Contribution ID: **77** Type: **Poster**

Comparative study of local structure for sputter deposited nitrogen doped zinc oxide thin films

Incorporation of N anion into ZnO crystal has been known to induce structural distortion and can cause dramatic change in its electronic structure. It has been reported that thin films with great variance in crystallinity and electrical properties such as highly crystalline p-type or amorphous high carrier mobility n-type ZnO films can be achieved by particular growth control of N doped ZnO or zinc oxynitride thin films using reactive sputtering deposition. In this work, we measured x-ray absorption spectroscopy (XAS) near Zn K edge energy to probe local atomic environment around Zn atom for nitrogen doped ZnO thin films, aiming at examining structural profile for those films by fitting variable to their extended x-ray absorption fine structure (EXAFS). Thin film samples were prepared using variety of RF magnetron sputtering depositions in order to investigate an influence of preparation method on the local structure. ZnO target sputtered with either continuous or gas timing flow of Ar and N2 reactive gases were utilized to coat thin films of undoped or nitrogen doped ZnO on a silicon substrate. The other samples were deposited on a glass substrate at high partial pressure of N2 with Zn target. XRD results confirmed that the deposited films were in Wurtzite ZnO crystalline phase. For EXAFS analysis, variables for the Wurtzite ZnO model were found reasonably fitted to each EXAFS spectrum within a range covering 2 nearest neighbor atomic shells surrounding the Zn center atom, thus details on Zn-O (or Zn-N) and Zn-Zn bond lengths, variance of atomic position attributed from structural disorder, and amplitude factors relevant to the number of atom on each scattering shell were extracted. Typically, it was found that N doped samples posed high degree of structural disorder and similar anion to cation ratio in opposition to the undoped ZnO. The thin film prepared with high partial pressure N2 gas tended to have relatively large bond lengths and low density of anion and cation in the Wurzite structure which could be due to the presence of other zinc oxynitride phase mixed in the sample. With an assist of principal component analysis (PCA), samples could be classified into groups according to the fitting variables. For example, N doped samples deposited using ZnO target could be grouped together, where as an undoped sample and the others were well distinguished. This study quantified structural feature for selected N doped thin film and suggested a rough guide on applying reactive gas sputtering deposition for tailoring local structure of the deposited film.

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Track Classification: Other related topics