Characterization of the ScAlMgO₄ cleaving layer by X-ray crystal truncation rod scattering

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SUPPLEMENTARY MATERIAL for
Characterization of the ScAlMgO$_4$ cleaving layer by X-ray crystal truncation rod scattering

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FIG. S1. Observed CTR scattering intensities of the clean ScAlMgO$_4$(0001) cleaved surface and calculated curves for the truncations shown in Fig. 1 of the article except for the [Al/MgO]$_2$ truncation, which is shown in Fig. 3 of the article.

FIG. S2. Real part of the atomic scattering factors ($f$) of neutral Sc, Al, Mg, and O (dashed lines) and Sc$^{3+}$, Al$^{3+}$, Mg$^{2+}$, and O$^{2-}$ ions (solid lines) as a function of momentum transfer of scattered X-ray divided by $4\pi$, where $2\theta$ is scattering angle and $\lambda$ is wavelength of X-ray.$^{S1}$ $f$ of O$^{2-}$ ion multiplied by occupancy ratio 0.73 (chained line) and that multiplied by occupancy ratio 0.84 and the Debye-Waller factor $e^{-M}$ for isotropic mean-square displacement parameter $U_{11} = U_{33} = 0.04$ Å$^2$ (long dashed line) are also shown. Scan ranges of the $hh + kl$ rods, $(hk) = (00), (01), (10)$, and $(11)$, are indicated by horizontal lines.

Imaginary part of the atomic scattering factors of neutral Sc, Al, Mg, and O are 0.7071, 0.1038, 0.0740, and 0.0128, respectively, at $\lambda = 1$ Å (12.4 keV).$^{S2}$


http://www.sasakiken.net/scatfac/scatfac.html