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Supporting information for article:

Quantitative analysis of dislocations in 4H-SiC wafers using synchrotron X-ray topography with ultra-high angular resolution

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Estimation of RC Width Using DuMond Diagram

In XRT, it is well known that the rocking curve of the sample is given by the convolution of two Darwin curves (the Darwin curve of the sample and the Darwin curve of the monochromator/conditioner). While the mathematical calculations for the convolution can be complicated, a good approximation of the resultant rocking curve can be obtained by the application of DuMond diagrams (DuMond, 1937; Sauvage, 1980; Caciuffo et al., 1987). In the following, we will briefly introduce the principles and demonstrate how the extremely narrow RC width of 0008 RCT is obtained.

DuMond diagram is drawn based on Bragg's law, where the wavelength is plotted as a function of diffraction angle, and the width of the DuMond band is determined by the Darwin width of the crystal. In DuMond diagrams, the region near the Bragg angle is usually enlarged and simplified as parallelograms (Fig. S1 (a) & (b)), the slope of which is determined by the d spacing of the diffraction plane. The DuMond diagram of 4H-SiC 11-28 GIT at an energy of 9 keV is shown in Fig. S1 (a), where the Si (111) DCM and SiC (11-28) are involved in the diffraction. The black parallelogram is the superimposition of two identical parallelograms of Si (111) as they are in (+, -) setting. The Darwin width of Si (111) defines the area shaded in blue, and it can be regarded as the range over which the effective Bragg diffraction condition for the third crystal is satisfied. A larger blue area usually indicates a broader RC for the sample, though the width of 4H-SiC 11-28 DuMond curve (the narrow red parallelogram in Fig. S1 (a)) is only 0.32″. The RC for the overall setup can be derived by translating the DuMond curve of 4H-SiC 11-28 along θ-axis (i.e. rock the sample around θ) and calculating the size of the intersecting region (the narrow dark region in Fig. S1 (a)). The schematic of the RC is shown in Fig. S1 (c), and the calculated full width at half maximum (FWHM) based on DuMond diagram is around 28″.

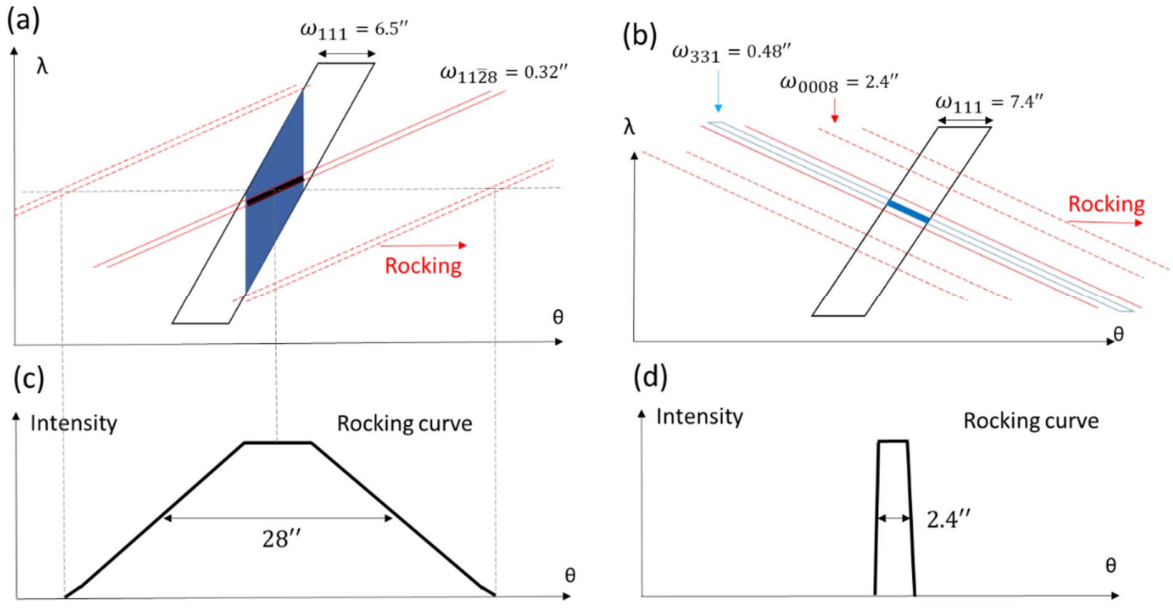

Figure S1 DuMond diagram of 4H-SiC 11-28 GIT at the energy of 9 keV (a) and 0008 RCT at the energy of 8 keV (b), ω is the Darwin width of the corresponding diffraction planes. The black and red band are the DuMond curve of the DCM and the sample respectively, which are exaggerated for illustration purposes. The narrow blue band in Fig. 2 (b) corresponds to the DuMond curve of Si (331). Schematic of 4H-SiC 11-28 rocking curve (c) and 0008 rocking curve (d) derived by translating 4H-SiC DuMond curve along θ axis.

