

Supporting Information

Article

High-Resolution Photoemission Study of Neutron-Induced Defects in Amorphous Hydrogenated Silicon Devices

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SI 1 Inelastic Mean Free Path

The inelastic mean free path IMFP may be calculated semi-empirically by the Tanuma-Powell-Penn equation (TPP-2M) [1], which depends on the material molecular mass (M), band gap (E_g),

density (ρ), and the number of free valence electrons (NV). IMFP predictions using TPP-2M are accurate to within 10%.

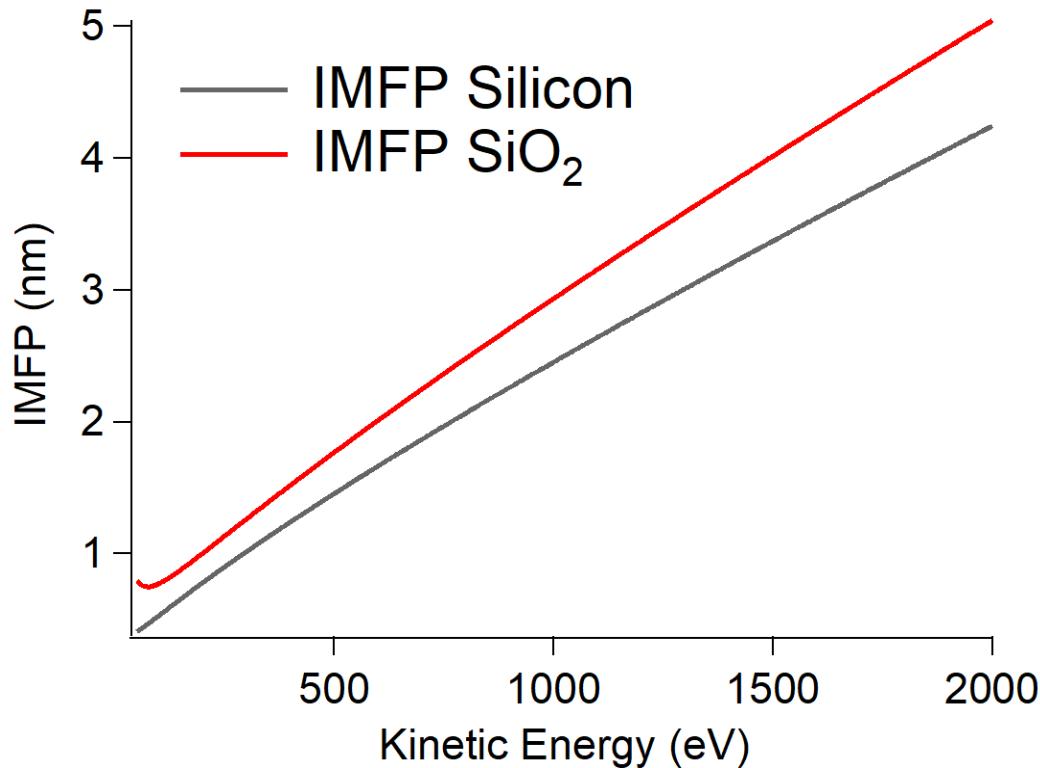


Figure S1 The IMFP for Si 2p photoelectrons in Si and SiO₂ as a function of Kinetic Energy.

SI 2 Comparison of XAS detection modes

In the Si L2,3 XAS edges the different sampling depths of Fluorescence Yield and the Total Electron Yield detection modes allow for discriminating the contribution of the spectra related to the coating oxide (above 104 eV) to the underneath crystalline silicon.

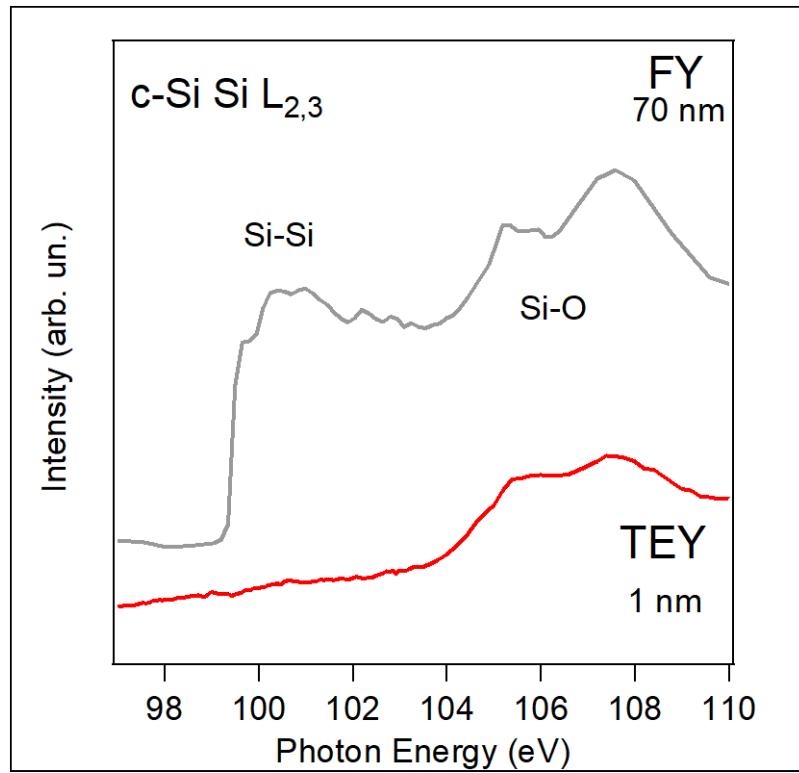


Figure S2 Comparison of Si L_{2,3} XAS edge taken in Fluorescence Yield (FY) and Total Electron Yield (TEY). The sample is crystalline Silicon with the layer of native oxide of about 3nm.

