Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information For

Role of S and Se atoms on the microstructural properties of kesterite $Cu_2ZnSn(S_xSe_{1-x})_4$ thin film solar cells

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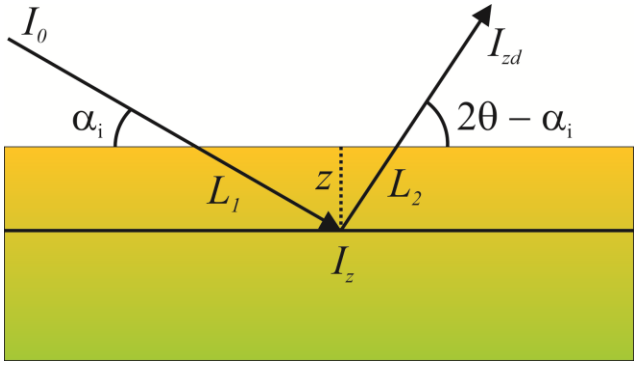

Figure S1. Schematic diagram of the X-ray diffraction through the sample in grazing incidence geometry. Based on the attenuation law, the incident beam I_0 after traveling through the sample and being reflected will be reduced to $I_{zd} = I_0 \cdot e^{-\mu(L_1+L_2)} = I_0 \cdot e^{-\mu\left(\frac{z}{\sin\alpha_i}+\frac{z}{\sin(2\theta-\alpha_i)}\right)}$. If the penetration depth z is defined as the depth at which the intensity of the X-rays is reduced to 1/e (about 37%) of its original value, then based on the ratio $I_0 = e \cdot I_{zd}$, the penetration depth can be calculated as $z = \frac{1}{\mu}\left(\frac{1}{\sin\alpha_i}+\frac{1}{\sin(2\theta-\alpha_i)}\right)^{-1}$.