However, the angular resolution in synchrotron X-ray RCT is significantly enhanced compared to that of GIT because of the presence of Si (331) conditioner. As shown in Fig. S1 (b), the DuMond curve of DCM has the width of 7.4″ at an energy of 8 keV. But the width of Si 331 DuMond curve is only 0.48″ according to (Caciuffo et al., 1987):

$$\omega_{331} = \sqrt{b}\omega_0 \quad (1)$$

where ω_0 is the intrinsic Darwin width of symmetric Si 331 and b is the asymmetric factor ($b = \frac{sin(\theta_B - \alpha)}{sin(\theta_B + \alpha)}$, θ_B is the Bragg angle and α is the angle between the diffraction plane and the surface, α is positive if the Bragg angle is bigger than the incident angle. In this experiment, α is 36.2° and θ_B is 38.5°). Hence, the width of Si 331 DuMond curve is extremely narrow since the asymmetric factor is very small. The DuMond curve of Si 331 (the blue band in Fig. S1 (b)) intersects that of the DCM at the narrow blue stripe, leaving a small effective diffraction range for 4H-SiC. Translating the DuMond curve of 4H-SiC 0008 across the blue strip along θ-axis and the resultant schematic of the RC is shown in Fig. S1 (d). A key point to make the RC as narrow as possible is to set the DuMond band of the sample parallel to that of the Si (331), which requires the d spacing of the sample diffracting planes to be almost the same with that of Si (331), and fortunately, the 0008 reflection satisfies this requirement. Eventually, the FWHM of 4H-SiC 0008 in RCT is only around 2.4″ based on DuMond diagram, and the value measured from experiment is 2.5″.

Calculation of Reflectivity

According to dynamical theory (Zachariasen 1945; Kikuta and Kohra 1970; Caciuffo et al., 1987), in the Bragg geometry and symmetric case, the diffraction pattern R_H for a non-absorbing crystal is given by:

$$R_H = \frac{1}{y^2 + (y^2 - 1)\cot^2\left[(\pi t/\Lambda)\sqrt{y^2 - 1}\right]}, \; |y| > 1$$

$$R_H = 1, \; |y| \leq 1 \quad \text{(S1)}$$

and the mean diffraction pattern is:

$$R_H = 1 - \sqrt{1 - y^2}, \; |y| > 1$$

$$R_H = 1, \; |y| \leq 1 \quad \text{(S2)}$$

y is deviation parameter as a function of $\Delta\theta$ (deviation from Bragg angle),

$$y = \frac{(\gamma_0/\gamma_H)\Delta\theta \sin 2\theta_B + \frac{1}{2}\chi_0(1-\gamma_0/\gamma_H)}{|C|\sqrt{\gamma_0/\gamma_H}\sqrt{\chi_H\chi_{\bar{H}}}} \quad \text{(S3)}$$

χ is the electric susceptibility, $\Lambda = \frac{\lambda\sqrt{\gamma_0\gamma_H}}{C\sqrt{\chi_H\chi_{\bar{H}}}}$ is the extinction length, $\gamma_0 = \gamma_H = cos\theta_B$, t is the crystal thickness, C is the polarization factor.

In the asymmetric case with absorption effect considered, the reflectivity R_H can be calculated as follows:

$$R_H = \mathrm{L} - \sqrt{L^2 - 1} \quad \text{(S4)}$$

$$L = \frac{\chi_{Hr}^2}{\chi_{Hr}^2+\chi_{Hi}^2}\left[y^2 + g^2 + \sqrt{\left(y^2 - g^2 - 1 + \frac{\chi_{Hi}^2}{\chi_{Hr}^2}\right)^2 + 4\left(gy - \frac{\chi_{Hi}}{\chi_{Hr}}\right)^2}\right] \quad \text{(S5)}$$

$$g = \frac{1+b}{2C\sqrt{|b|}}\frac{\chi_{0i}}{\chi_{Hr}} \quad \text{(S6)}$$

$$y = \frac{1+b}{2C\sqrt{|b|}}\frac{\chi_{0r}}{|\chi_{Hr}|} + \frac{\mathrm{b}\Delta\theta \sin 2\theta_B}{|C|\sqrt{|b|}|\chi_H|} \quad \text{(S7)}$$

The asymmetric factor b is given in previous section. Using the equations above, Fig. 3-17 in Zachariasen's book can be reproduced and the measured diffraction intensity of 4H-SiC 0008 in PWT is in good correlation with the calculated reflectivity (Fig. 2 in the main text).

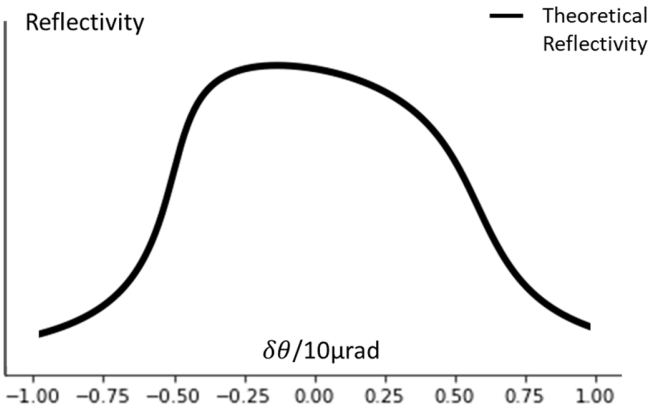

Figure S2 Reflectivity of 4H-SiC 0008 calculated from dynamical theory.