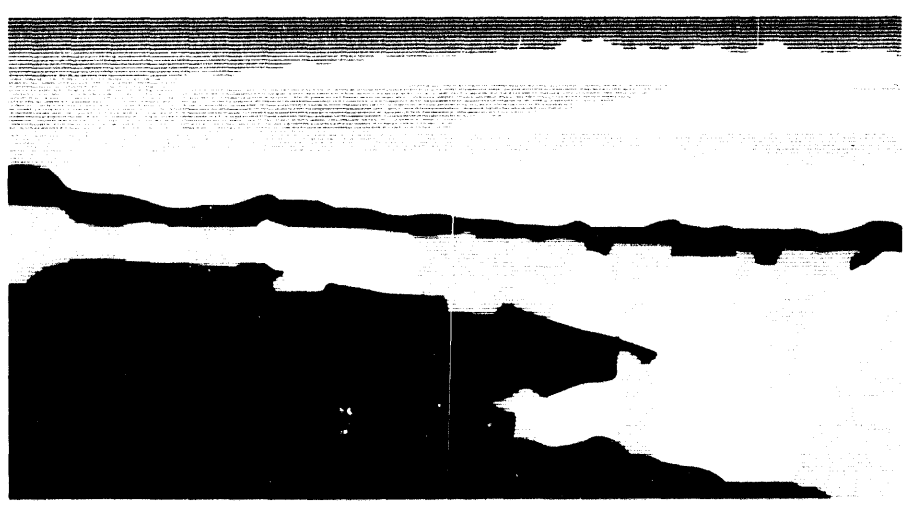
Submitted to: J. Alloys Compounds



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MAGNETIC PHASES IN UNiGe

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UNiGe is one of 14 UT(Si,Ge) compounds which were reported to adopt the orthorhombic $CeCu_2$ -type structure (space group Imma) [1] or its ordered ternary version of the TiNiSi type (Pnma) [2]. Note that the lattice constants *a, b, c* in the TiNiSi notation correspond to *b, a, c* in the $CeCu_2$ -type lattice.

A number of papers on UNiGe polycrystals report a magnetic phase transition to antiferromagnetic ordering around 40-44 K [1,3-5]. Based on powder neutron-diffraction results, Murasik et al. [6] claimed that UNiGe crystallizes in the $CeCu_2$ -type structure with Ni and Ge atoms being randomly distributed on copper sites. Moreover, an antiferromagnetic structure with a propagation vector **q** = (1/2,0,1/2) and uranium magnetic moments (μ = 1.37+0.07 μ_B at 13 K) oriented along the *a* axis is proposed

below T = 43.3 K. The possibility of the first order magnetic phase transition was considered. In contradiction, Kawamata et al. [7] claim that they observed on a UNiGe single crystal at 10 K only magnetic reflections which coincide with nuclear ones, which they naturally interpreted in terms of the identical size of the magnetic and chemical unit cell. This not very satisfactory situation about UNiGe has motivated our further studies on a single crystal reported previously [8]. The original measurements of the magnetization curves at 4.2 K (up to 38 T) and temperature dependence of magnetic susceptibility were completed by an extended study of the magnetization, specific heat and electrical resistivity as a function of temperature and magnetic field. Moreover, we performed neutron diffraction experiments on a powder sample and on the single crystal.

The temperature dependence of the specific heat shown in Fig. 1 exhibits a sharp peak at 41.5 K and a broad anomaly around 50 K in a good agreement to data published by Kawamata et al. [8]. The peak at 41.5 K corresponds to the first-order magnetic phase transition mentioned above. Anomalies at this temperature were observed also in the temperature dependence of magnetic susceptibility and electrical resistivity. The powder neutron diffraction pattern at 3 K consists of pure nuclear reflections consistent with the TiNiSi-type structure and magnetic reflections pointing to AF structure of U moments $\mu_B \approx 1.4\ \mu_B$ (within the b-c plane) with a propagation vector $\mathbf{q}$ = (0,1/2,1/2). This pattern remains generally unchanged up to 41.5 K. Temperature scans of several magnetic reflections made on the single crystal reveal only a week decrease of uranium magnetic moment with increasing temperature (see Fig. 2). At 40 K, the moment amounts still to about 90% of its low temperature value. Then it steeply decreases in the close vicinity of the magnetic phase transition at 41.5 K. The magnetic state between 41.5 and 50 K is not fully understood up to now. The slight anomalies around 50 K observed also in both the temperature dependence of the susceptibility and resistivity are indicative of a magnetic phase transition from paramagnetic state

