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X-ray fluorescence holography studies for an ordered and disordered Cu_3Au crystal

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X-ray fluorescence holography (XFH) is a three-dimensional method of atomic structure imaging. The fine structure in directional dependence of fluorescence yield originates from an interference of the beam incident on the sample with waves scattered at the atomic sites [1]. Element sensitivity for multi-component crystals is feasible by measuring distinct fluorescence from particular kind of atoms. However, recently it was demonstrated that matrix effects, such as beam attenuation and indirect excitation result in losing chemical resolution, therefore a numerical correction for these effects is required [2].

In this work we demonstrate the XFH analysis performed for a Cu_3Au (001) single crystal sample in ordered and disordered phase. In the ordered $L1_2$ phase Cu atoms occupy three non-equivalent positions, therefore the measured signal is the sum of the three different local structure. The disordered fcc phase poses the same position of atoms as the ordered one but differ in the average occupancy of the atomic sites. This makes Cu_3Au an ideal test sample to demonstrate sensitivity of XFH to the change of site occupancy.

In the experiments we used a tabletop setup equipped with a low-power 50 watt Mo tube combined with collimating polycapillary optics and HOPG monochromator [3]. Cu K and Au L fluorescence spectra were collected using an energy resolved silicon drift detector. The transition from the ordered to the disordered phase was carried out through annealing and quenching the ordered sample. An x-ray fluorescence and a ToF-SIMS analysis showed that during this procedure polycrystalline thin Cu_2O layer precipitated on the sample. We show that the matrix effects correction restores chemical resolution in the XFH maps as well as it is able to remove the influence of the top layer.

Figures 1(a) and 1(b) show XFH maps recorded for Cu_3Au sample. Because of the similarity between $L1_2$ and fcc structures, the difference between the XFH maps recorded for different phases is small [figure 1(a)]. However, subtraction of Au and Cu maps [figure.1 (b)], clearly demonstrates the differences in the experimental data.

Figures 1(c) and 1(d) present electron density maps reconstructed from XFH data. The plots demonstrate full three-dimensional reconstruction of atomic positions. Moreover, the intensities of maxima agree with the theoretical electron density at the given atomic sites. This indicates the possibility of direct and precise determination of atomic sites occupancy using XFH.

The possibility of performing XFH experiments using a low power laboratory x-ray source reveal the possibility of future x-ray holographic experiments at SOLARIS [4].

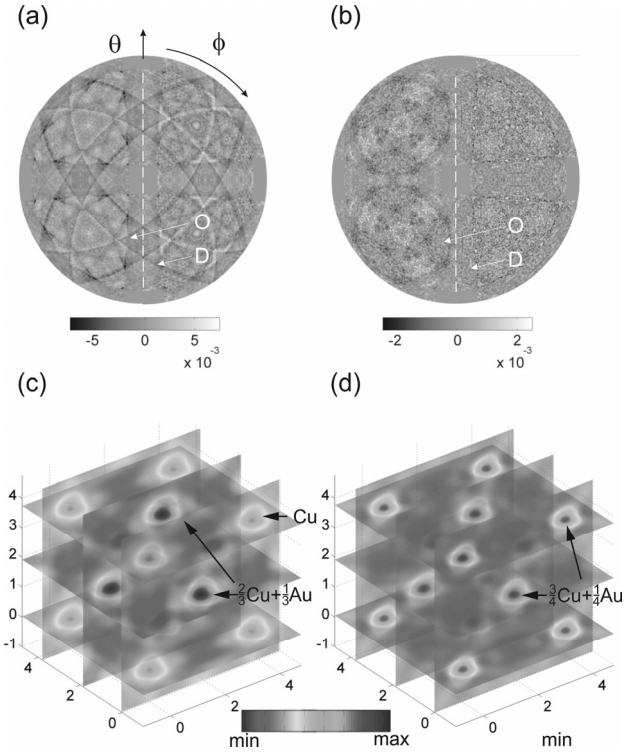

Figure 1. (a) XRF hologram recorded by measuring Cu fluorescence. (b) Holographic data obtained by subtraction of XRF holograms recorded for Cu and Au. (O, D) denotes ordered and disordered phase, respectively. (c,d) Three-dimensional linear regression reconstruction of the electron density from XFH maps recorded for Cu fluorescence from ordered (c) and disordered sample (d). Labels describe the theoretical average occupancies of atomic sites.

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