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Detection of vancancies by using XAS, is it possible? The case of ZnO

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The occurrence of high temperature ferromagnetism (HTFM) in transition-metal-doped ZnO systems has attracted much attention in the last years. In particular, the Mn–Zn–O system has been widely studied and large efforts have been aimed at finding Curie temperatures above room temperature (RT). However the origin of that magnetic behaviour has not been explained yet. While doubts rise about the role of the 3d cations, several types of defects, such as oxygen and zinc vacancies, as well as hydrogen, oxygen and zinc interstitials, have been proposed by different authors to induce HTFM [1]. Aiming at determine the exact type of defect that causes the HTFM in these systems several experimental tools, such as x-ray absorption spectroscopy, have been applied. However, based on similar experimental spectra, different authors report opposing conclusions regarding the nature of defects involved in the observed HTFM [2,3]. These results pose serious doubts about the real capability of XAS to determine the presence of vacancies in these systems and, consequently, to shed light on the origin of the magnetism in these systems. Here we report a XANES study at both Mn and Zn K-edges in Zn(0.95)Mn(0.05)O thin films prepared with different sputtering gases (pure Ar, Ar/N2 and Ar/O2). We have studied the local order around Mn in the films, by means of ab initio XANES calculations. During this study, a special emphasis has been paid to determine the role played by both vacancies and structural distortions associated with the substitution of Zn by Mn in the ZnO host. Our results indicate that XANES is not sensitive to the presence of randomly distributed vacancies. On the contrary, the observed modifications of the XANES spectra are associated with the structural distortion around Mn sites, which rules the magnetic behaviour of these Mn:ZnO thin films in terms of the different sputtering gases involved in the preparation.

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