Supplementary Information (SI) for RSC Advances.

Precise Dopant Detection and Transport Properties of Boron Ion-Implanted Silicon Solar Cells

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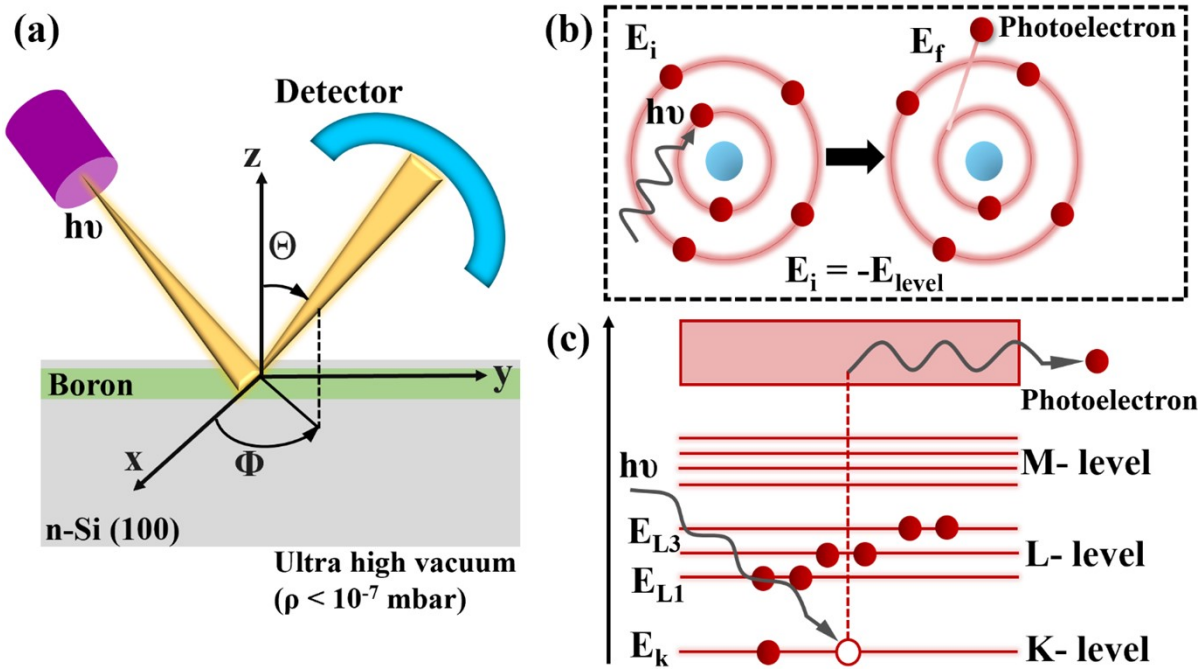

Figure S1 (a) Principle of X-ray photoelectron spectroscopy, (b) Mechanism of X-ray photoelectron spectroscopy, and (c) Photoelectric effect.

1. SRIM/TRIM Simulation (raw data)

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==================================================================
        SRIM version ---> SRIM-2013.00
        Calc. date   ---> September 11, 2025
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Disk File Name = SRIM Outputs\Boron in Silicon.txt
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Ion = Boron [5] , Mass = 11.009 amu

Target Density = 2.3212E+00 g/cm3 = 4.9770E+22 atoms/cm3

======= Target Composition ========

Atom Name	Atom Numb	Atomic Percent	Mass Percent
Si	14	100.00	100.00

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Bragg Correction = 0.00%

Stopping Units = MeV / (mg/cm2)

