Compositional intermixing at CdS/Cu(In,Ga)Se$_2$ rough interface studied by x-ray fluorescence

S. Kim, Y. L. Soo, G. Kioseoglou, and Y. H. Kao

Department of Physics, State University of New York at Buffalo, Amherst, New York 14260

K. Ramanathan and S. K. Deb

National Renewable Energy Laboratory, 1617 Cole Blvd., Golden, Colorado 80401

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The effects of compositional intermixing and high interfacial roughness in a series of CdS/Cu(In,Ga)Se$_2$ heterojunctions have been investigated using the technique of angular dependence of x-ray fluorescence. In the present case, the average interfacial roughness actually exceeds the nominal thickness of CdS film. A method of data analysis has been worked out to account for the large roughness and this technique allows a possibility of nondestructive determination of the concentration profile of both CdS and Cu(In,Ga)Se$_2$ as well as the effective roughness parameters in the system. © 2002 American Institute of Physics.

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I. INTRODUCTION

Advances in modern photonic and electronic devices depend crucially on the capability to control the physical and chemical properties of layer-structured semiconductors. To this end, a fundamental understanding of the morphology of interfaces in multiplayer systems is needed.\(^1\) This problem is especially important for the development of thin film materials for photovoltaic (PV) applications.\(^2\) However, many currently available techniques for probing the microscopic structure of buried interfaces in layered materials are inevitably detrimental or abrasive, making it difficult to reliably characterize the interface morphology for as-made specimens or materials after special processing needed in actual device applications. Development of nondestructive methods for characterizing buried interfaces would seem highly desirable.

X-rays from synchrotron radiation now afford many useful approaches for probing the atomic depth profile and morphology of buried interfaces, as well as defects in layer-structured materials. To examine the compositional depth profile without perturbing the material structure under study, the angular dependence of x-ray fluorescence (ADXRF) technique is particularly useful. This nondestructive method is also element specific, well suited for probing the depth profile of selected atomic species in complex systems. It can therefore be employed for solving the problem of ubiquitous intermixing of constituent components across the heterointerfaces, as usually found in some advanced layer-structured PV materials.

In comparison with other existing methods such as scanning transmission electron microscopy (STEM)\(^3\) and secondary ion mass spectrometry (SIMS)\(^4\) most commonly used for interface characterization, this x-ray technique offers many outstanding advantages, e.g., (i) Nondestructive probing of buried microstructures, (ii) No need for a vacuum enclosure, suitable for large-scale on-line evaluation of PV materials, and (iii) Continuously variable x-ray probing depth from about 3 nm to microns controlled by varying the incidence angle and wavelength of the x-rays, allowing the possibility to examine deep buried layers even for interfaces with high roughness. Since little attention has been given so far to quantitatively determine the concentration profile for rough surfaces, we have applied the ADXRF technique to investigate the rough interface formed between thin films of CdS and Cu(In,Ga)Se$_2$; this class of material now holds a record of highest sunlight conversion efficiency in practical solar cell applications.\(^5\)

II. EXPERIMENT

The Cu(In,Ga)Se$_2$(CIGS) thin films were grown at National Renewable Energy Laboratory (NREL) by a three-stage process as described in detail elsewhere.\(^6\) For the present synchrotron radiation experiment, CIGS thin films of about 2.5 \(\mu\)m in thickness were grown on Corning 7059 glass substrates. The resulting films were compositionally very similar to the ones used in the fabrication of high efficiency solar cells.\(^6\) For the purposes of comparison and also for calibrating the x-ray fluorescence intensities, a prototype CIGS sample (S1694-1) was made with a CIGS thin film coated on Corning 7059 glass. For sample S1694-2, a thin layer of CdS with a thickness approximately 40 nm was deposited on the CIGS film as prepared in the previous sample, using an aqueous solution containing 0.0015 M CdSO$_4$, 1.5 M NH$_4$OH, and 0.15 M thiourea at 60 °C. The sample S1694-3 was prepared by the same procedure as for S1694-2, but subjected to a postgrowth heating at 200 °C in air for 5 min.

The x-ray experiments were performed at beamline X3B1 of the National Synchrotron Light Source (NSLS) in Brookhaven National Laboratory. A schematic diagram of the experimental setup is shown in Fig. 1. The energy of incident photons was selected by using a Si(111) double-crystal monochromator. A two-axis goniometer with angular...
resolution of 0.001° was used to control the grazing incidence angle between the incident x-ray beam and the sample surface. The x-ray fluorescence photons from the irradiated samples were collected by using an energy-dispersive solid state Si(Li) detector and the intensity of Se Kα or Cd Kα was measured as a function of incidence angle using a single-channel pulse-height analyzer. All the ADXRF measurements were taken with x-ray photon energy of 28 keV.

