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Neutron-Diffraction Investigation of UPSe and UAsS

By

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As a further extension of our neutron-diffraction investigations of magnetic properties of UXY compounds (X pnigogen, Y chalcogen) (1, 2), we have determined the magnitude of the magnetic moment at 4 K and refined the crystal structure parameters in UPSe and UAsS.

Polycrystalline samples were obtained as described in (3). The lattice constants were derived from X-ray powder photographs obtained in a Guinier camera and refined by the method of least squares. Both UPSe and UAsS crystallize in the PbFCl type of structure. The space group is P4/nmm with

$$2\ U \qquad \text{in } 2c; \quad 1/4,\ 1/4,\ u; \quad 3/4,\ 3/4,\ \bar{u};$$

$$2\ S\ (\text{or Se}) \text{ in } 2c; \quad 1/4,\ 1/4,\ z; \quad 3/4,\ 3/4,\ \bar{z};$$

$$2\ P\ (\text{or As}) \text{ in } 2a; \quad 3/4,\ 1/4,\ 0; \quad 1/4,\ 3/4,\ 0.$$

The crystallographic parameters u and z up to now have not yet been determined.

The diffractometer DN-500 at the Świerk reactor EWA was used for obtaining neutron-diffraction patterns at 4 and 300 K. The neutron wavelength was (1.32 ± 0.01)Å. As an example neutron diffraction diagrams obtained for UAsS are shown in Fig. 1. Room temperature neutron intensities were used for the calculations and a squares refinement of the u and z parameters. The results are collected in Table 1. Neutron scattering amplitudes for U, P, As, Se, and S as reported in (5) were adopted. No temperature factor was allowed for. Calculated and observed intensities are compared in Table 2.

Comparing neutron-diffraction patterns taken at 4 and 300 K one can see the presence of a magnetic contribution to the (101) reflections. This, together with the observed lack of a contribution to the (001) reflection, permitted to conclude that both investigated compounds are ferromagnetic with the magnetic moments aligned
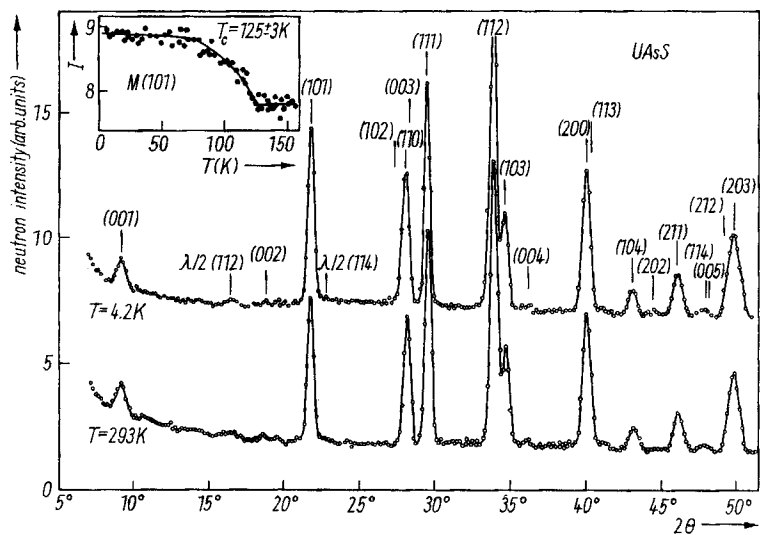
Fig. 1. Neutron-diffraction patterns of UAsS taken at room and liquid helium temperature

Table 1

The crystallographic and magnetic data for UPSe and UAsS

compound	a (Å)	c (Å)	u	
UPSe	3.951 + 0.006	8.185 + 0.008	0.2610 + 0.0040	
UAsS	3.884 + 0.005	8.176 + 0.006	0.2839 + 0.0020	
	z	R (%)	$\mu_f (\mu_B)$	T_c ($^\circ$K)
UPSe	0.6435 + 0.0029	7.75	1.35 + 0.10	110 + 3
UAsS	0.6314 + 0.0049	8.39	1.24 + 0.10	125 + 3

Table 2

A comparison of calculated and observed neutron intensities for UPSe and UAsS

hkl	UAsS		UPSe	
	$I_{obs.}$	$I_{calc.}$	$I_{obs.}$	$I_{calc.}$
001	45	49	1	0
002	4	10	41	27
101	147	194	21	29
102				
110	167	175	331	335
003			139	123
111	262	277	304	341
103	140	121	264	230
200				
113	231	214	381	370
104	46	40		
202	3	0		
211	45	70		
114				
005	14	16		
212				
203	190	168		

The scaling factors are UPSe: $k = 0.0111 \pm 0.0003$, UAsS: $k = 0.101 \pm 0.0002$.

along the c-axis, in accordance with previous magnetic measurements (3, 4).

The temperature dependence of the magnetic contribution to the (101) peak gave the Curie points for both samples. The magnitude of the magnetic moment of the uranium ion was calculated from the above magnetic contribution using the form factor for the $5f^2$ configuration, the uranium atomic parameter, and the scaling factor determined from room temperature neutron intensities.

The obtained data are summarized in Table 1.

References

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