

Element-specific structural analysis of Si/B₄C using resonant X-ray reflectivity. Corrigendum

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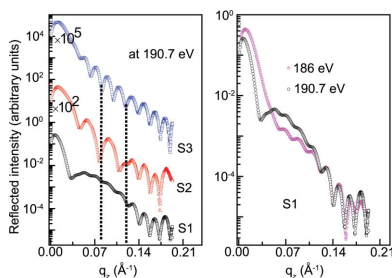
Errors in the article by Nayak, Pradhan & Lodha [*J. Appl. Cryst.* (2015), **48**, 786–796] are corrected.

It has come to the authors' attention that the paper published by Nayak *et al.* (2015) contains the following errors: (i) an error in the calculated electron density contrast (*i.e.* fraction of electron density difference, $\Delta\rho/\rho$) between the Si and B₄C layers and (ii) a numerical error during conversion of the measured angular reflectivity to $q_z = 4\pi\sin\theta/\lambda$. Regarding (i), $\Delta\rho/\rho$ across the Si/B₄C interface is 0.5%, not 0.05%. This $\Delta\rho/\rho$ is still one order of magnitude lower than what can be measured using hard X-ray reflectivity (XRR). Regarding (ii), the reported q_z range in Figs. 3–10 of the original article exceeds the actual measured angle. The original data files were modified by mistake and are not retrievable. To show that the proposed methodology and the conclusion drawn are not affected by the error in q_z , fresh measurements on freshly prepared similar samples were performed.

Three different samples were fabricated on Si wafers using electron beam evaporation with varying spatial position of the B₄C layer (40 Å) in the Si film (300 Å). The B₄C layer is at the top, middle and bottom of the Si film in samples S1, S2 and S3, respectively. A tungsten layer with thickness ~10 Å is located between the substrate and the thin film. In the B₄C layer, elementary boron is incorporated through co-deposition. The XRR profiles of the three samples, measured using a Cu K α source, are nearly identical in nature [similar to Fig. 2(b) in the original paper]. Considering Si and B₄C as a single layer, the fitted thicknesses (roughnesses) are 350 (1) Å [7.5 (5) Å], 352 (1) Å [6.5 (5) Å] and 353 (1) Å [7.0 (5) Å], for S1, S2 and S3, respectively. Thus, our original conclusion that XRR is not sensitive to the low-contrast Si/B₄C interface ($\Delta\rho/\rho = 0.5\%$) still stands.

The microstructural sensitivity of the resonant soft X-ray reflectivity (R-SoXR) to the low-contrast Si/B₄C interface is demonstrated near the B K edge of B₄C (Fig. 1a). R-SoXR measurements were done in s-polarization geometry using the Optics Beamline on the BESSY synchrotron (Sokolov *et al.*, 2014). The enhanced scattering strength strongly modulates the R-SoXR owing to reflection from the Si/B₄C interface (similar to Fig. 3 in the original paper). This provides experimental evidence for the sensitivity of resonant reflectivity to the spatial variation of position of a low-contrast interface structure.

To obtain spectroscopic information on S1, R-SoXR measurements are performed across the B K edge of



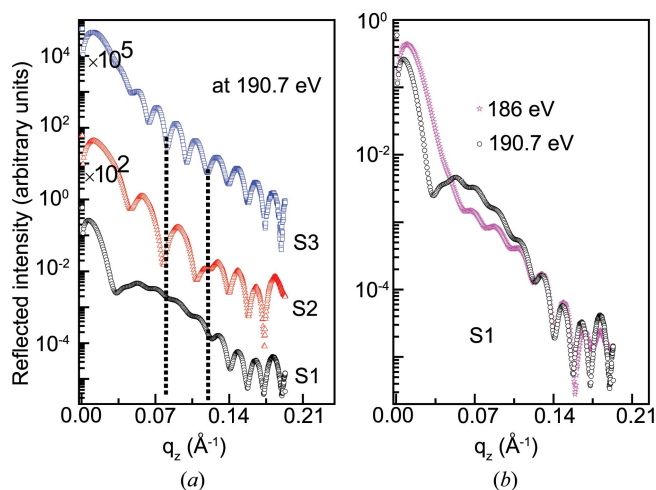


Figure 1
 (a) Measured R-SoXR of samples S1, S2 and S3 at 190.7 eV. (Measured data of S2 and S3 are shifted vertically for clarity.) (b) R-SoXR at two different photon energies near the B *K* edge of elementary boron for sample S1.

elementary boron at two selected energies of 186 and 190.7 eV (Fig. 1*b*). R-SoXR undergoes a strong variation with a significant change in the amplitude and shape of the oscillations [similar to Fig 4(*c*) in the original paper] due to the strong variation of the optical constant of boron. This indicates the presence of elementary boron in S1. Similarly, R-SoXR measurements across the B *K* edge of B₂O₃ (194.1 eV) indicate that the reflection spectra are nearly identical in nature [similar to Fig 4(*b*) in the original paper], showing the absence of B₂O₃. In S1 of the original paper the elementary boron was oxidized, but in the fresh sample S1 elementary boron is not oxidized. Similarly, in S2 and S3, we observed that only elementary boron is present in the B₄C layer (similar to Fig. 5 of the original paper).

The atomic percent of resonating element and the distribution were quantified near the B *K* edge of elementary boron for S1, S2 and S3. The fitting procedure of R-SoXR is similar to that described in the original paper. In S1, the optimized values for the thicknesses (roughnesses) of the Si and B₄C

layers are 294 Å (5 Å) and 42 Å (13 Å), respectively. A carbon-contaminated layer at the top of the B₄C layer is considered, with thickness 11.5 Å and roughness 6.5 Å. An intermixed layer at the Si/B₄C interface is also considered, with thickness 11.5 Å and roughness 7.5 Å. The best-fit results reveal that the B₄C layer is composed of 80 (3)% of B₄C and 20 (3)% of B. The interlayer is composed of 80% of Si and 20% of (80% B₄C + 20% B). Similarly for S2, the average thicknesses (roughnesses) of the W, Si, interlayer I (B₄C-on-Si), B₄C, interlayer II (Si-on-B₄C) and Si layers are 8 (1) Å [4.0 (5) Å], 138 (1) Å [8.5 (5) Å], 13 (1) Å [4.0 (5) Å], 41 (1) Å [6.5 (5) Å], 13 (1) Å [5.5 (5) Å] and 148 (1) Å [7.0 (5) Å], respectively. The B₄C layer is composed of 80 (3)% of B₄C and 20 (3)% of B. The interlayer is composed of 80% of Si and 20% of (80% B₄C + 20% B). Similarly, for S3, the thicknesses (roughnesses) of the W, B₄C, interlayer (Si-on-B₄C) and Si layers are 8 (1) Å [5.0 (5) Å], 41 (1) Å [5.5 (5) Å], 12 (1) Å [6.0 (5) Å] and 301 (1) Å [7.5 (5) Å], respectively. The B₄C layer is composed of 80 (3)% of B₄C and 20 (3)% of B. The interlayer is composed of 80% of Si and 20% of (80% B₄C + 20% B). The results are consistent with Figs. 6–10 of the original paper.

This corrigendum identifies and corrects errors in the original paper that have come to our attention. On addressing these errors and conducting a fresh set of measurements on new similar samples, we have established that our methodology and original conclusions regarding the quantitative estimation of the structural and chemical profile of layers in the Si/B₄C system still stand.

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