III. STUDY OF LAYERED-STRUCTURE WITH THE ADXRF METHOD

For some thin-film solar cell systems, such as heterojunctions formed between CdS and single crystals of CuInSe₂ (CIS) and those between CdS and CdTe, the interface is rather smooth and the ADXRF analysis can usually be aided by measurements of grazing incidence x-ray scattering (GIXS) which provides direct information on the interfacial roughness as well as the layer thickness. A combination of these two techniques can be very useful for probing the interface morphology, as demonstrated in our previous experiments.7,8

In the present case, however, the interfacial roughness in our CdS/CIGS heterojunctions is usually around several hundred angstroms. This roughness is actually comparable to or even become greater than the thickness of the CdS film deposited. Such a high interfacial roughness, usually coupled with intermixing of elements, leads to the presence of a transitional region with high density variations of the constituent components CdS and CIGS. In the interface region, the material density varies with depth. Since the refractive indices are functions of density, a simple critical angle can not be defined in this case. To overcome these difficulties, a method to incorporate the density variation is needed for treating the optical properties in the transitional region of high interfacial roughness [see Sec. B of Appendix]. A comparison of the ADXRF data with this type of model calculations then affords a method to probe the concentration profile of a selected atomic species (CdS or CIGS) in the present case. Using this model, we are now able to characterize the compositional variation around the interface and also taking into account the effects of high interfacial roughness.

IV. THEORETICAL BACKGROUND

The ADXRF technique has been established in the past decades as a nondestructive, element-specific probe for concentration depth profiling based on the fact that the x-ray penetration depth changes from nanometers to micrometers when the angle of incidence passes through the critical angle. Since the first report on grazing incidence x-rays for spectrochemical analysis of solid samples made by Yoneda and Horiuchi in 1971,9 many groups have extended this technique to a variety of applications including the determination of concentration profile,10 analysis of a small amount of material on top of an optically flat substrate,11 determination of contaminants on semiconductor wafers,12 study of impurity concentration distribution in bulk material,13 thin films and layer structures,14,15 methodological demonstrations of the technique,15,16 studies on rough surfaces,17,18 and theoretical analysis of the effects of x-rays on solids.14,19 However, quantitative concentration profiling for rough interfaces has not been well studied.

X-ray fluorescence intensity $I_a$ (number of photons emitted per unit area per unit time due to atoms of a selected element $a$), taking into account the absorption of radiation in the layer and neglecting the enhancement effects due to secondary fluorescence or absorption of fluorescence radiation, can be generally expressed as:14

$$I_a(\theta) \propto \int dz \left( -\frac{dS_a(\theta)}{dz} \right) \Phi_a(z),$$

where $\theta$ is the grazing incidence angle, $S_a$ is the $z$ component (perpendicular to the interface) of the Poynting vector, and $\Phi_a(z)$ is the concentration depth profile of a specific atomic species $a$ in the $z$ direction, i.e., $\Phi_a(z) = C_a(z)\rho(z)$, where $C_a$ is the mass fraction of element $a$ and $\rho$ the material density. The x-ray fluorescence intensity $I_a$ of element $a$ is proportional to the absorption of incident x-ray beam by sample ($-dS_a/dz$) and the concentration of the element $a(\Phi_a)$. Quantitative determination of x-ray fluorescence intensity thus requires a detailed knowledge of the field distribution (in terms of layer parameters such as density, elemental composition, and thickness) convoluted with the concentration profile in the layered structure. The functional dependence of x-ray fluorescence intensity on these parameters is nonlinear due to the variation of $S_a$, the x-ray fluorescence signals are thus sensitive to these parameters.

