

Directory in which a single XSW data set is stored: /home/francois/Lab/Programming/XSW progs/PGI3_Torricelli/branches/Published_version/Example data sets/N1s_hBN on Cu(111) angluarResolved

Theoretical reflectivity and phase Import experimental data Fit reflectivity Fit photoelectron yield Argand diagram Geometry, About, License

(1) DCM (σ-polarized light) (2) Substrate (3) ☐ σ- (4) ☒ n-polarized light $P_{\text{Ref}} = -0.9925$

(5) Edit DCM $(\zeta=0^\circ, P_{\text{Ref}}=1, b=-1.00)$ (4) $\zeta=0.00^\circ$ $b=-1.000$ $\xi=3.50^\circ$ $\theta=86.50^\circ$

(6) Element: Si (7) Crystal system: Cubic Type: diamond
a (Å) = 5.4309
b (Å) = 5.4309
c (Å) = 5.4309
 $\alpha \beta \gamma (^\circ) = 90.0 \quad 90.0 \quad 90.0$
Checked values: Yes
DW method: Gao
DW Temperature = 77.0 K
(hkl) = 1 1 1
Debye-Waller = 0.2253
(B_n in Å²)
 $F_0 = 113.5438+15.9018j$
 $F_H = -60.3573-11.1800j$
 $F_{\bar{H}} = -60.3573-11.1800j$
 $d_{hkl} = 3.136$ Ang
Bragg energy =

(8) Cu (9) 6H-SiC (10) Cubic Hexagonal
faceCentered HEX Wurtzite
3.6149 3.08129
3.6149 3.08129
3.6149 15.11976
90.0 90.0 90.0 90.0 90.0 120.0
Checked values: Yes
DW method: Gao Zywiez
DW Temperature = 300.0 K 300.0 K
(hkl) = 1 1 1 0 0 0 6
Debye-Waller = 0.5747
 $F_0 = 116.1454+13.6065j$
 $F_H = 85.5677+13.1650j$
 $F_{\bar{H}} = 85.5677+13.1650j$
 $d_{hkl} = 2.087$ Ang
Bragg energy = 2975.85 eV

(11) Photon energy range: ± 10.0 eV

(12) Structure factors, reflectivity and phase