SI 3 Si 2p core level deconvolution

The Si 2p spectra were deconvoluted into chemically-shifted components using Linear for $h\nu=700$ eV and linear or Shirley background for 1400 eV, Voigt doublets with spin-orbit splitting 0.6 eV, 2p_{3/2}-2p_{1/2} intensity ratio of 1.5, Lorentzian width 100-150 meV, and Gaussian width \geq experimental resolution.

Table S1 Example of fit parameters used for the global fit of the Si2p core level taken at 700 eV and 1400 eV for No irradiated spectra and 1400 eV for Irradiated and annealed samples. For the component of the non-stoichiometric Silicon oxides components see ref.2

Component	Binding Energy Si 2p _{3/2} (eV)	No Irradiated $h\nu=700$	No Irradiated $h\nu=1400$ eV	Irradiated	Annealed
		Gaussian Width	Gaussian Width	Gaussian Width	Gaussian Width
c-Silicon (c Si-Si)	99.4	0.35	0.75	0.7	0.75

a-Si&Dangling Bonds (Dis Si)	99.1	0.31	0.85	0.75	0.8
Si-H	99.7	0.36	0.7	0.75	0.75
Si-C	100.1	0.35	0.7	0.7	0.8
SiOx	102.-100.4	1.9	-	1.9	1.7
SiO2	103.5	2.1	2.4	2.0	1.8

SI-4 Effect of sputtering on the Si2p XPS

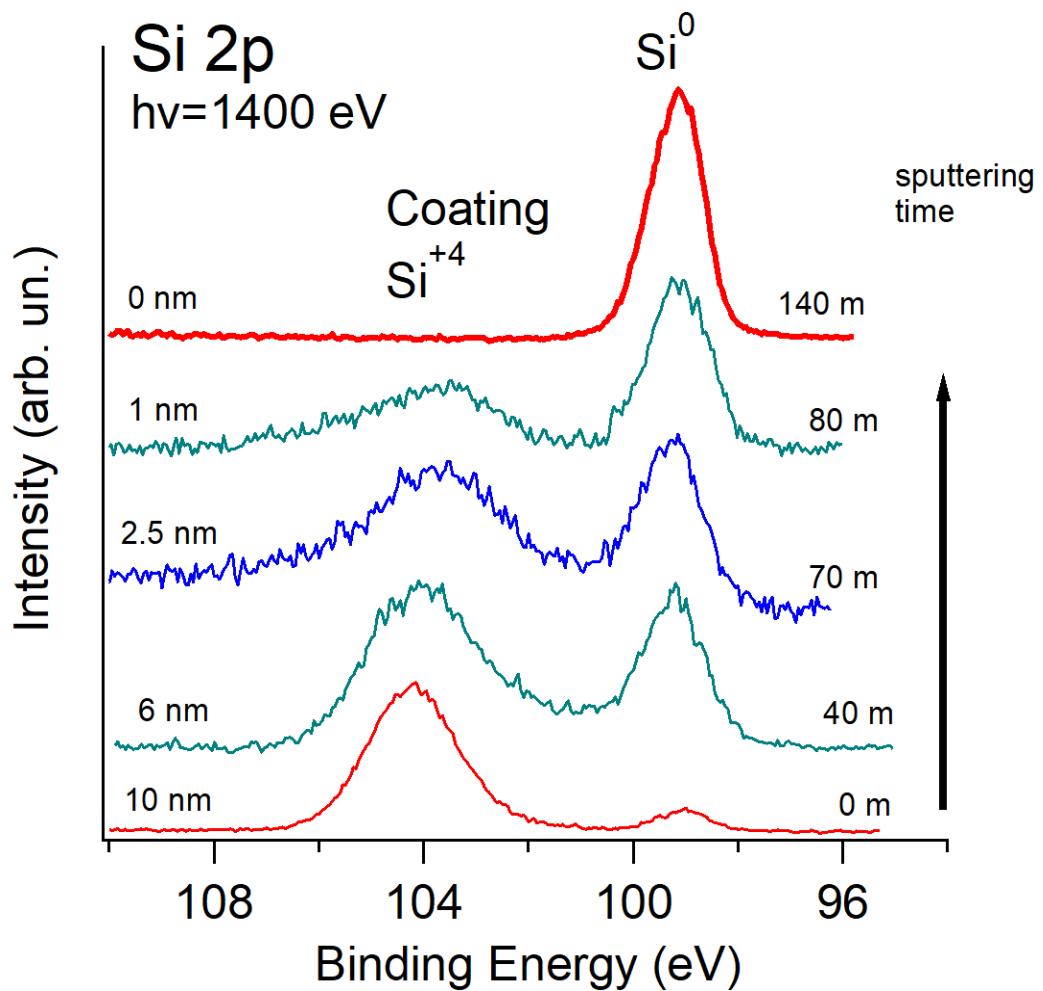


Figure S3 Example of Si 2p evolution as a function of the sputtering time of a a-Si:H reference film, indicating the disappearance of the coating contribution after 140 minutes.

References

- 1) S. Tanuma, C. J. Powell, and D. R. Penn, "Calculation of electron inelastic mean free paths (IMFPs) VII. Reliability of the TPP-2M IMFP predictive equation" *Surf. Interface Anal.* 35, 268 (2003)
- 2) F. J. Himpel, F. R. McFeely, A. Taleb-Ibrahimi, J. A. Yarmoff, G. Hollinger "Microscopic structure of the SiO₂/Si interface" *Phys- Rev. B* 38, 6084 (1988).