Consider a layer-structured system consisting of $N$ layers labeled $j = 1, 2, ..., N$, where the effects of $x$-rays on each layer are characterized by a complex refractive index $n_j = 1 - \delta_j - i\beta_j$. In an idealized situation, if the interfaces are all so smooth that the effects due to interfacial roughness can be neglected, the coefficients of reflection $r_j$ and transmission $t_j$ at the $j$th interface (between the $j$th and $(j+1)$th layers) can then be obtained from the well-known Fresnel’s formulas in optics:

$$r_j = (k_{z,j} - k_{z,j+1})/(k_{z,j} + k_{z,j+1}),$$

$$t_j = 2k_{z,j}/(k_{z,j} + k_{z,j+1}),$$

where $k_{z,j} = k\sqrt{n_j^2 - \cos^2 \theta}$ is the $z$ component of the wave vector in layer $j$, $k = 2\pi/\lambda$ is the modulus of the wave vector.
in a vacuum (layer $j=0$), $\lambda$ is the x-ray wavelength, and $\theta$ is the grazing angle of incidence. The transmitted field $E_j^t$ and reflected field $E_j^r$ at the interface $j$ can be found from the recurrence relations:

$$E_j^t = a_j^2 X_j E_j^t$$
$$E_j^r = a_j^2 E_j^t/(1 + a_j^2 + X_{j+1} r_j),$$

where $a_j = \exp(-i\theta k_{a,j}), d_j$ is the thickness of layer $j$, and $X_j = (r_j + a_{j+1} X_{j+1})/(1 + a_{j+1} X_{j+1} r_j), j = 0, 1, 2, ..., N-1$. For a very thick substrate, $X_N \approx 0$, since there is no need to consider the reflection occurring at its bottom.

For a layered system with rough interfaces, a Gaussian probability density with standard deviation $\sigma_j$ is commonly assumed to represent the root-mean-square deviation $\sigma_j$ of the $j$th interface atoms from a perfectly smooth plane such that

$$P_{\text{Gauss}}(z) = \frac{1}{\sqrt{2\pi \sigma_j^2}} e^{-z^2/2\sigma_j^2}. \quad (3)$$

It follows that the depth variation of the refractive index $n(z)$ between the $j$th and $(j+1)$th layers can be represented by an error function resulting from an integration over $z$ of the density probability $P_{\text{Gauss}}(z)$ in this region:

$$n(z) = n_j + \frac{n_{j+1} - n_j}{2} \text{erf}\left(\frac{z - z_0}{\sqrt{2} \sigma_j}\right). \quad (4)$$

Incorporation of interfacial roughness in a layered structure can be divided into two categories depending on the value of interfacial roughness by a criterion that $\sigma_j |k_{a,j}| < 1$ (low roughness) or $\sigma_j |k_{a,j}| > 1$ (high roughness). A more detailed description of the ADXRF method applied to the study of a multilayer structure, as well as techniques used for model calculations, is presented in the Appendix.

V. RESULTS AND DISCUSSION

The Se $K\alpha$ ADXRF raw data for the bulk CIGS and the two CdS/CIGS samples are shown in Fig. 2(a). The fluorescence intensity increases gradually with grazing incidence angle (or the penetration depth) of the x-rays, which actually indicates that the critical angle for the samples is not clearly defined due to the high density variation caused by the rough interfaces. As we expected from the field distribution, the observed Se $K\alpha$ intensity for the CIGS sample (S1694-1) is higher than that for the other two samples (S1694-2 and S1694-3) which are coated with a thin CdS layer.

The Cd $K\alpha$ ADXRF data are shown in Fig. 2(b). The fluorescence spectra show the following features characteristic of a thin film: a steep increase at low angles, a maximum, and a plateau. The small maximum around 0.09° arises from an interplay between the field distribution and the concentration variation of Cd atoms, as analyzed in the Appendix. The signal reaches a plateau at high angles since all the Cd atoms are exposed to the incident x-rays which have already penetrated throughout the entire system. By a comparison of the intensity levels at high angles between samples, sample S1694-3 shows more CdS and the distribution of CdS is deeper than that of sample S1694-2.

Calculations of the Se $K\alpha$ and Cd $K\alpha$ intensity for the samples studied have been performed using Eqs. (1)–(4), (A1) and (A2) (see Appendix) with a model for the concentration profile of the constituent components. By a comparison of the theoretical calculations with experimental data, the concentration profile of the components CdS and CIGS can be determined.

