

**All Experimental Details can be found at <https://doi.org/10.1021/acsami.2c01225>**

### **GIXRD and XRR**

The data is structured as followings. All Grazing Incidence X-ray diffraction (GIXRD) and X-ray Reflectometry (XRR) data have been measured on the same Bruker D8 Discover diffractometer and inside an Anton Paar XRK 900 Reactor Chamber under vacuum ( $P < 5 \times 10^{-4}$  mbar) unless otherwise specified. The measured data, stored as .brml files, are converted to (i) .raw data files (<file name>\_exported.raw) and (ii) text files (<file name>\_exported.xye) using Bruker Diffrac Eva 4.1.1 software. The file name is structured as follows:

<Date of measurement(YYYYMMDD)>\_<sample name and conditions>\_<measurement type (XRR/GIXRD)>\_Incident beam optics\_Exit\_slit\_size in mm (ES)\_<secondary beam optics (e.g. Soller slit or AS (acceptance Slit) and RS (receiving slit, slitsize in mm)>\_<incident angle (GIXRD only)>\_<2Theta range in degrees>\_<Orientation/mode of detector (0D)>\_<presence of attenuator (e.g. NoCuFoil or Cu0.1 (with 0.1 mm the thickness in mm)>

Example:

20210702\_HT\_763-  
1\_HfCleaned\_2000s\_Annealing\_800C\_PEO\_InSitu\_GiXRD\_GM\_ES\_0.1\_Soller\_theta\_0.2deg  
\_2Theta\_20\_75\_0D\_NoCuFoil

Subsequently, the data is stitched using the home-written Python 3 code '20220323 XRR\_Data\_conversion'. This creates a file ending with '\_treated'.

The data is analyzed using the open source software GenX 3 (available at <https://sourceforge.net/projects/genx/>). The fits can be found in the .hgx files that can be opened with GenX. The fits are exported as text files ending with '\_fit000.dat'. The corresponding scattering length density (SLD) profiles are exported as '\_SLD000.dat' text files. All fitted parameters are stored in '20210929\_fit\_Parameters\_Si\_Solar\_Cells\_XRR.xlsx'

### **Lifetime data**

The lifetime data can be found in the folder 'Lifetime'. Lifetime data measured by Photo-Conductance Decay (PCD) on symmetrical samples made from c-Si substrates and featuring passivating contacts annealed at different temperature from 800 °C to 900 °C. PCD was performed after annealing and after further hydrogenation of the samples.

The data were used to evaluate the surface passivation of the samples, quantified by the implied open-circuit voltage (iVoc) and the emitter recombination current density ( $J_0$ ).