to a sort of magnetic ordering. Preliminary neutron diffraction studies by SCD at LANSCE and E3 at BENSC revealed between 41.5 and 50 K an incommensurate magnetic structure with a temperature dependent propagation vector in the *b-c* plane. Further neutron diffraction studies are under way.

The magnetization curves at 4.2 K display metamagnetic transitions in fields B parallel to *b* (at 17 and 25 T) and B parallel to *c* (at 3 and 10 T) reflecting changes of antiferromagnetic structure towards the parallel alignment of moments in high fields (M = 1.45 μ_B /f.u.). A weak linear magnetic response to field B parallel to *a* (M = 0.23 μ_B/f.u.) manifests a huge magnetic anisotropy. In order to study the microscopic origin of different magnetic states between the transitions we have started neutron diffraction experiments on the UNiGe crystal in magnetic fields. So far we have measured the behaviour in fields up to 6 T along the c-axis. The phase above 3 T (amounting $M = 1/3\, M_S$) is consistent with the propagation vector **q** = (0,1/3,1/3), which yields + + - stacking of uranium magnetic moments locked in the *b-c* plane) along both the *b*- and *c*-direction. The pronounced hysteresis of the metamagnetic transition seen on the magnetization curve was reproduced when measuring h,k/2,l/2 and h,k/3,l/3 reflections with increasing and decreasing magnetic field as shown in Fig. 3. The first transition in fields along the b-axis cannot be reached by static magnetic fields available at neutron beams. Considering the dramatic difference in the magnetoresistance response on the first metamagnetic transition in fields along the *c*- and *b*-axes displayed in Fig. 4, we can conclude that **q** of the magnetic structure above 17 T (B parallel to *c*) cannot be equal to (0,1/3,1/3).

The up to now observed features of magnetic structures in UNiGe confirm the conclusions, which we made previously from bulk experiments suggesting that the strong bonding of 5f orbitals along the a axis leads to a huge magnetic anisotropy characterized by uranium magnetic moments perpendicular to this direction, which seems to be a general feature in UTX compounds with the TiNiSi-type structure.

ACKNOWLEDGMENTS

This publication is based on work sponsored by the U.S. Czechoslovak Science and Technology Joint Fund in cooperation with the MSMT CR and the U.S. Department of Energy under project Number 93039. It was also supported in part by the division of Basic Energy Sciences of the U.S. Department of Energy and by the "Nederlandse organisatie voor Wetenschappelijk Onderzoek (NWO)". The experiments of V.S. at BENSC are sponsored by an EC grant within the Go West programme.

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FIGURE CAPTIONS

Fig. 1 C/T vs T plots displaying the specific heat behaviour of UNiGe.

Fig. 2. Temperature dependence of several 0,k/2,l/2 reflections of UNiGe

Fig. 3. Field dependence of the magnetization (top), and 0,2/3,4/3 (middle) and 0,3/2,5/2 (bottom) reflections of UNiGe in the magnetic filed applied along the c-axis.

Fig. 4. Longitudinal magnetoresistance in UNiGe in the magnetic field applied along the *a*-, *b*- and *c*-axis.