For the CIGS samples (S1694-1), $\Phi_S(z)$ in Eq. (1) is not a simple constant because of the high top surface roughness (or high density variation). This effect of surface roughness is illustrated in Fig. 3. If, in an idealized situation, the interface between CIGS and air is completely smooth, then the Se $K\alpha$ intensity should follow the dotted line in Fig. 3. The Se $K\alpha$ intensity is very low at angles below the critical angle of bulk CIGS, mainly caused by the evanescent wave near the surface, the x-rays start to penetrate deeper into the material when it reaches the critical angle, thus the result shown in the dotted line of Fig. 3 also serves as an indication of the photon flux distribution inside the material. However, the actual density variation of CIGS near the top surface most probably takes the form of an error function due to the roughness effect (as discussed more quantitatively in the Appendix), such a rough surface then allows the x-rays to penetrate into the material at low angles, and this leads to a gradual increase of fluorescence intensity below the critical angle (usually defined only for an ideal smooth surface, as indicated by a rapid rise of a calculated intensity shown by
the dotted line). At high incidence angles greater than 0.1°, the density distribution approaches that of a bulk CIGS and \( \Phi_{\text{Se}}(z) \) then becomes a constant in Eq. (1). Using the method described in the Appendix (Sec. B) the experimental ADXRF data (circles in Fig. 3) can be fitted quite well with the solid line pertaining to a rough surface using the parameters shown in Table I. This result shows that the ADXRF method is useful for determining the parameters in order to quantify the actual density variation of a material near its rough surface.

The Se \( K\alpha \) and Cd \( K\alpha \) data obtained with sample S1694-2 are shown in Fig. 4(a). The interpretation for Se \( K\alpha \) intensity shown in Fig. 4(a) is somewhat similar to Fig. 3, except that an additional CdS layer has been added on CIGS. Hence the Se \( K\alpha \) intensity starts to rise at a higher angle to allow the x-rays to penetrate through CdS and the fluorescence intensity of sample S1694-2 is naturally lower than that of the sample without CdS (see Fig. 2) due to the effects of attenuation.

The general shape of Cd \( K\alpha \) intensity is different from that of Se \( K\alpha \) intensity, because Cd atoms only reside in the CdS layer and in the interfacial region. For an illustration purpose, a model calculation for Cd \( K\alpha \) intensity arising from a smooth CdS layer of 400 Å in thickness with a uniform density on CIGS is shown as a dotted line in Fig. 5. Below the critical angle of the CdS layer, the Cd \( K\alpha \) intensity is low due to the evanescent fields. A steep rise occurs at the critical angle of this material, and it starts to decrease due to an interplay between the changes in penetration depth of the x-rays and the thickness of the CdS layer. At higher angles, the Cd \( K\alpha \) intensity shows a plateau because all the Cd atoms have already been exposed and yielded the same fluorescence. A shallow maximum therefore appears at an angle prior to the plateau region. All these features: a low intensity below the critical angle, a rapid rise, a maximum, and a plateau at high angles can be viewed as the generic characteristics of fluorescence intensity variation from elements contained in a thin film with low roughness.

For a CdS layer with high roughness on its surface and also at the interface with CIGS, the Cd \( K\alpha \) intensity starts to rise at low angles and more gradually as a function of the incidence angle. There also appears a shift of the maximum, mainly due to density variations in the mixture of CdS and CIGS. These changes are demonstrated by the solid curve in Fig. 5. It can be seen from the drastic differences between the solid and dotted curves in Fig. 5 that the ADXRF method is quite sensitive to the structural variations in the layered structure, thus it is useful for quantitative characterization of the interface morphology.
Simultaneous curve fitting to both the Cd Kα and Se Kα data requires iterative comparisons between the experimental data and theoretical calculations. In our data analysis, usually an initial model of the density variation \( \rho(z) \) and the composition profile \( C_i(z) \) of both constituents CdS and CIGS were assumed for each sample and followed by reiterative processes of adjusting the input parameters to reach a final satisfactory agreement between theory and experiment. The density variation and composition profiles in the mixture of CdS and CIGS are obtained from the final set of parameters. The solid lines in Fig. 4 were obtained by this procedure, and the agreement between experimental results and theoretical calculations is quite satisfactory. The data for sample S1694-3 is also in very good agreement with theoretical calculations (not shown here). The parameters obtained are summarized in Table I with the density variations and the concentration profiles of CdS and CIGS for sample S1694-2 shown in Fig. 6.

