

X-ray Absorption Spectroscopic on the Phase Transition of Cd₂Re₂O₇

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The geometrically frustrated pyrochlore oxides, such as Cd₂Re₂O₇, have attracted much attention and been investigated extensively. It was reported that Cd₂Re₂O₇ exhibits anomalous second-phase transition at $T=200\text{K}$. This transition is also accompanied with an ideal cubic to a tetragonal structural phase transition. It undergoes another first-order phase at $T=120\text{K}$ as well as the structure transition from one tetragonal to another. Moreover, the compound was recently discovered to reveal superconductivity at about 1 K and is the first one found in the pyrochlore family.

We conducted the X-ray diffraction as well as Re L₃-edge extended X-ray absorption fine structure (EXAFS) at different temperatures to investigate the local structure of Cd₂Re₂O₇. Temperature-dependent Re L₃-edge X-ray absorption near edge spectra (XANES) of Cd₂Re₂O₇ for normal incident ($\theta = 0^\circ$) are showed in Fig. 1. The pre-peak at 10544.5 eV is ascribed to the transition from Re $2p_{3/2}$ into the continuum free-electron like states. As noted, the spectra show no clear change under the phase transition. Fig.2 (a) and 2(b) present the normalized Re L₃-edge EXAFS oscillation $\chi(k)$, weighted by k^2 and its corresponding Fourier Transform (FT) amplitude of the $k^3\chi$ data, respectively. The peak position for the first shell was observed around 1.9 Å at room temperature and shift to a larger bond length when the temperature decreases. As observed, full width of half maximum (FWHM) for first-shell peak at 20 K is larger than all the others. As known, Debye Waller factor should be smaller at lower temperature, thus the corresponding peak should have been narrower. The broaden peak at at lowest temperature (20K) implies that the peak might have at least two components. In order to understand the variation of the geometry structure of different temperature, we performed the single crystal X-ray diffraction experiments of single crystal Cd₂Re₂O₇ between 300K and 90K.

Table 1 shows the bond length of Re and its surrounding oxygen which formed the octahedral. Comparing the XRD and EXAFS we observed the bond length for Re first shell (Re-O) with smaller variation at 295K and 160K. At 90 K (below the first-order phase transition) the bond length for apical and plane oxygen are around 1.925 Å and 1.935 Å, respectively. This explains the Re L₃-edge FT amplitude of EXAFS has FWHM of first-shell peak at 20 K than others. The average bond length increases with decreasing temperature which is also consist with our EXAFS FT

data.

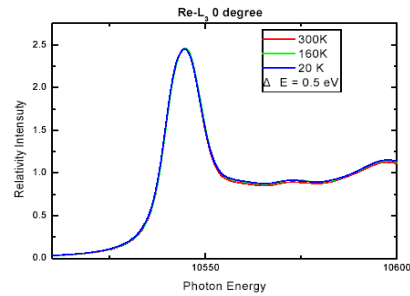


Figure 1. Temperature-dependent Re L₃-edge XANES of Cd₂Re₂O₇

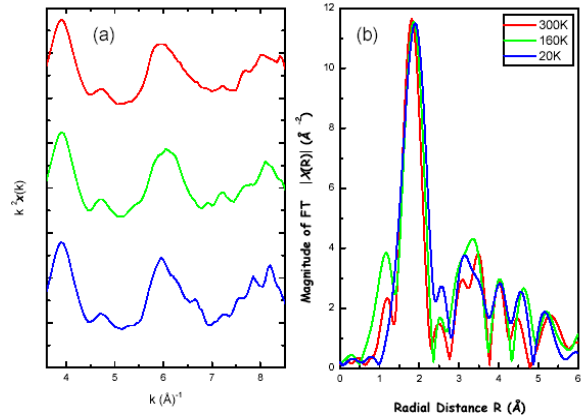


Figure 2. (a) Re L₃-edge EXAFS oscillations $\chi(k)$ weighted by k^2 ; (b) Magnitude of the FT of the EXAFS χk^2 data.

Table 1 Bond length [Å] for Cd₂Re₂O₇

300K		
Re-O1	1.927(3)	
Re-O1	1.927(3)	
Re-O1	1.927(3)	
200K		
Re-O11	1.932(6)	
Re-O12	1.926(6)	
Re-O13	1.932(6)	
Re-O14	1.925(6)	
<Re-O>	1.9298	
120K		
Re-O11	1.935(7)	
Re-O12	1.925(5)	
Re-O13	1.935(8)	
<Re-O>	1.9316	