See bottom of Table for other Stopping units

Ion Energy	dE/dx Elec.	dE/dx Nuclear	Projected Range	Longitudinal Straggling	Lateral Straggling
10.00 keV	3.912E-01	3.418E-01	400 A	231 A	173 A
11.00 keV	4.103E-01	3.346E-01	437 A	248 A	187 A
12.00 keV	4.285E-01	3.277E-01	475 A	264 A	200 A
13.00 keV	4.460E-01	3.210E-01	512 A	280 A	212 A
14.00 keV	4.628E-01	3.145E-01	549 A	295 A	225 A
15.00 keV	4.791E-01	3.083E-01	587 A	310 A	237 A
16.00 keV	4.948E-01	3.024E-01	624 A	324 A	249 A
17.00 keV	5.100E-01	2.967E-01	661 A	338 A	261 A
18.00 keV	5.248E-01	2.912E-01	698 A	352 A	272 A
20.00 keV	5.532E-01	2.809E-01	771 A	379 A	295 A
22.50 keV	5.910E-01	2.691E-01	863 A	410 A	323 A
25.00 keV	6.449E-01	2.584E-01	952 A	439 A	350 A
27.50 keV	6.955E-01	2.487E-01	1038 A	465 A	375 A
30.00 keV	7.417E-01	2.398E-01	1122 A	490 A	399 A
32.50 keV	7.834E-01	2.316E-01	1204 A	512 A	422 A
35.00 keV	8.210E-01	2.240E-01	1306 A	534 A	449 A
37.50 keV	8.551E-01	2.170E-01	1364 A	554 A	464 A
40.00 keV	8.860E-01	2.105E-01	1442 A	573 A	484 A
45.00 keV	9.407E-01	1.988E-01	1595 A	609 A	522 A
50.00 keV	9.874E-01	1.885E-01	1746 A	642 A	557 A
55.00 keV	1.028E+00	1.794E-01	1895 A	673 A	591 A
60.00 keV	1.063E+00	1.713E-01	2042 A	701 A	622 A
65.00 keV	1.094E+00	1.639E-01	2188 A	728 A	653 A
70.00 keV	1.121E+00	1.573E-01	2332 A	754 A	681 A
80.00 keV	1.169E+00	1.458E-01	2618 A	802 A	736 A
90.00 keV	1.211E+00	1.361E-01	2901 A	845 A	788 A
100.00 keV	1.249E+00	1.278E-01	3180 A	886 A	837 A
110.00 keV	1.286E+00	1.205E-01	3455 A	923 A	883 A
120.00 keV	1.323E+00	1.142E-01	3727 A	958 A	927 A
130.00 keV	1.359E+00	1.085E-01	3995 A	991 A	969 A
140.00 keV	1.396E+00	1.035E-01	4259 A	1021 A	1009 A