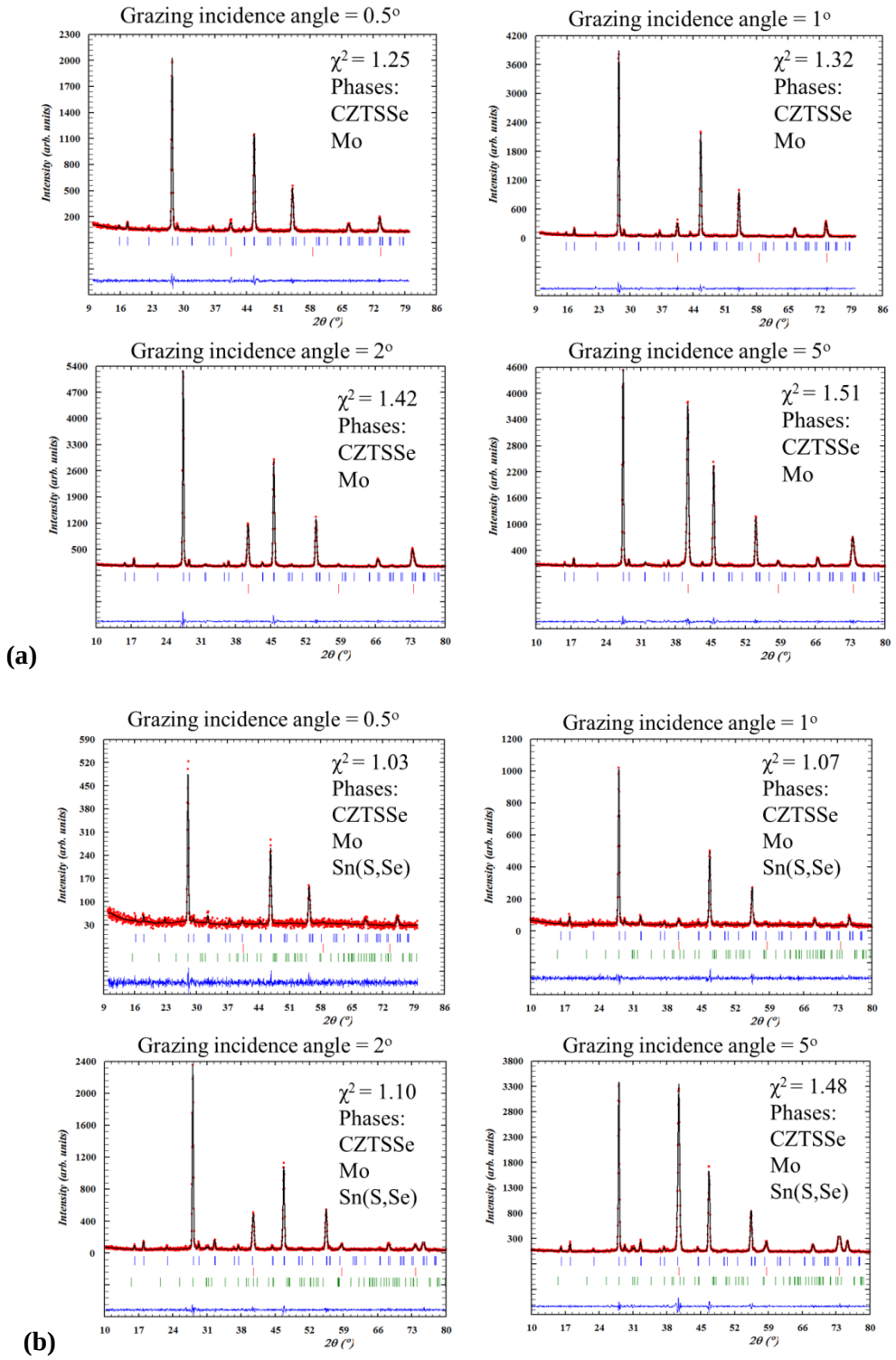

Figure S2. Le Bail fits of the XRD patterns measured with 0.5, 1, 2 and 5° incidence angles of two representative CZTSSe samples with (a) [S] / ([S] + [Se]) = 0.27 and (b)) [S] / ([S] + [Se]) = 0.65 anion compositions.

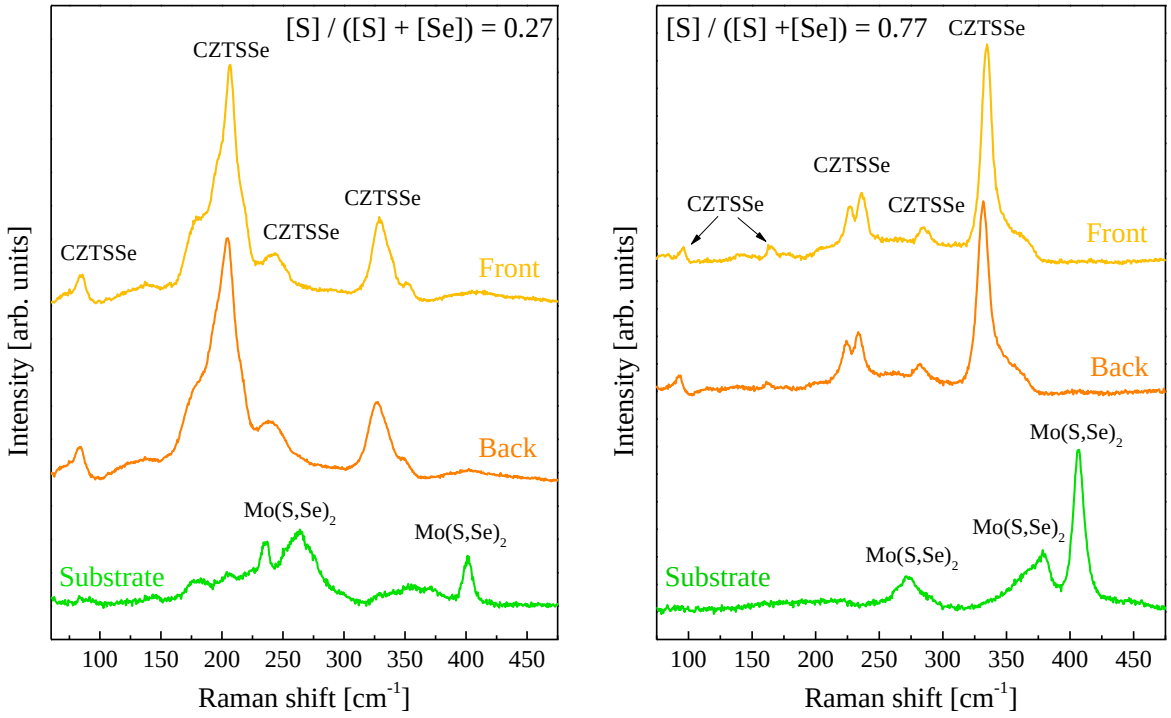

Figure S3. Raman spectra of front, back and substrate for two representative CZTSSe samples measured with 532 nm excitation wavelength.