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Local Structure Around Sn in CeCoIn_{5-x}Sn_x

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Abstract

The local structure around Sn dopants in CeCoIn_{5-x}Sn_x has been probed by extended x-ray absorption fine structure (EXAFS) technique. Our fit results for both $x = 0.12$ and $x = 0.18$ clearly indicate the dopant Sn atoms predominantly occupying the planar In(1) site. These results are consistent with the quasi-two-dimensional electronic properties of CeCoIn₅ and will be discussed in relation to the observed bulk properties.

Key words:

Heavy-Fermion compounds, X-ray absorption spectroscopy

CeCoIn₅ is an ambient pressure superconductor with a superconducting transition temperature (T_c) of 2.3 K [1]. Recent experiments, however, have shown that T_c is easily suppressed by the replacement of In by Sn [2]. The mechanism by which Sn suppresses superconductivity is not understood well. It is therefore important to determine the local structure of the dopant atom in order to understand the microscopic origin for the suppression of T_c . We have performed extended x-ray absorption fine structure (EXAFS) investigations on CeCoIn_{5-x}Sn_x system at the Sn K -edge. In this work, we present x-ray absorption measurements and analysis and discuss the results in relation to the observed properties.

Details of sample growth and characterization are described elsewhere [1,2]. Single crystals of CeCoIn_{5-y}Sn_y ($y = 0.2, 0.3$) were grown in In flux in the ratio Ce:Co:In:Sn=1:1:20: y . Microprobe analysis reveals an actual Sn concentration $x \sim 0.6y$; hence, in what follows, the microprobe deduced actual Sn concentration will be used. The samples were found to crystallize in the primitive tetragonal HoCoGa₅-type structure [3]. Sn K -edge absorption spectra were measured in fluorescence mode using a Canberra 32-element germanium detector and a half-tuned double-crystal Si(220) monochromator at beamline 11-2 of the Stanford Synchrotron Radiation Laboratory (SSRL). Pellets of the single crystal samples were ground with a mortar and pestle and passed through a 20 μ m sieve. The powdered material was then brushed onto adhesive tape and several layers were stacked together. The samples were mounted in a liquid helium flow cryostat. The EXAFS data were analyzed using the REXAFS software package [4]. The EXAFS function $\chi(k)$ was extracted from the measured absorption coefficient $\mu(k)$ according to $\chi(k) = \mu(k)/\mu_0(k) - 1$, where $\mu_0(k)$ is a smooth background function, the photoelectron wave vector $k = \hbar^{-1}[2m(E - E_0)]^{1/2}$, m is the elec-

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tron rest mass, E is the incident energy and E_0 is the threshold energy. Structural refinement of the EXAFS data was done in R -space by fitting data to theoretical standards generated by FEFF7 [5].

In the 115 compounds In atoms reside in two crystallographically inequivalent sites. In atoms at the planar site (In(1) site) are surrounded by 4 Ce and 8 In near neighbors, at distances 3.268 Å and 3.286 Å, respectively. On the other hand, In atoms at the low symmetry In(2) site have 2 Co and 1 In immediate near neighbors at 2.723 Å and 2.879 Å, respectively, followed by 4 In at 3.268 Å, and 2 In and 2 Ce neighbors at a distance 3.286 Å. To help us compare the difference between the two sites, we have generated a theoretical EXAFS function $\chi(k)$ for the two sites. The Fourier transform (FT) of the simulated EXAFS function for both sites is presented in the Fig. 1 insert. Note that for the In(2) site, in the low R region, there is a well resolved peak at ~ 2.4 Å, which is mainly due to the 2 Co and 1 In near neighbors (due to the phase shift of the photoelectron at the absorbing and backscattering atoms, the peak positions are shifted by small known amounts from the actual pair distances). In addition, the peak at ~ 3.0 Å, which is due to Ce and In neighbors, is higher for the In(1) site since there are higher coordination numbers, namely 4 Ce and 8 In, as compared to the In(2) site, which has 2 Ce and 6 In neighbors at this distance. By comparing the Sn data with the simulation (Fig. 1 insert), one can learn the following: the small amplitude between 2–2.5 Å strongly suggests that Sn is predominantly occupying the In(1) site.

The fraction of Sn atoms going to the In(1) site has been estimated by detailed fits to the EXAFS signal. By allowing the contribution from each site to vary, a linear combination of both sites were fit to the data. The coordination distances, and the pair distribution widths (σ 's) were also allowed to vary in the fits. Only single scattering paths were included in the fits. Consistent with the observed FT features, the fit results show a major fraction of Sn atoms predominantly occupying the In(1) sites. Despite the fact that there are 4 times as many In(2) sites as In(1) sites, we find the fraction of Sn atoms going to the In(1) site is 0.5(1) and 0.7(1), for $\text{CeCoIn}_{4.82}\text{Sn}_{0.18}$ and $\text{CeCoIn}_{4.88}\text{Sn}_{0.12}$, respectively. With the exception of the Sn-Co pair, which shows a small contraction, the pair-distance results compare very well with those of CeCoIn_5 obtained from previously reported diffraction results [6]. A plot showing the best fit spectra, along with data, is exhibited in Fig. 1.

Our findings are particularly significant when one considers the observed bulk physical properties of Sn doped CeCoIn_5 samples. As noted above, superconductivity is easily destroyed with Sn doping and the results of our study appear to be related with the 2D-like nature of superconductivity in these systems. Sn

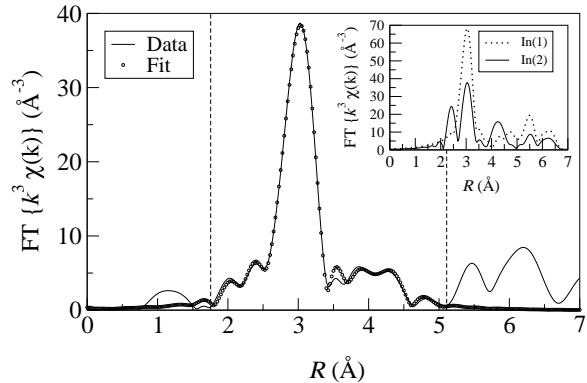


Fig. 1. A low temperature (30 K) Sn K -edge Fourier transform (k^3 weighted) for $\text{CeCoIn}_{4.82}\text{Sn}_{0.18}$. Solid line indicates data; open circles indicate theoretical fit. The fit range, 1.75-5.10 Å, is indicated by the dashed vertical line. The k -range for the fit is 3.0-14.8 Å $^{-1}$. Insert shows a FEFF simulation of Fourier transforms (k^3 weighted) for the In(1) and In(2) sites.

doping, therefore, alters the electronic and magnetic structure of the quasi-2D CeIn_3 -like planes leading to the strong suppression of T_c . This result is in complete agreement with the critical field measurements in the $a-c$ plane, a study which suggests a two dimensional nature of superconductivity in CeCoIn_5 [7].

In conclusion, the local structure of Sn dopants in $\text{CeCoIn}_{5-x}\text{Sn}_x$ ($x = 0.12, 0.18$) has been probed by EXAFS. Our fit results show that the majority of Sn atoms reside on the planar In(1) sites. The results of this study suggest that T_c suppression is due in part to the perturbation of the Ce-In planes by Sn doping, consistent with the 2D-like electronic structure of CeCoIn_5 .

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