As shown in Table I, the average height of the density variation (or an effective interfacial roughness) is very high around 1000 Å for the CIGS sample S1694-1. For the two heterojunction samples S1694-2 and S1694-3 which are coated with a thin CdS layer, the density variations of the mixture of CdS and CIGS are much less than that of sample S1694-1. This may be due to a “filling effect” from the CdS layer. From the parameter \( S_{\text{com}} \) in Table I, which describes the composition of CdS and CIGS, we can estimate a length for the distribution of CdS. The transitional region due to intermixing of CdS with CIGS is very large in this case, about 1200 Å (S1694-2) and 1500 Å (S1694-3) within 68% of statistical confidence. Heat treatment may be responsible for the deeper distribution of CdS in sample S1694-3 than in sample S1694-2. These are much greater than the thickness (about 400 Å) of the CdS layer deposited on CIGS. In this case of high roughness, the usual definition of CdS film thickness is not meaningful. However, from the concentration profiles given in Fig. 6, it is possible to define an effective thickness of CdS in the heterojunctions by integrating the concentration profile over the sample depth and dividing it by the normal bulk density of CdS. This gives rise to an effective thickness of CdS around 380 Å for sample S1694-2 and around 410 Å for sample S1694-3. It should also be noted that the sensitivity for the determination of the parameters for samples S1694-2 and S1694-3 is somewhat higher due to simultaneous analysis of Se Kα and Cd Kα data as compared to the case of sample S1694-1 (see Table I).

**VI. CONCLUSION**

The ADXRF method has been applied to a study of interfaces in CdS/CIGS heterojunctions. The interfacial roughness in this system is quite high, it actually exceeds the thickness of the CdS layer of about 400 Å. The previous method for depth profiling is only valid in the cases of low roughness below 50 Å, so it is not applicable here. In the present work, an improved data analysis method has been developed to account for the high interfacial roughness, with an emphasis on a determination of the concentration profile for each of the two components CdS and CIGS. This method allows us to achieve very good agreement between experimental data and theoretical calculations. As a result, the concentration profile in the transitional region between CdS and CIGS has been obtained for both constituents, and the effective interfacial roughness as well as the effective thickness of CdS have also been determined. We have thus demonstrated that the ADXRF method is useful for a general study of compositional intermixing around very rough interfaces in the heterojunctions needed for PV applications.

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APPENDIX: INVESTIGATION OF MULTILAYER SYSTEMS BY THE ADXRF METHOD

A. Applications to multilayer systems with low interfacial roughness

For the simple case of a multilayer system with low interfacial roughness such that \( \sigma_j / k_{z,j} < 1 \), the modified Fresnel’s coefficients can be used to account for the effects of interfacial roughness. Assuming a Gaussian distribution of the interfacial roughness, the standard Fresnel’s coefficients \( r_j \) and \( t_j \) can be conveniently replaced by \( \tilde{r}_j = r_j \exp \left( -2k_{z,j} \sigma_j^2 \right) \) and \( \tilde{t}_j = t_j \exp \left( \left( k_{z,T} - k_{z,j} \right)^2 \sigma_j^2 \right) \), with the appearance of the Debye–Waller-like exponential factors in order to incorporate the effects of interfacial roughness. In the hard x-ray regime, this “low roughness limit” approximation is only valid for multilayer systems with interfacial roughness \( \sigma_j \) values generally lower than about 50 Å.

For very thin films, the x-ray fluorescence intensity \( I_{aj} \) arising from the atoms of a selected element \( a \) in layer \( j \) can be simplified as

\[
I_{aj} \propto \Phi_{aj} d_j |E_j^u + E_j^s|^2 = C_{aj} \rho_j d_j |E_j^u + E_j^s|^2, \quad (A1)
\]

where \( \Phi_{aj} \) is the concentration of element \( a \) in layer \( j \), \( C_{aj} \) the mass fraction of element \( a \) in layer \( j \), and \( \rho_j \) the density of layer \( j \). The intensity is proportional to the total number per unit area \( C_{aj} \rho_j d_j \) of the element \( a \) in layer \( j \).

B. Applications to multilayer systems with high interfacial roughness

In the more general case, the roughness effects on the Fresnel’s coefficients can not be simply represented by a single parameter \( \sigma_j \). For layer systems with high interfacial roughness \( \sigma_j / k_{z,j} \gg 1 \), the Debye–Waller-like exponential factors are no longer applicable. In some cases, the average interfacial roughness can even become larger than the film thickness in the system. A different approach for the variation of refractive indices with depth is needed.

To account for the effects of high interfacial roughness, the depth dependence of refractive indices can be derived from the density variation of the system through the dependence of the optical constants \( \delta_j \) and \( \beta_j \) on density. In this treatment, the interfacial roughness is expressed in terms of compositional variation pertaining to each of the constituent components in a transitional zone between two dissimilar materials. Mathematical analysis of the rough interface can be carried out by dividing the density transitional zone into a series of virtual layers each with a step-wise change of density. From the depth dependence of the density variation, one can then calculate the refractive indices and hence the fluorescence intensity to make comparison with the experimental data.