150.00 keV	1.434E+00	9.901E-02	4519 A	1050 A	1047 A
160.00 keV	1.472E+00	9.492E-02	4774 A	1076 A	1084 A
170.00 keV	1.511E+00	9.120E-02	5025 A	1101 A	1119 A
180.00 keV	1.550E+00	8.780E-02	5271 A	1125 A	1152 A
200.00 keV	1.631E+00	8.179E-02	5749 A	1169 A	1215 A
225.00 keV	1.733E+00	7.547E-02	6322 A	1218 A	1287 A
250.00 keV	1.837E+00	7.017E-02	6868 A	1260 A	1352 A
275.00 keV	1.941E+00	6.564E-02	7389 A	1297 A	1411 A
300.00 keV	2.043E+00	6.172E-02	7888 A	1329 A	1464 A
325.00 keV	2.145E+00	5.830E-02	8365 A	1359 A	1513 A
350.00 keV	2.243E+00	5.527E-02	8824 A	1385 A	1558 A
375.00 keV	2.340E+00	5.258E-02	9265 A	1408 A	1600 A
400.00 keV	2.433E+00	5.016E-02	9690 A	1429 A	1638 A
450.00 keV	2.610E+00	4.601E-02	1.05 um	1468 A	1707 A
500.00 keV	2.774E+00	4.255E-02	1.13 um	1501 A	1767 A
550.00 keV	2.925E+00	3.962E-02	1.20 um	1530 A	1820 A
600.00 keV	3.062E+00	3.711E-02	1.27 um	1555 A	1868 A
650.00 keV	3.186E+00	3.492E-02	1.33 um	1577 A	1911 A
700.00 keV	3.299E+00	3.301E-02	1.40 um	1597 A	1951 A
800.00 keV	3.493E+00	2.979E-02	1.52 um	1636 A	2021 A
900.00 keV	3.649E+00	2.719E-02	1.64 um	1670 A	2082 A
1.00 MeV	3.775E+00	2.505E-02	1.75 um	1699 A	2137 A
1.10 MeV	3.875E+00	2.325E-02	1.86 um	1726 A	2186 A
1.20 MeV	3.955E+00	2.170E-02	1.97 um	1750 A	2231 A
1.30 MeV	4.018E+00	2.037E-02	2.08 um	1773 A	2273 A
1.40 MeV	4.067E+00	1.921E-02	2.18 um	1794 A	2312 A
1.50 MeV	4.105E+00	1.818E-02	2.29 um	1814 A	2349 A
1.60 MeV	4.134E+00	1.726E-02	2.39 um	1833 A	2384 A
1.70 MeV	4.156E+00	1.644E-02	2.49 um	1851 A	2417 A
1.80 MeV	4.171E+00	1.570E-02	2.60 um	1868 A	2450 A
2.00 MeV	4.188E+00	1.442E-02	2.80 um	1912 A	2511 A
2.25 MeV	4.189E+00	1.310E-02	3.06 um	1971 A	2582 A
2.50 MeV	4.178E+00	1.202E-02	3.31 um	2028 A	2649 A
2.75 MeV	4.159E+00	1.112E-02	3.57 um	2082 A	2713 A
3.00 MeV	4.135E+00	1.035E-02	3.83 um	2134 A	2774 A
3.25 MeV	4.108E+00	9.691E-03	4.09 um	2186 A	2834 A
3.50 MeV	4.080E+00	9.114E-03	4.35 um	2236 A	2892 A
3.75 MeV	4.051E+00	8.607E-03	4.61 um	2286 A	2949 A
4.00 MeV	4.022E+00	8.157E-03	4.88 um	2335 A	3004 A
4.50 MeV	3.964E+00	7.394E-03	5.41 um	2489 A	3113 A
5.00 MeV	3.909E+00	6.769E-03	5.96 um	2638 A	3219 A
5.50 MeV	3.855E+00	6.249E-03	6.51 um	2782 A	3323 A
6.00 MeV	3.804E+00	5.807E-03	7.07 um	2922 A	3426 A
6.50 MeV	3.755E+00	5.428E-03	7.64 um	3059 A	3528 A
7.00 MeV	3.707E+00	5.098E-03	8.22 um	3193 A	3628 A
8.00 MeV	3.618E+00	4.551E-03	9.39 um	3648 A	3828 A
9.00 MeV	3.533E+00	4.117E-03	10.59 um	4070 A	4027 A
10.00 MeV	3.453E+00	3.763E-03	11.82 um	4470 A	4226 A

Multiply Stopping by	for Stopping Units
2.3211E+01	eV / Angstrom
2.3211E+02	keV / micron
2.3211E+02	MeV / mm
1.0000E+00	keV / (ug/cm2)
1.0000E+00	MeV / (mg/cm2)
1.0000E+03	keV / (mg/cm2)
4.6637E+01	eV / (1E15 atoms/cm2)
8.2629E-01	L.S.S. reduced units