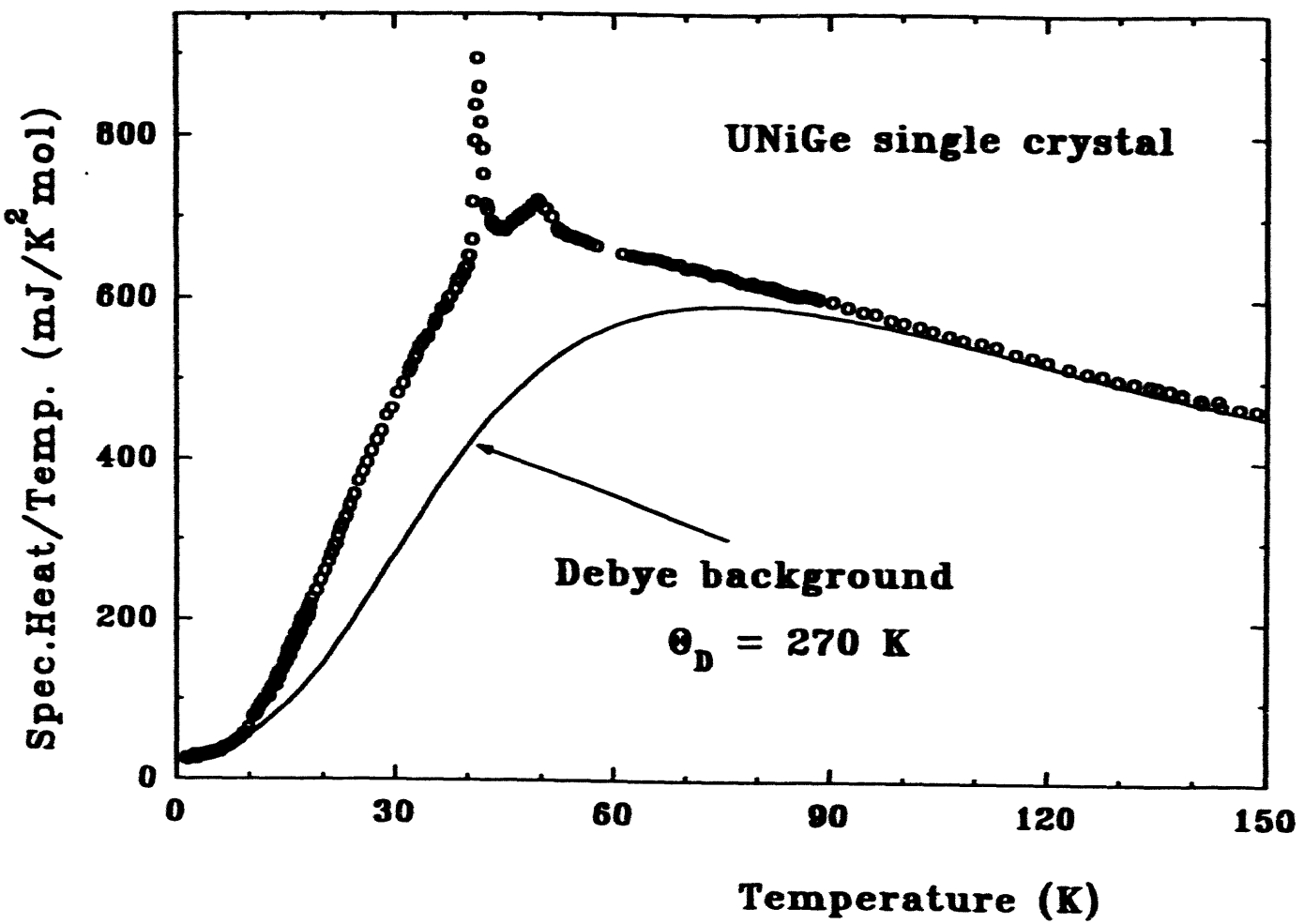