As an illustrative example, we consider the case of a rough interface between bulk CIGS and air, as schematically shown in Fig. 7. This analysis is applicable to sample S1694-1, in which the CIGS layer is so thick that no x-rays can penetrate into the glass substrate. The rough surface of CIGS is represented by a series of virtual layers with step-wise increasing density beginning from a value close to zero (in air) at the left-hand side and up to the bulk density at the right-hand side. For simplicity, we assume that the stoichiometry of CIGS for this calculation is in the so-called (112) structure, i.e., Cu(In_{0.5}Ga_{0.5})Se_2, and the compositional distribution is the same for all the virtual layers. From Eq. (4), we obtain an error function for the density profile \( \rho(z) \) in the following form:

\[
\rho(z) = \frac{\rho_0}{2} \left( 1 + \text{erf} \left( \frac{z-z_0}{S} \right) \right), \quad (A2)
\]

where \( \rho_0 \) is the density of bulk CIGS (≈ 5.4 g/cm^3), \( z \) the depth into CIGS in Å, \( z_0 \) a point with maximum probability in a Gaussian distribution, and \( S \) is a parameter which effects the profile of density variations. An example of density profile is shown in the lower part of Fig. 7. In Eq. (A2), an effective root-mean-square roughness \( \sigma_{eff} \) can be defined as \( S = \sqrt{2} \sigma_{eff} \). The effect of density fluctuations (or effective roughness) on x-ray fluorescence intensity is closely related to the value of \( S \). Theoretical calculations of Se Kα for a smooth surface gives a critical angle at 0.09°, but the fluorescence intensity of bulk CIGS (sample S1694-1) increases gradually at low angles due to the density variation, which implies that the surface has a high roughness. Using this method, we are able to fit the experimental data of ADXRF very well for sample S1694-1 (see Fig. 3) with \( S = 1400 \pm 300 \) Å. This result shows that the CIGS film prepared by the present method yields a very rough top surface.

For the calculations of ADXRF for the two CdS/CIGS/glass samples (S1694-2 and S1694-3), we neglect the effect of the glass substrate for the same reason as for S1694-1. The sample structure for calculations is assumed to consist of an admixture of CdS and CIGS in the transitional region and connected to the region of a bulk CIGS deep in the samples. The depth dependence of the material density takes a similar form of an error function as in Eq. (4). For the transitional...
zone of intermixed components, the compositional distribution is naturally CdS rich at the top surface \((z=0)\), and gradually becomes CIGS rich at the depth where the un-mixed bulk CIGS begins. It perhaps should be noted that the data can not agree with a model assuming a uniform compositional distribution of CdS and CIGS. Furthermore, the agreement between theory and experiment can be improved by introducing another error function for the compositional distribution \(C_d(z)\) for CdS and CIGS in the calculation of x-ray fluorescence intensity using Eq. (1), the final results for sample S1694-2 are shown in Fig. 4.

Another useful parameter \(D_{\text{eff}}\) can be introduced to represent the effective thickness of CdS buried between the rough top surface and the CdS/CIGS interface. This effective thickness \(D_{\text{eff}}\) is obtained by integration of the concentration depth profile for CdS in Fig. 6 and divided by the density of bulk CdS \((\approx 4.8 \text{ g/cm}^3)\). The values obtained are also included in Table 1.

As a concluding remark, we note that all the statements and analysis discussed so far are all based on the depth dependence of the concentration \(\Phi_d(z) = C_d(z) \rho(z)\) for each component CdS and CIGS. Due to the high interfacial roughness in the samples (as schematically illustrated in Fig. 7), no information can be obtained about the microscopic interdiffusion between CdS and CIGS at the very rough boundaries separating these two components. These boundaries can no longer be thought of as a simple plane perpendicular to the sample growth direction \((z)\) as in the usual cases. As a matter of fact, these boundaries are not in the \(xy\) plane, and consequently, the response of the region with composition intermixing to incident electromagnetic waves is dominated by the large interfacial roughness (or large density variations) within which a thin "layer" of CdS has been distributed. Any changes in the electronic band structures caused by the intermixing between CdS and CIGS will most likely be overshadowed by the large density variations of the material.