ESRF

Experiment title:
EXAFS study of the supersonic phase transition in Silver Iodide

Experiment number:
HC-347

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Names and affiliations of applicants (*indicates experimentalists):

G. Dalba*, P. Fornasini*, R. Grisenti*
INFM, Dipartimento di Fisica, University di Trento, 1-38050 Povo (Trento), Italy
F. Rocca*
Centro CNR-ITC di Fisica degli sati aggregati e impianto ionico, 1-38050 Povo, Italy

Report:

EXAFS was measured at the Ag K edge in AgI as a funtion of temperature from 77 K to 480 K. The final aim was to obtain a better understanding of the mechanism of the β to α supersonic phase transition, expected at about *420* K. The k-range of the EXAFS signal extended up to 20 $Å^{-1}$. The 1st-shell contribution was separated by Fourier filtering. A separate analysis of phase differences and logarithm of amplitude ratio was done by the cumulant method. The preliminary results (even cumulants from the amplitude analysis) are here summarized.

When the data analysis is limited to $k_{max}=10\ Å^{-1}$, the 2nd and 4th cumulants regularly grow with temperature (C_2 following an Einstein law, C_4 a cubic parabola) [Fig. 1] in good agreement with previous results at the Ag K edge in β phase (ref. [1]); the behaviour at the phase transition is consistent with the one previously found at the I L3 edge (ref. [2]). An analysis extended beyond $k_{max}=10\ Å^{-1}$ cannot be limited to the 4th cumulant for temperatures higher than 300 K due to the poor convergence properties of the cumulant series of the highly asymmetric distribution of distances [1]. The good quality of experimental data allowed to extend the amplitude data analysis up to 16.5 $Å^{-1}$ by including also the 6th cumulant. The 2nd and 4th cumulants [Fig. 2, triangles] are in remarkably good agrement with the cumulants obtained from the analysis limited to 10 $Å^{-1}$ [Fig. 2, *circles]; also the* temperature dependence of the 6th cumulant is

meaningful.

A few conclusions can be drawn from these still preliminary results:

a) good quality data can be measured up to high k values also at high temperatures in AgI, guaranteeing a meaninfull use of higher order cumulants;

b) the regular temperature dependence of cumulants in β phase suggests that disorder is of purely thermal nature, with high enharmonic contributions;

c) the relatively small variations of cumulants at the phase transition previously observed [2] are confirmed.

[1] G. Dalba, P. Fornasini, R. Getter, and F. Rocca, Phys. Rev. B 52 (1995) 149.

[2] G. Dalba, P. Fornasini, R. Getter, S. Cozzini, M. Ronchetti, F. Rocca, Solid St. Ionics 69 (1994), 13.

Fig. 1: reference 77 K.
Cumulant analysis 3.5 - 10 Å^{-1}

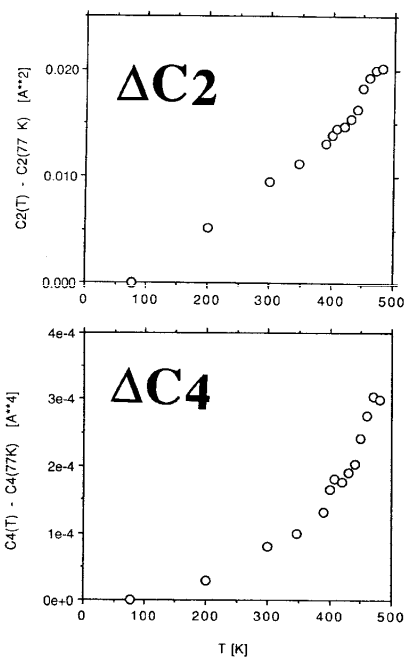

Fig. 2: reference 400 K
Cumulant analysis 3.5 - 16.5 Å^{-1}