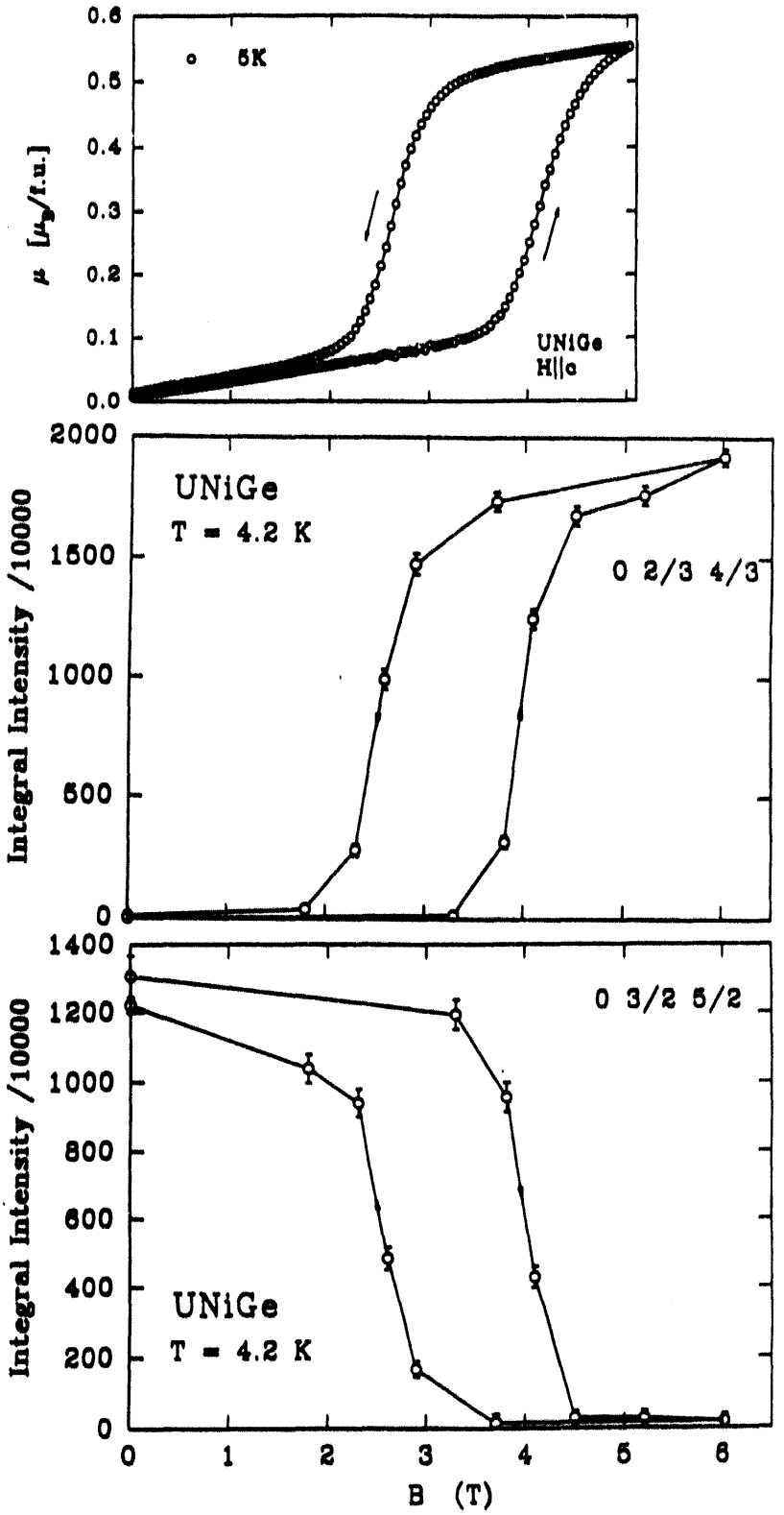