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2. FEFF Simulation

DFT based FEFF simulation for NEXAFS analysis

```
# # Silicon                                        FEFF 9.6.4
# # POT  SCF  30  3.0000   0, NO core-hole, AFOLP (folp(0)= 1.150)
# # Abs   Z= 8 Rmt= 0.766 Rnm= 0.921 K  shell
# # Pot 1 Z=14 Rmt= 1.016 Rnm= 1.234
# # Pot 2 Z= 8 Rmt= 0.766 Rnm= 0.921
# # Pot 3 Z= 5 Rmt= 0.974 Rnm= 1.120
# # Gam_ch=1.559E-01 H-L exch Vi= 3.000E-01 Vr=-2.000E+00
# # Mu=-7.238E+00 kf=2.635E+00 Vint=-2.309E+01 Rs_int= 1.376
# FMS rfms= 6.0000
# # PATH  Rmax=-1.000,  Keep_limit= 0.00, Heap_limit 0.00  Pwcrit= 2.50%
#  S02=0.900  Temp=   0.00  Debye_temp=   0.00  Global_sig2= 0.00000
#  Curved wave amplitude ratio filter   4.000%
#    file        sig2 tot  cw amp ratio   deg  nlegs   reff  inp sig2
#    0/   0 paths used
#  xsedge+ 50, used to normalize mu          4.2389E-03
#  ---------------------------------------------------------------------
# omega    e    k    mu    mu0     chi     @#
   488.321   -54.615  -3.600  3.68831E-03  3.69638E-03 -8.06787E-06
   498.684   -44.252  -3.200  4.62384E-03  4.61250E-03  1.13378E-05
   507.828   -35.108  -2.800  5.97809E-03  5.94563E-03  3.24599E-05
   515.752   -27.184  -2.400  8.04756E-03  8.01046E-03  3.70981E-05
   522.458   -20.478  -2.000  1.14445E-02  1.14875E-02 -4.30391E-05
   527.944   -14.992  -1.600  1.76104E-02  1.80617E-02 -4.51313E-04
   532.212   -10.724  -1.200  3.07173E-02  3.28007E-02 -2.08344E-03
   535.260    -7.676  -0.800  6.79051E-02  7.64953E-02 -8.59026E-03
   537.088    -5.848  -0.400  2.53631E-01  2.92046E-01 -3.84152E-02
   537.509    -5.427  -0.223  5.19782E-01  5.93103E-01 -7.33217E-02
   537.698    -5.238   0.000  7.43104E-01  8.46636E-01 -1.03531E-01
   537.850    -5.086   0.200  9.24040E-01  1.05712E+00 -1.33084E-01
   538.308    -4.628   0.400  1.16873E+00  1.39124E+00 -2.22513E-01
   539.070    -3.866   0.600  1.17567E+00  1.51353E+00 -3.37860E-01
```

540.136	-2.800	0.800	1.11987E+00	1.52551E+00	-4.05638E-01
541.508	-1.428	1.000	1.09666E+00	1.49373E+00	-3.97075E-01
543.184	0.248	1.200	1.15499E+00	1.44269E+00	-2.87705E-01
545.166	2.230	1.400	1.53030E+00	1.38391E+00	1.46388E-01
547.452	4.516	1.600	1.94280E+00	1.32400E+00	6.18798E-01
550.042	7.106	1.800	1.71842E+00	1.26692E+00	4.51505E-01
552.938	10.002	2.000	1.53542E+00	1.21492E+00	3.20494E-01
556.138	13.202	2.200	1.44235E+00	1.16910E+00	2.73254E-01
559.644	16.707	2.400	1.27067E+00	1.12970E+00	1.40972E-01
563.453	20.517	2.600	1.28043E+00	1.09652E+00	1.83909E-01
567.568	24.632	2.800	1.33014E+00	1.06895E+00	2.61186E-01
571.988	29.052	3.000	1.20902E+00	1.04627E+00	1.62749E-01
576.712	33.776	3.200	1.08112E+00	1.02769E+00	5.34304E-02
581.741	38.805	3.400	9.70634E-01	1.01238E+00	-4.17427E-02
587.075	44.139	3.600	8.83491E-01	9.99636E-01	-1.16144E-01

****Additional data if required, are available from the corresponding author on reasonable request.**