ESRF

Experiment title: Separation of the influences of martensitic distortion and of superconductivity on the electron momentum density of V_3Si		**Experiment number:** HE-578
Beamline: ID 15B	**Date of Experiment:** from: 10-Apr-99 to: 20-Apr-99	**Date of Report:** 23 September 1999
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Report:

Since the advent of ceramic high-T_c superconductors research on A15 compounds has been pushed aside, although still the latter are technologically much more important and yet not completely understood. The A15 compound V_3Si has a $T_c \approx 17.1$ K that depends somewhat on the stoichiometry and crystalline perfection of the material. In addition and even more dependent on stoichiometry and perfection, it undergoes a low-temperature martensitic transition that starts at 20.5 K and that is practically completed when reaching T_c according to Ref. [1].

Our previous studies [2, 3] of single-crystal samples of V_3Si have been aiming at three-dimensional Compton-scattering data with the idea to investigate whether there are characteristic features of the electronic structure already at a resolution $\Delta p > \Delta \cdot m/p$ at room temperature and to provide experimental benchmark data for theoretical calculations. The discrepancy between the experimental reciprocal form factor $B(\vec{s})$ in the resolution-limited range $1\,Å \leq s \leq 3.5\,Å$ and our theoretical calculations for linear vanadium chains has made the validity of the popular chain model less likely [2]. Apart from the higher experimental resolution and encouraged by the referees, the project HS-553 [3] has comprised low-temperature Compton measurements including the transition to the superconducting state for the first time for a comparison between the normal state and the superconducting state of V_3Si. The sample had maximum excess of vanadium, and its heat-capacity data showed no martensitic transition. The remarkably large and directionally dependent effect we found made a corroboration with a stoichiometric sample necessary, which was to enable us to separate the effects of martensitic distortions and superconductivity.

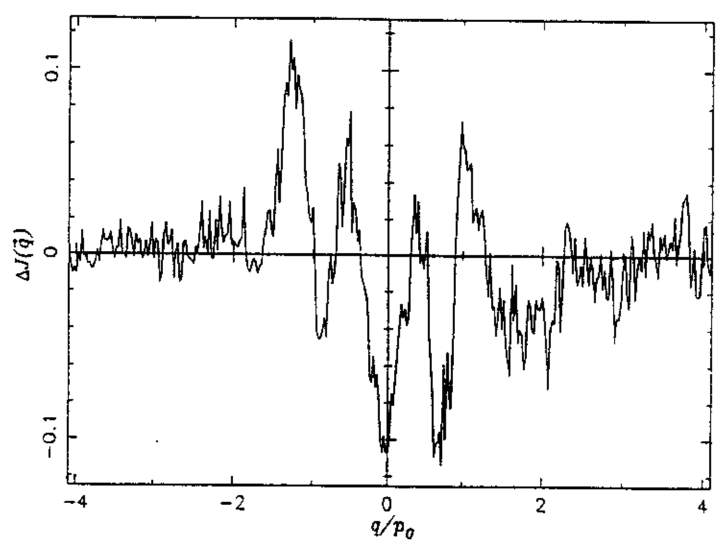
We were right with our scepticism that originated from the shape and momentum range of the observed effect. It has been an artefact indeed — caused not by an inhomogeneous vanadium distribution, but by small amounts of solid air condensed in spite of the high-vacuum conditions and detected quite at the beginning of our new measurements when checking the sample position by optical surveying. Regularly repeated degassing at higher temperatures has helped to avoid the artefact this time.

With a rotating-crystal diffraction measurement at gradually lowered temperatures we could beautifully observe the small martensitic distortion, continuously increasing with decreasing temperature. It saturates well below T_c and shows no discontinuity at T_c itself. In spite of very good statistics the Compton-profile data do not differ between 25, 18 and 10 K. This means that at the two transitions the single-particle electronic structure changes only marginally, if any. The difference in the position-space deformation density between room temperature and 13.5 K that has been reported by Staudenmann et al. [4] should be redetermined.

The second success of our experiment is the proof that the electronic range of coherence extends beyond 5.5 Å along the V—V chains and is therefore metal-like (⟨100⟩ direction), whereas the coherence range in the direction of the V—Si bonds hardly exceeds 4 Å like in insulators (⟨210⟩ direction). The two figures (directional difference in the Compton profile and the long-range reciprocal form factor on an absolute scale, so far based on the high-energy-side data alone) visualise the clear distinction. The chain model has to be revisited, and more elaborate theoretical calculations can now be calibrated against our data that could be measured only with the excellent spectrometer at beamline ID 15B.

[1] L. R. Testardi, Rev. Mod. Phys. **47**, 637 (1975).
[2] T. Asthalter, Dissertation, Konstanz 1997; see also the application for project HS-553 (1997/98).
[3] T. Asthalter, M. Walter, W. Weyrich, Report on project HS-553 (1998).
[4] J.-L. Staudenmann, B. DeFacio, C. Stassis, Phys. Rev. B **27**, 4186 (1983), and refs. therein.

V_3Si Compton profile difference: [210] − [100]



V_3Si reciprocal form factors