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Nondestructive Characterization of Atomic Profiles in Layer-Structured Photovoltaic Materials Using the Method of Angular Dependence of X-ray Fluorescence(ADXRF)

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Abstract

Angular dependence of x-ray fluorescence technique has been applied to the study of atomic density profile in composite systems. This method is shown to be useful for probing the microstructures and intermixing of constituent elements in layer-structured photovoltaic materials.

I. **Introduction**

It is well known by now that further development of advanced photovoltaic (PV) technology will make extensive use of layer-structured materials. This approach will depend crucially on the technical capability to prepare layer structures with high quality interfaces. To this end, a clear understanding and quantitative characterization of the microscopic structure and density profile around the inferfacial region would seem highly desirable. A basic problem in this area of research still remains unsolved is the intermixing of constituent elements across the interfaces. An example can be found in the case of CdS/Cu(In,Ga)Se_2 heterojunctions. This class of PV materials has already demonstrated a record high efficiency of 18.8%; however, the problem of microstructure and intermixing of atoms around the heterointerface is still poorly understood.

Recent development of the technique of angular dependence of x-ray fluorescence (ADXRF) using synchrotron radiation has shown that it is very useful for nondestructive characterization of layer-structured CdS/CdTe PV materials.[1, 2] This method is element-specific and nondestructive, it can provide valuable information about the density profile of selected elements in a composite system, thus is particularly useful for the study of element intermixing across the interfaces. In essence, when an x-ray beam impinges on a layer structure, its penetration depth varies from nanometers to micrometers as the grazing incidence angle passes through the critical angle of the material, the fluorescence yield (FY) of a specific element measured as a function of angle can therefore provide information on the depth profile of that selected element in the material. For a multilayer material consisting of very thin films, the x-ray FY can be described by the following equation[3]:

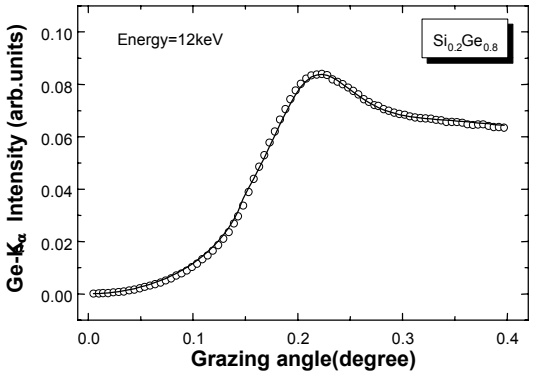
$$I_{aj} \propto C_{aj} \rho_j D_j \mid E^t_j + E^r_j \mid^2 \qquad (1)$$

where I_{aj} is the primary x-ray fluorescence intensity of a particular element a in layer j, C_{aj} the mass fraction of element a in layer j, ρ_j the density of layer j, D_j the thickness of layer j, E^t_j and E^r_j the transmitted and reflected fields at the top of layer j, which are functions of the roughness σ, and the incidence angle θ. By a comparison of the calculated and measured FY, information about the depth distribution of selected elements in the layer material can be obtained.

II. **Examples of ADXRF Applications**

A typical ADXRF result is shown in Fig. 1. In this figure, the Ge-K_α FY is plotted as a function of grazing incidence angle for a SiGe layer grown on Si(100) by molecular beam epitaxy. The nominal concentration of Ge is 80%, and the nominal thickness is 150Å. The data were taken at Beamline X3B1 at the National Sybchrotron Light Source using x-ray photon energy of 12 keV. The solid line

Fig.1. Typical ADXRF for a SiGe layer grown on Si(100). The raw data (open circle) are fitted with theoretical calculation (solid line) based on equation (1).



in Fig.1 is a fit to the raw data by using Eq. (1). From the close agreement between theory and experiment, the actual Ge concentration of the SiGe layer has been determined to be 56% throughout the entire SiGe layer. This corrected Ge concentration is also consistent with other experimental results including x-ray diffraction and x-ray absorption fine structure (XAFS) obtained with the same sample.

The problem of element intermixing in a CdS/$CuInSe_2$ junction has been investigated using the ADXRF method.[4] Figure 2 shows some preliminary data taken with x-ray energy at 28keV.

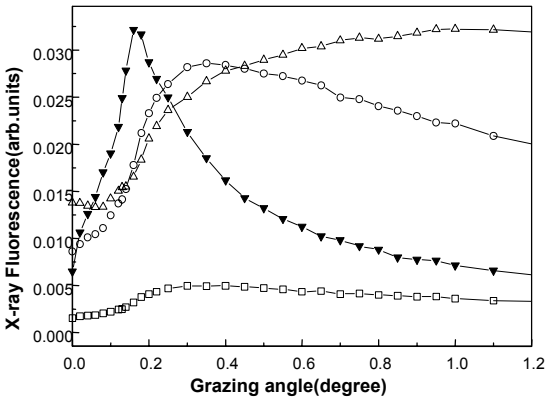


Fig.2. ADXRF data for different elements in a CdS/$CuInSe_2$ heterojunction taken with incident x-ray energy at 28keV: In(triangles), Se(circles), Cu(squares), and Cd(inverted triangles). All the data are subject to a geometrical factor correction.

While detailed quantitative analysis of these results are in progress, it is useful to compare the experimental results with a simulation of the Cd FY in this system. In Fig. 3, the angular dependence of Cd-K_α FY is shown for the cases with and without a 10% Se diffusion from the bulk $CuInSe_2$ to the CdS top layer. For simplicity, the Se atoms are assumed to be uniformly distributed in the CdS layer. The gross feature of these curves are seen to be similar to the Cd FY data shown in Fig. 2 (after a geometrical factor correction). This example also shows the sensitivity of the

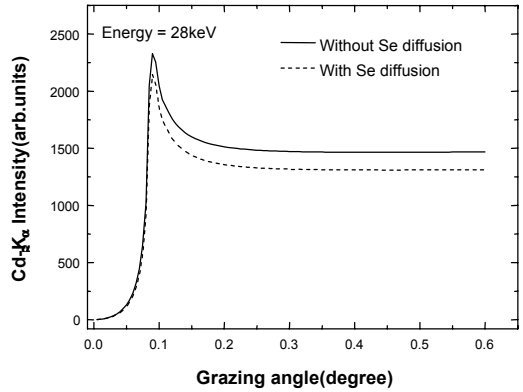


Fig.3. Simulation for Cd-K_α FY profile in a CdS/$CuInSe_2$ heterojunction : (a)without Se diffusion into the CdS layer (b)with 10 % Se diffusion into the CdS layer.

ADXRF method for detecting changes in the density profile of selected elements. When this plot is analyzed in conjunction with a similar plot for Se FY, more detailed information about Se diffusion can be obtained. Likewise, the same technique can be applied to probing the density profiles related to the diffusion of Cu or In into the CdS layer, and S or Cd into $CuInSe_2$.

III. **Conclusion**

In summary, we have demonstrated by way of examples that the ADXRF technique can be conveniently applied to studying the changes in density profiles of selected elements in a composite system. This method is therefore specifically useful for investigating the problems of atomic profile and element intermixing in layer-structured PV materials.

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IV. **References**

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