UNiGe single crystal
Debye background
θ_D = 270 K
Spec.Heat/Temp. (mJ/K^{2}mol)
Temperature (K)
0
200
400
600
800
0
30
60
90
120
150

Fig. 1

Fig. 3


5K
μ [μB/f.u.]
UNiGe
H||a
UNiGe
T = 4.2 K
0 2/3 4/3
Integral Intensity /10000
0 3/2 5/2
UNiGe
T = 4.2 K
Integral Intensity /10000
B (T)

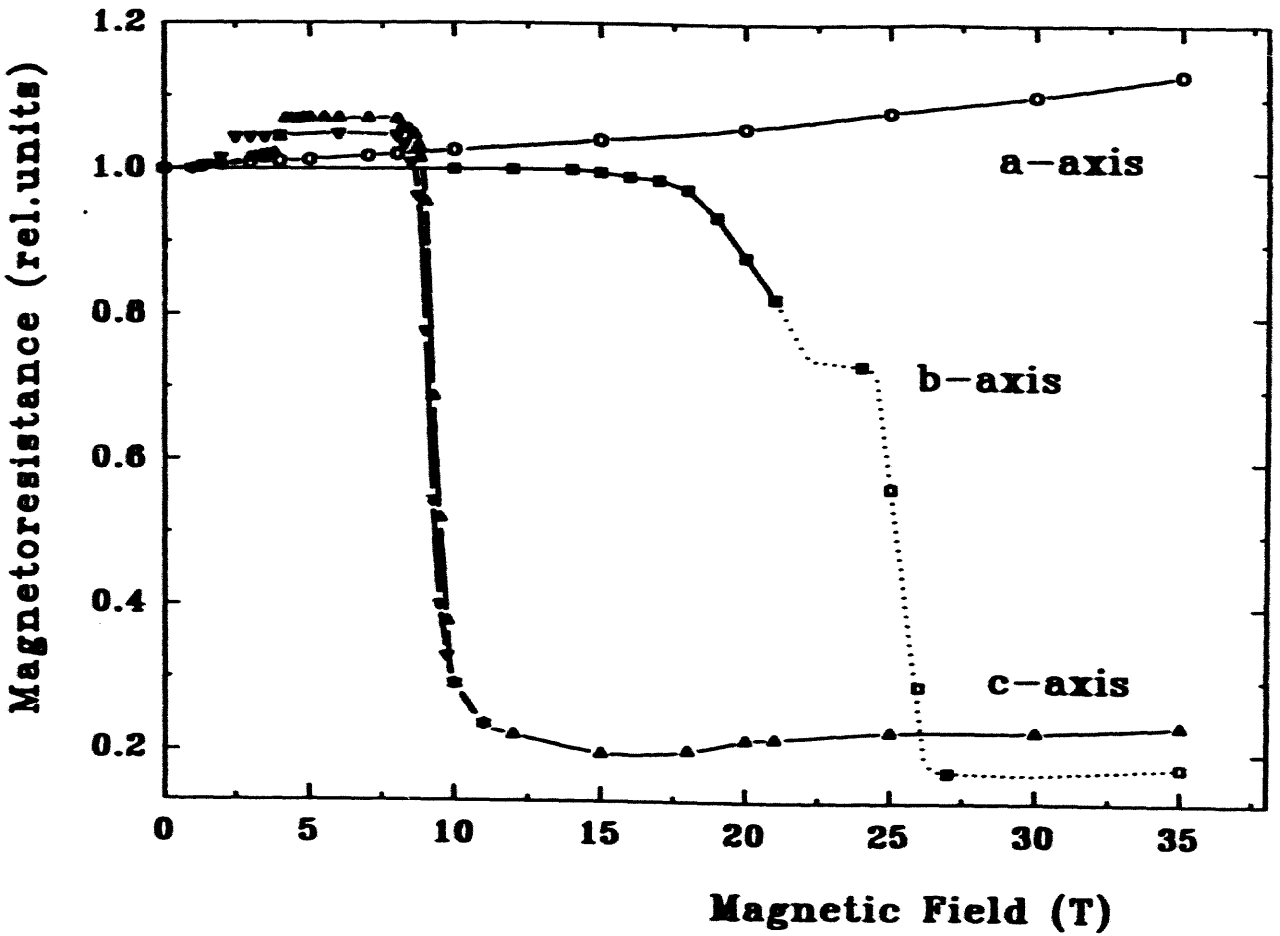

Magnetoresistance (rel.units)
1.2
1.0
0.8
0.6
0.4
0.2
0
5
10
15
20
25
30
35
Magnetic Field (T)
a-axis
b-axis
c-axis

