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X-Ray Diffuse Scattering Holography of a Mn-doped GaAs layer

The experiment was carried out on the material science beamline ID11 at European Synchrotron Radiation Facility. X rays of energy 30 keV were chosen in order to achieve good spatial resolution in the reconstructed image. The small layer thickness required the measurements to be carried out with a condition of total reflection in order to hinder penetration of incident x-ray photons into the bulk. The beam was incident on the sample at were recorded on a 16-bit CCD the grazing angle of 0.7 deg., i.e. slightly below the critical angle. Scattering patterns were recorded on a camera FreLon2k16 covering 94×94 mm^2 detection field using 2048×2048 pixels of the size of 46×46 μm^2. It was possible to measure diffuse scattering patterns from different parts of the wafer under identical geometrical conditions. The experiment itself consisted of the collection of two high precision diffuse scattering patterns: the first one from the GaMnAs layer and the second one from the GaAs substrate on the etched half of the same wafer.

Specifically, in the case of GaMnAs layers, the diffuse scattering pattern of a doped layer is compared to that of GaAs. Fig. 1(a) shows the simulated hologram calculated as a difference of simulated diffuse scattering pattern of eight unit cells of GaMnAs containing a Mn atom in a substitutional position and those of undoped GaAs of the same volume. The axes of the images correspond to the crystallographic axes of the sample and a photon energy of 30 keV was used for the calculation. A real-space image of a plane (100) reconstructed from this hologram exhibits peaks in the positions of neighbouring gallium atoms (Fig. 1(b)). A similar hologram of a cluster of GaMnAs with Mn atom in the interstitial position with fractional coordinates ½, ½, ½ and the reconstructed image of the nearest neighbours of the Mn atom are depicted in Fig. 1(c) and (d), respectively. Evidently, the difference of diffuse scattering patterns of GaMnAs and GaAs depends essentially on the site of the manganese atom. Its real-space

reconstruction provides the local atomic structure around the dopants, making it possible to distinguish between the substitutional and interstitial Mn sites.

The diffuse scattering pattern of GaMnAs as recorded on the CCD detector is shown in Fig. 2(a). The same pattern of a bulk GaAs was measured under identical geometrical conditions. Fig. 2(b) shows the difference of these intensity patterns, equal to the real part of the hologram [Kopecký, M. (2004). *J. Appl. Cryst*. **37**, 711-715], transformed to the co-ordinates of wave vectors; it is a top view on a spherical cap in the reciprocal space. The bottom half of the image originally shielded by the sample was completed using known sample symmetry. Three selected planes of atoms parallel to the (001) crystallographic plane were reconstructed using Helmholtz-Kirchhoff integral theorem (Fig. 3).

In summary, the positions of manganese atoms doped in a thin GaMnAs layer were determined by means of x-ray holography with atomic resolution and found that the closest neighborhood of Mn atoms corresponds to Mn atoms in substitutional positions. No evidence of interstitials was observed. At the given Mn content of 0.02, this result is in agreement both with theoretical predictions [Jungwirth, et al.(2005). Phys. Rev. B72, 165204(1-13] and with experimental data on lattice constant expansion of Mn doped GaAs [Zhao, et al. (2005). Appl. Phys. Lett. 86, 071902(1-3)]

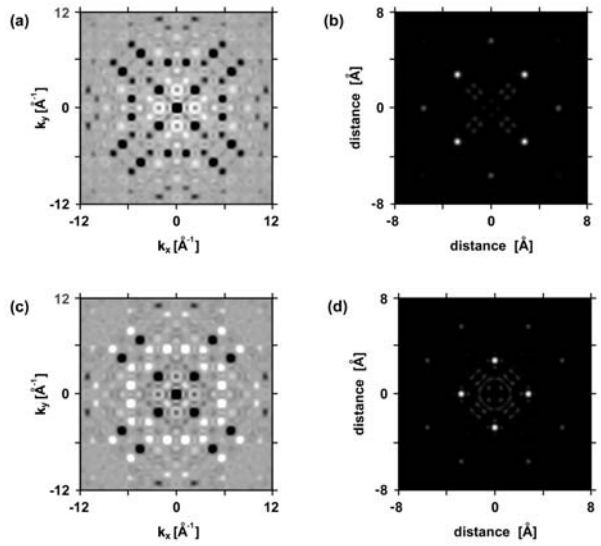

Figure 1

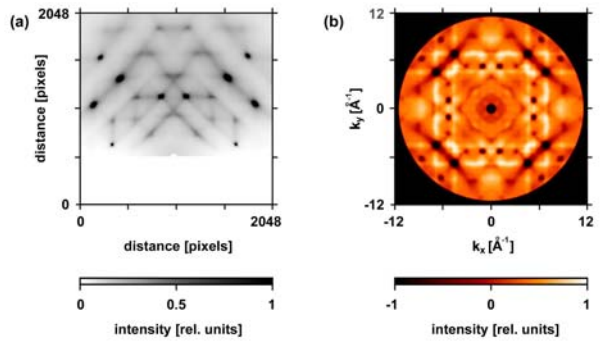

Figure 2

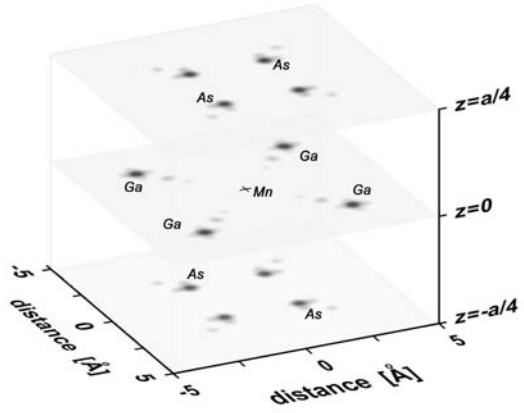

Figure 3