	Experiment title:	Experiment number:
	Temperature dependence of the degree charge order in Yb_4As_3	HE 1213
Beamline: BM28	Date of experiment: from: 1.5.2002 to: 5.5.2002	Date of report: 23.4.2003
Shifts: 12	Local contact(s): Danny MANNIX	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Urs Staub SLS, Paul Scherrer Institut, Switzerland

Bruce Patterson SLS, Paul Scherrer Institut, Switzerland

Clemens Schulze SLS, Paul Scherrer Institut, Switzerland

Report:

Electronic charge localization leading to metal-insulator type of phase transitions has attracted great interest in the past. A particular interesting material is Yb_4As_3, where a first order charge order transition is observed at approximately 290K. The charge order in Yb_4As_3 leads to a structural phase transition from cubic ($I\bar{4}3d$) at ambient temperatures to hexagonal; R3c symmetry below T_{CO}. At ambient temperatures, chemical considerations assuming As^{3-} lead to an intermediate valence of Yb of 2.25. In this work we have performed a resonant X-ray scattering on a strained crystal to obtain direct information on the temperature evolution of the charge order.

The energy dependence of the integrated (330) reflection is presented for different temperatures in figure 1. These data have been collected with use of polarization analysis and correspond to the unrotated light in the □□□ channel. No intensity could be detected in the □□□channel, indicating the charge origin of the reflection. These data show that at the maxima located at 8941 eV, there is almost

no temperature dependence between 12 and 150K. The temperature dependence at lower energies, e.g. off resonance at 8900 eV, is significantly larger, even though it is still small. In a previous study, the energy dependence of this reflection was described by to be simply proportional to $(f_a\text{-}f_b)^2$ with f_a and f_b corresponding to the scattering factors of the Yb^{2+} and Yb^{3+} ions, respectively. The contribution of the movement of the ions within the unit cell originated by the charge ordering has been neglected. Now, with the true crystal structure at hand (HE1171), the energy dependence of this reflection is calculated and the result is shown in figure 2. The observed data have been corrected for absorption. The qualitative agreement shows that the intensity at resonance is still dominated by difference of $f_a\text{-}f_b$ squared as previously assumed. However, off resonance, the observed intensity is significantly larger than that obtained from the calculation. The energy dependent calculation shows a peak that is less sharp and more symmetric compared to the observed one. These deviations are likely caused by the imperfect first principle calculations of the energy dependent scattering factors. They may overestimate the width of the white line feature for the imaginary parts of the scattering factors (XANES), which would directly lead to a narrower peak in the energy dependence. This is would also lead to an increase in the ratio between the on resonant and off resonant intensity as observed in the experiment.

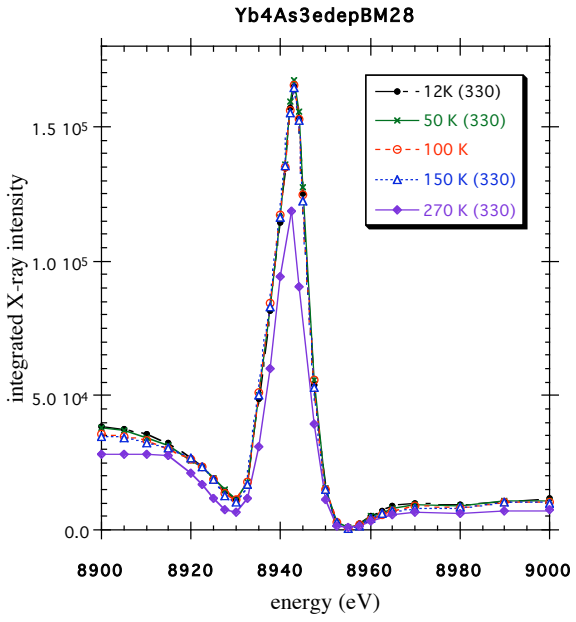

Fig. 1 Energy and temperature dependence of the (330) reflection.

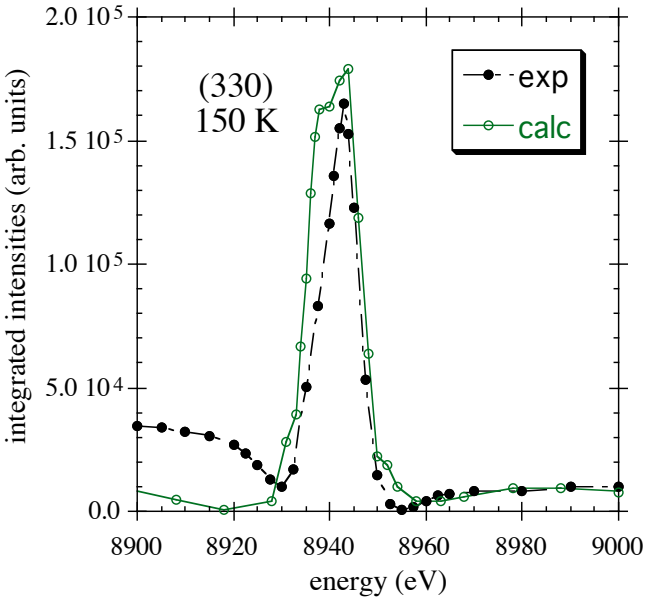

Fig. Energy dependence of the (330) reflection (experiment and calculation).