Maximum-Entropy Electron-Density Maps for the Si(111) 7×7 Surface

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Maximum-entropy electron density maps have been calculated for the first time for a two-dimensional surface structure using X-ray diffraction data. In-plane reflections observed from a clean Si(111) 7×7 surface are given phases obtained from a refined model and used as a constraint in a maximization of Shannon-Jaynes entropy. The map calculated using 84 fractional-order reflections with a maximum 1.135 Å resolution clearly resolves all the 102 atoms of the Takayanagi dimer-adatom-stacking fault model. Electrons are concentrated on the atomic sites showing peaks at the adatom locations more than twice as high as the mean of the other atomic peaks, which have more uniform heights than in a Fourier map calculated from the same data. The maximum entropy method does not assume zero amplitudes for missing reflections, which extends the resolution of the data and improves the sampling of reciprocal space. The atomic positions determined from the map are in good agreement with those from a least-squares refinement. It was evidenced that the 102 atoms are visible in a map calculated from a reduced data set with 20 strongest reflections.

Left: ME electron-density map calculated for Si(111) 7×7 surface from 84 in-plane X-ray reflections. Contour lines are drawn for density levels, 0, 1, 2, 2.0, 4.0, 10.0, 20.0, 40.0, 50.0 and 60.0 in units of $e/\text{\AA}^2$. The maximum density is $72.6 e/\text{\AA}^2$.

Right: Conventional Fourier synthesis from the same 84 structure factors with phases from the model. Regions of negative densities are shaded. Contour lines are drawn for density levels 0, 5.0, 10.0, 20.0, 30.0, 40.0, 50.0, 60.0 $e/\text{\AA}^2$.