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Supporting information for article:

Retrieving the configuration of grain boundary structure in polycrystalline materials by extraordinary X-ray reflection analysis

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In this supporting document, we depict additional simulation details, as well as the intensity configurations of the interfaces ascribed in Table 1 as most probable.

Concerning the simulation of extraordinary peaks, it begins with a reduced crystal size of 30 unit cells in all spatial directions. As distinct tilt angles were probed with a 0.1° step, some orientations (with the angular tolerance depicted in the main text) have shown the appearance of grain boundary peaks. In these cases, two distinct procedures were carried out. First, the simulation was repeated only for the tilted inclusion of atoms (which generated the boundaries), as well as only for the host crystal without the tilted inclusion. This step was necessary to verify whether the diffraction peak was a result of truncated crystal surfaces. Such condition was not verified. The second step is then carried out with the tilted grain inclusion and intends to provide peaks with closer reciprocal space width in comparison with the measured data. It consists in elongating the simulated crystal along the defect axis in a cylindrical rod, with the grain boundary plane aligned along the rod longitudinal axis. This type of simulation was performed solely to the conditions that maximized the simulated peaks of a given grain boundary (as depicted in the main text), using one longitudinal (defect plane) axis with 200 unit cells, while other directions remained with a size of 30 unit cells .

Figure S1 shows, similarly to Figure 4 and 5 of the main text, the intensity of the extraordinary peaks observed at $2\theta = 29.32°$ and $2\theta = 41.95°$ as a function of the interface tilt angle.

