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Investigation of the crystal structure of URu_2Si_2 by high-resolution X-ray diffraction

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Abstract

We report thermal expansion measurements on URu_2Si_2 by high-resolution X-ray diffraction done with a relative longitudinal resolution of 3×10^{-6}. Besides the abnormal thermal expansion, no lattice distortion indicating a transition into another space group was observed, i.e. the crystal remains tetragonal down to 3 K.

Keywords: Heavy fermion; Magnetism; Supraconductivity; X-ray diffraction

URu_2Si_2 is a tetragonal heavy fermion superconductor which has a magnetic phase transition at $T_N \sim 17.5$ K. The origin of this transition remains an enigma despite considerable experimental and theoretical effort [1]. The size of the small uranium magnetic moment at low temperature ($\sim 0.03\mu_B$) is incompatible with the huge anomalies observed in thermodynamic and transport properties at T_N. Various ideas have been put forward in Refs. [2–6]. For example, it has been suggested that a quadrupolar phase transition could occur near T_N [3–5,10,11] or the transition at T_N could be primarily structural [6]. A high-resolution X-ray diffraction investigation of the crystal structure at low temperature is therefore of interest. This contribution reports such a work.

The measurements were done at the triple crystal diffractometer of the high-energy beamline ID15A at the ESRF (Grenoble, France). An X-ray beam of ~ 114 keV was used in the non-dispersive mode. In this mode the beam divergence does not play any role [7]. Since the setup becomes already dispersive with the mismatch of the monochromator and sample scattering vectors [8], one has to use reflections with monochromator and sample interplanar spacings as close as possible.

The measured mosaicity of our crystal at ID15A is $\sim 0.01^\circ$.

In Fig. 1 we display two longitudinal scans recorded either below or above T_N. Each diffraction pattern can be described by the sum of two Lorentzian functions, reflecting the fact that the region probed by the measurement is slightly inhomogenous within our resolution ($\sim 3 \times 10^{-6}$), i.e. the crystal is not perfect. If a structural transition, for instance from tetragonal to orthorhombic, occurs [6,9] at T_N, i.e. the a lattice parameter becomes different from b, reflections $[h\,0\,0]$ and $[0\,k\,0]$ would be characterized by different interplanar spacings. As the crystal would certainly be twinned this would result in a splitting of the Bragg peak. Since we do not observe any splitting of the [4,0,0] Bragg reflection, we infer that URu_2Si_2 remains tetragonal down to 3 K. This result obtained by a microscopic experimental method is consistent with the result of the investigation of the elastic response by macroscopic methods [9].

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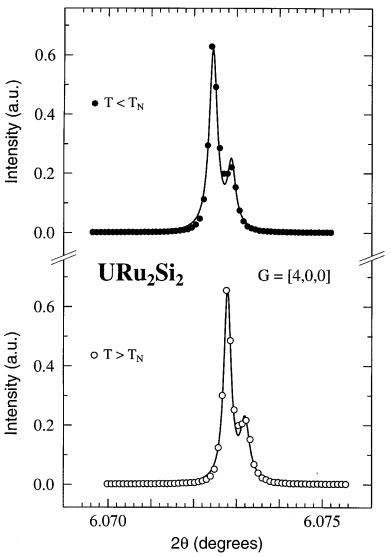

Fig. 1. X-ray intensity as a function of the scattering angle 2θ recorded for the scattering vector $G = [4,0,0]$. The upper and lower panels present the pattern recorded below (at 14.38 K) and above (20.22 K) the Néel temperature, respectively. The solid line in each panel is a fit with the sum of two Lorentzian functions. These results show that URu_2Si_2 remains tetragonal in the ordered state.

In Fig. 2 we present the thermal variation of the lattice parameter c. The solid line displays the computed variation of this parameter obtained from the integration of the thermal-expansion data [9]. It is rewarding that the two experimental techniques yield consistent results although we note that the effect of the phase transition is more pronounced in the X-ray data than in the thermal-expansion data.

In conclusion, within an accuracy of 3×10^{-6}, there is no lattice distortion in URu_2Si_2, i.e. the crystal remains tetragonal down to 3 K. This dismisses neither the possibility of a quadrupolar ordering [3–5,10,11] since this

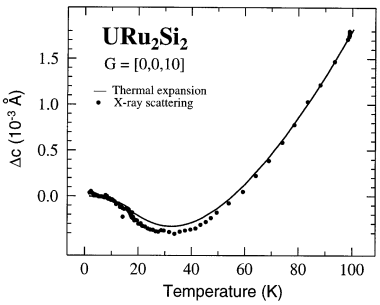

Fig. 2. Thermal variation of the lattice parameter c of URu_2Si_2 as measured in this work by high-energy X-ray diffraction (points) and deduced from the thermal-expansion measurements of Kuwahara et al. (solid line) [9].

order could be antiferromagnetic nor the valence fluctuation mechanism [6] because the distorsion due to the fluctuation could be smaller than 3×10^{-6}.

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