SUPPLEMENTARY MATERIAL TO

Computational diffraction reveals long-range strains and disorder in molecular dynamics simulations of irradiated single crystals

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Cell orientations

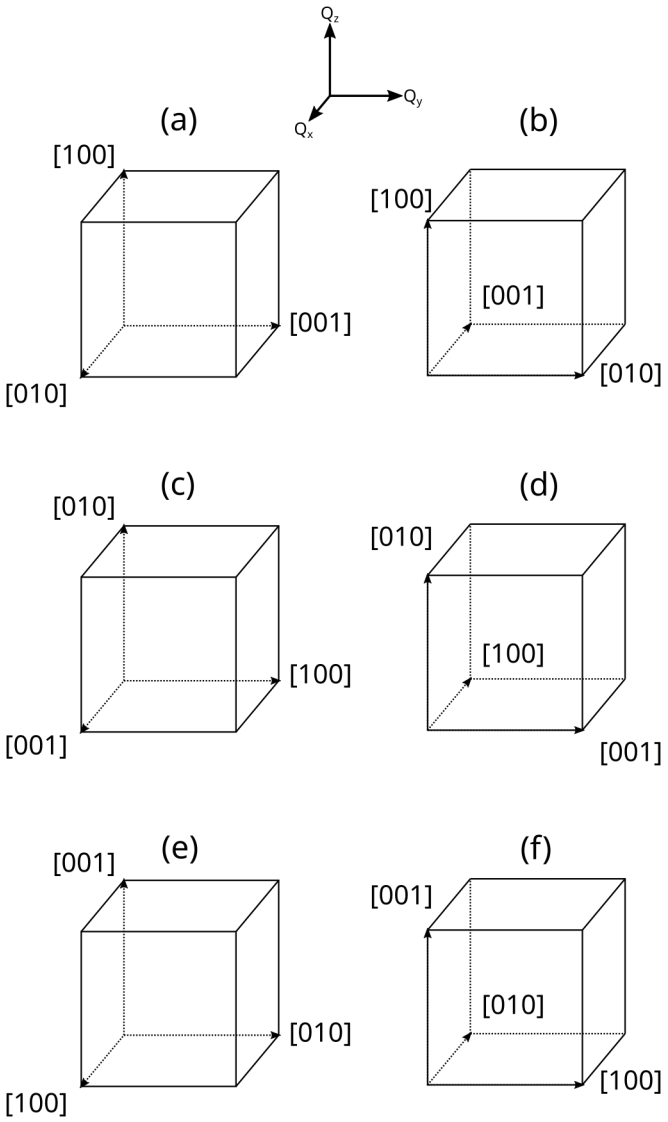

Fig. S1.The 6 different cell orientations used in this work. Labels (a-f) correspond to those of Fig. 4 in the article.

Effect of Q_y integration

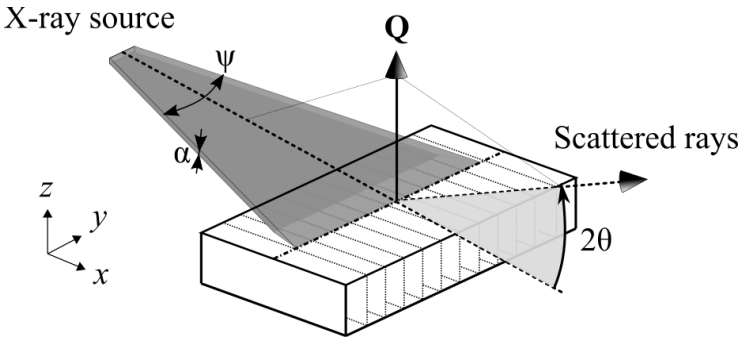

Fig. S2. Schematic illustration of the scattering geometry. The scattered photons are collected within the (x, z) plane, defined by the incident and the scattered beam. In the (x,z) plane the beam is parallel (α ~ 0), whereas it is divergent in the y direction (ψ>0). For completeness, the scattering vector **Q** *is also indicated.*

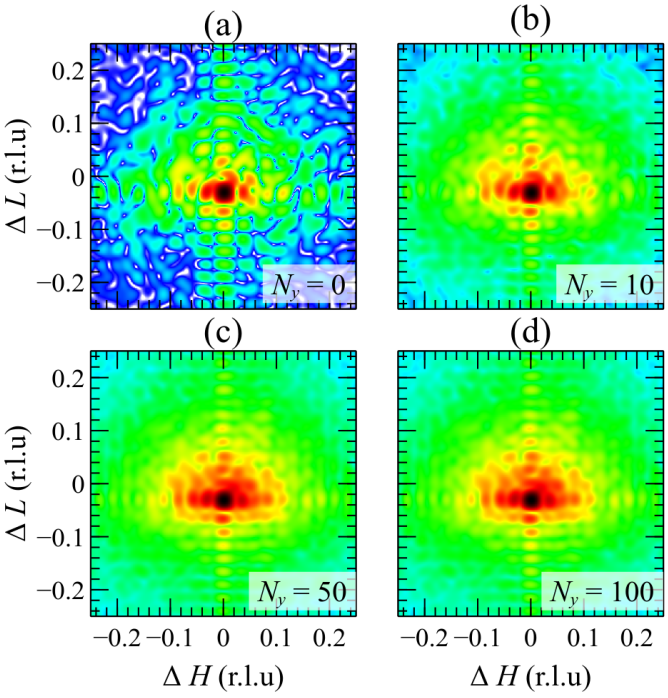

Fig. S3. Effect of the number of planes included in Eq. 1. (a) without any averaging the RSM displays a significant speckle pattern. (b) increasing the number of sections N_y results in a smoothing of the intensity distribution. When the number of (x,z) sections is higher than 50 (c, d), no evolution is observed. The intensity is plotted on a logarithmic scale using a usual red-yellow-green-blue color scale. The axes are graduated in reciprocal lattice units (r.l.u), i.e. multiples of the reciprocal space basis vectors.