ESRF	**Experiment title:** Local structure around Ge substitutional impurities in Ag	**Experiment number:** HS529
Beamline: BM29	**Date of Experiment:** from: 17-Jan-1998 to: 21-Jan-1998	**Date of Report:** 22-Aug-1998
Shifts: 12	**Local contact (s):** A. Filipponi	*Received at ESRF:* 31 AOUT 1998

Names and affiliations of applicants (*indicates experimentalists):

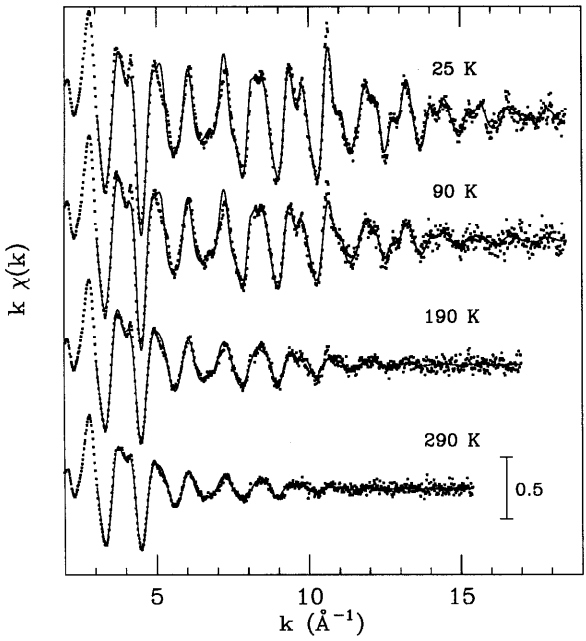
*A. Filipponi - Dipartimento Di Fisica, Università dell' Aquila, I-67010 Coppito L' Aquila - Italy
*M. Borowski - E.S.R.F., B. P. 220, F-38043 Grenoble - France
*F. Natali - E.S.R.F., B. P. 220, F-38043 Grenoble - France

Report:

We have collected high quality fluorescence-yield x-ray absorption spectra of substitutional Ge impurities in Ag. Samples were prepared under high purity conditions in a high vacuum furnace by alloying suitable amounts of Ge and Ag in graphite crucibles. The present measurement were performed on an Ag(l.5% Ge) sample which has been equilibrated for several hours at high temperature. With such a concentration the Ge impurities can be considered virtually isolated in the Ag f.c.c. lattice.

The sample quality was checked by x-ray diffraction and resulted to be a single phase f.c.c. structure with no residual c-Ge impurities within the sensitivity of 2 x 10^{-4}. Moreover a direct comparison between the diffraction patterns of Ag:Ge and Ag collected with a resolution of $\Delta\theta$ = 0.03 degrees full width at half maximum revealed a lattice expansion of about 10^{-4} in agreement with the expected behaviour.

X-ray absorption spectra have been collected with a fine energy sampling at constant Δk = 0.03 $\AA^{-1}$ intervals up to the highest energies where the signal was expected to be visible. Measurements were taken at 25 Ii, 90 Ii, 190 Ii, and 295 K in a closed-cycle He cryostat. The fluorescence signal was detected with a 13-element solid state detector with energy discrimination to eliminate scattering and spurious Ag fluorescence counts. The small concentration makes the distortion due to self-absorption effects negligible, still however it is sufficient to provide an excellent fluorescence signal. Successive spectra have been accumulated during several hours at each temperature point to achieve a total of about 10^7 counts above edge resulting in a noise to signal ratio of about 3x 10^{-4} in the EXAFS signal.



EXAFS spectra have been analysed in the framework of a multiple-scattering analysis [l] including contributions up to the fifth neighboring shell.

Specific multiple scattering signals were included in the modelling of the Ge-Ag-Ag contributions for the third and fourth shells. The agreement between model and experimental signals can be appreciated in the above figure. The structural parameters have evidenced local distortions from the ideal f.c.c. lattice. In particular the first neighbour Ge-Ag bond is slightly contracted with respect to the ideal lattice, whereas the Ag-Ag bonds connecting first and third (or fourth) shell atoms is expanded. These findings reconcile the paradox of a small impurity atoms producing an average expansion of the lattice. These results, which are presented in details elsewhere [2], demonstrate the possibility to investigate by a multiple-scattering EXAFS analysis the local structure around substitutional impurities in solids beyond the first neighbour shell. These findings open the way to further experimental and theoretical investigations.

[l] A. Filipponi, A. Di Cicco, and C. R. Natoli, Phys. Rev. B 52, 15122 (1995).
A. Filipponi and A. Di Cicco, Phys. Rev. B 52, 15135 (1995).
[2] A. Filipponi, M. Borowski, and F. Natali, Europhysics Letters (submitted 1998).