

## Where does Pauling's bond length interconnect with Vegard's law in a mixed crystal? : An x-ray Fluorescence holographic study

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### Introduction

In order to bridge experimental results for the atomic structure in mixed crystals between x-ray diffraction (XD) showing a Vegard's law [1] and x-ray absorption fine structure (XAFS) indicating preservations of each Pauling's bond length [2], an x-ray fluorescence holography (XFH) experiment was carried out on  $\text{Zn}_{0.4}\text{Mn}_{0.6}\text{Te}$  single crystal for drawing a three-dimensional (3D) atomic image around the Zn atom [3].

### Experimental procedure

The  $\text{Zn}_{0.4}\text{Mn}_{0.6}\text{Te}$  and ZnTe single crystal samples were grown by a Bridgeman method. The XFH holograms were recorded at nine incident x-ray energies of 11.0-15.0 keV in steps of 0.5 keV, and the 3D atomic image was constructed using Barton's algorithm [4] by superimposing the holograms, which can highly suppress the false twin images.

### Results and discussion

An example of the obtained 3D atomic images around the Zn atoms was given in Fig. 1 of Ref. [5]. The images of the first neighbor Te atoms appear at the proper positions assumed by the XAFS [2] within the error bars.

Solid and empty circles in Fig. 1 indicate the image intensities of the Te atoms on the (100) plane in  $\text{Zn}_{0.4}\text{Mn}_{0.6}\text{Te}$  and ZnTe, respectively. As shown in the figure, the image intensities in ZnTe gradually decreases with increasing the distance from the central Zn atom. On the other hand, those at the first, third, and fifth neighbor Te atoms are highly suppressed in the mixed crystal  $\text{Zn}_{0.4}\text{Mn}_{0.6}\text{Te}$ .

The magnitude of the XFH image intensity highly depends on the positional randomness of the atoms.

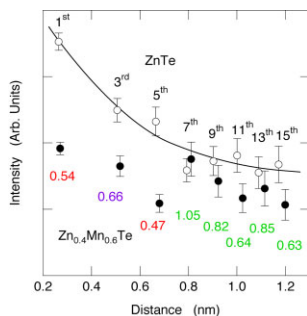


Fig. 1 The image intensities of Te atoms on the (100) plane in  $\text{Zn}_{0.4}\text{Mn}_{0.6}\text{Te}$  and ZnTe.

Since the XD result shows the sharp Bragg peaks even for the mixture [1], we started to consider a model by assuming that each atom always locates on a sphere with a distance from averaged lattice position,  $d_{\text{dis}}$ , and fluctuates from the sphere with a proper mean-square displacement obtained from the XAFS [2].

Figure 2 shows the  $d_{\text{dis}}$  dependence of the image intensity of Te atoms normalized with respect to the  $d_{\text{dis}} = 0$  values, i.e., the values of the perfect ZnTe crystal. The averaged intensity ratio for the distant Te atoms beyond the seventh is about 0.73, which corresponds to  $d_{\text{dis}} \sim 0.014$  nm as indicated by the circles on the solid curve. The first neighbor Te atom, where only the angular fluctuation is taking into account with a cross atomic configuration, gives a similar  $d_{\text{dis}}$  value of 0.016 nm indicated by the circle on the dotted curve.

In conclusion, the present XFH measurement has successfully observed the lattice distortion in the  $\text{Zn}_{0.4}\text{Mn}_{0.6}\text{Te}$  mixed crystal in the intermediate range, and built bridges between that farsighted XD [1] and the nearsighted XAFS [2] measurements at about five neighbors.

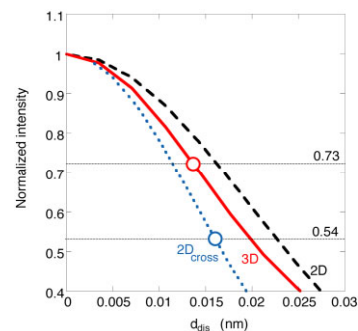


Fig. 2 The  $d_{\text{dis}}$  dependence of the normalized XFH intensity of the Te atoms.

### References

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