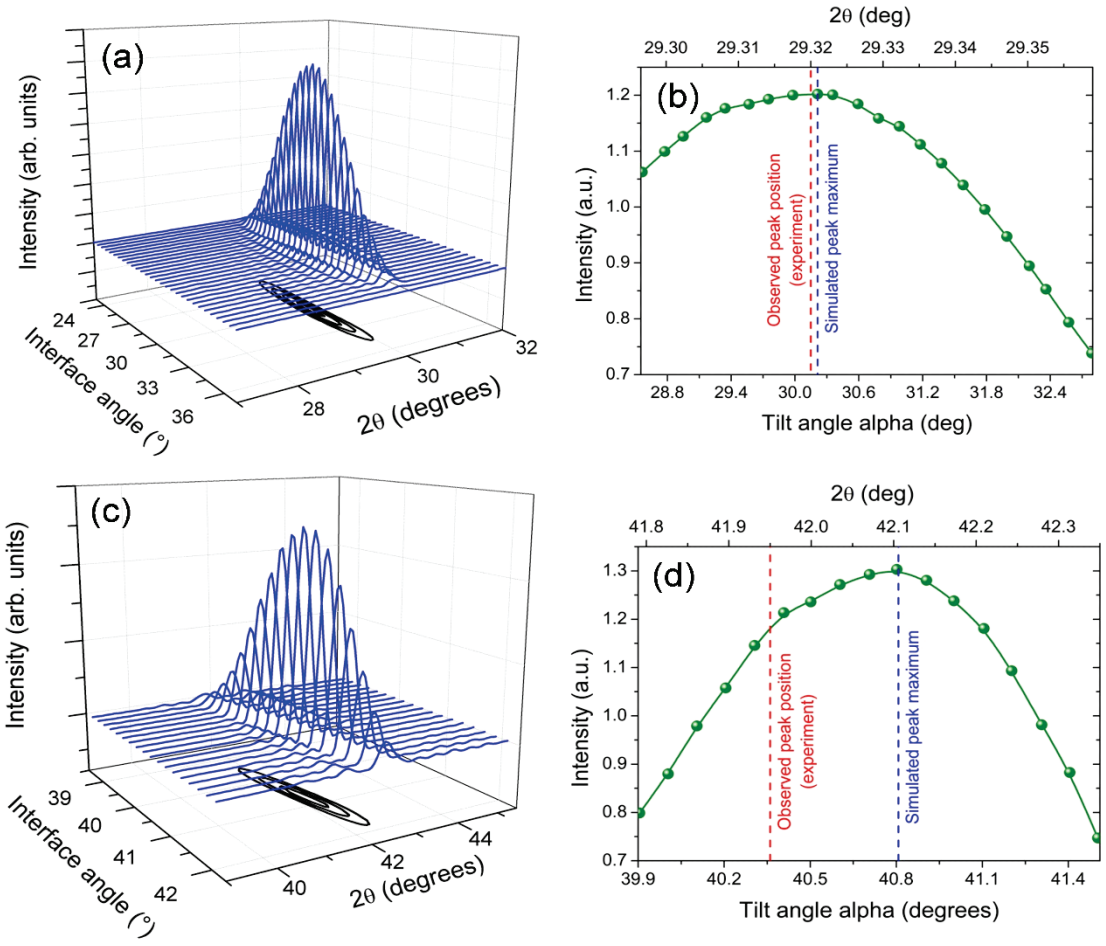

Figure S1 (a) Simulated intensity profile for the interface peak at 2θ = 29.32° plotted with respect to the interface angle and scattering angle. (b) Detailed view of the simulated maximum intensity. (c). Simulated intensity profile for the interface peak at 2θ = 41.95° plotted with respect to the interface angle and scattering angle. (d) Detailed view of the simulated maximum intensity.

Figure S2 shows the relative intensity of the four retrieved extraordinary peaks, displayed with respect to the processing procedure applied to the samples of Figure 7. Although a quantitative comparison is not recommended here (samples have distinct textures), large changes on all peak intensities can be ascribed to the reduction of the total volume of grain boundary interfaces that diffract at these peak positions.

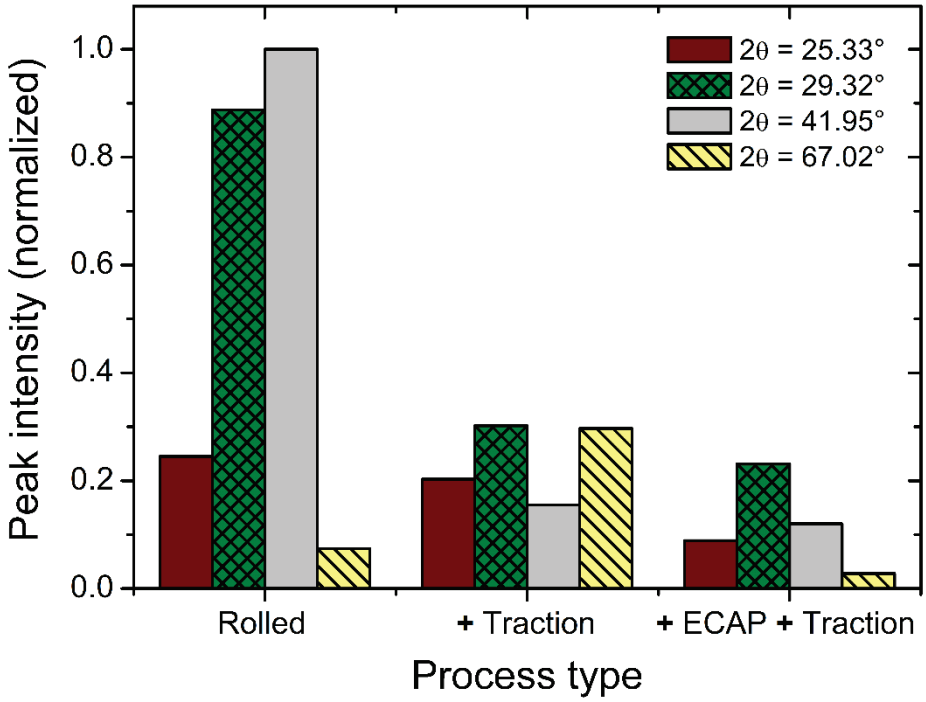

Figure S2 Relative intensity of extraordinary peaks as a function of processing type.