Fig. 4

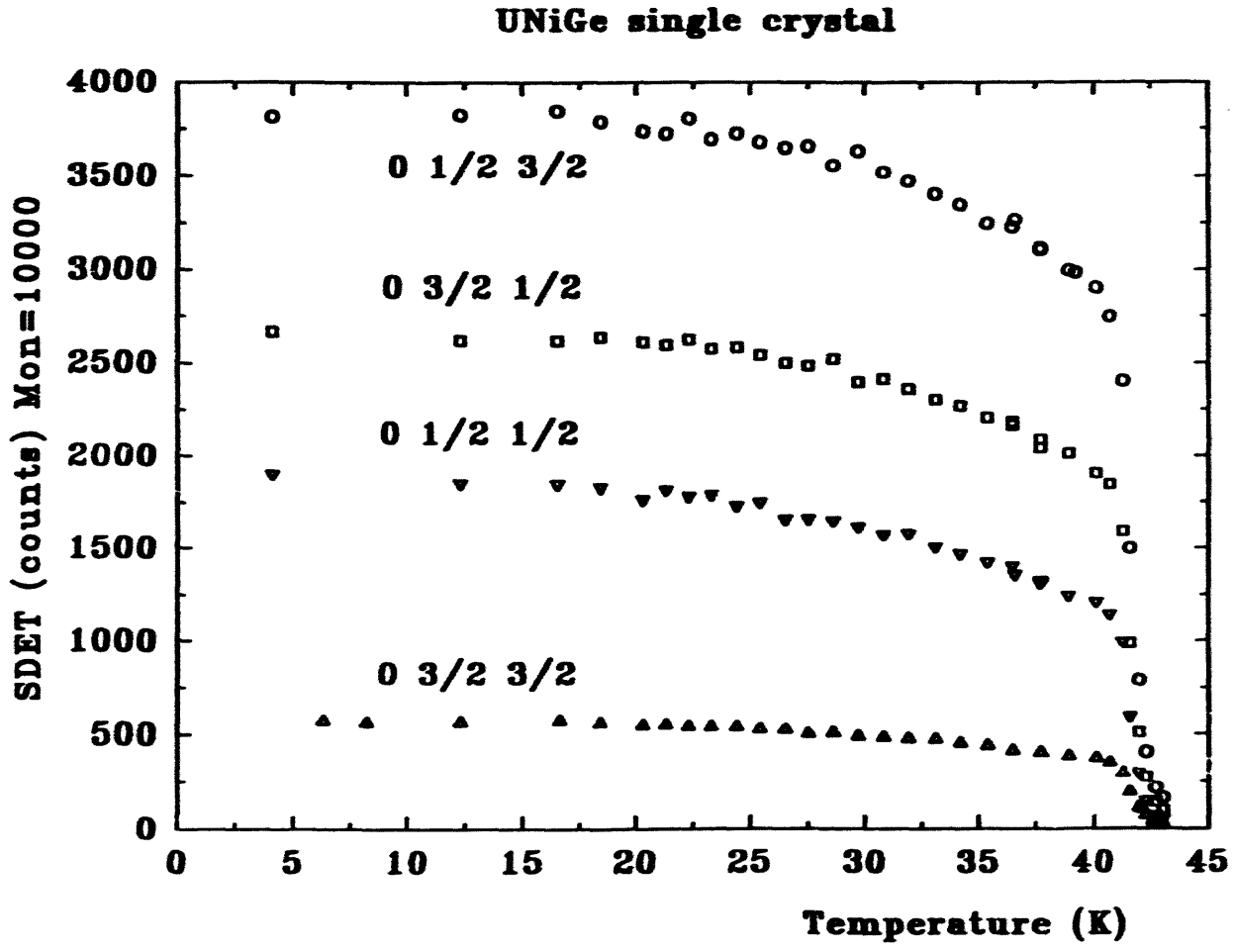

UNiGe single crystal
SDET (counts) Mon=10000
4000
3500
3000
2500
2000
1500
1000
500
0
0 1/2 3/2
0 3/2 1/2
0 1/2 1/2
0 3/2 3/2
0
5
10
15
20
25
30
35
40
45
Temperature (K)

Fig. 2

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