## FOUNDATIONS

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Supporting information for article:

Direct recovery of interfacial topography from coherent X-ray reflectivity: model calculations for a one-dimensional interface

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## 1) Details on the Topographic Structures in Figures 2-5:

Figures 2-3: The illumination function is centered at $\mathrm{n}=220$ with a size of 240 sites, while the surface island is located at $\mathrm{n}=191$ with a size of 51 sites.
Figure 4: A single island is located with its center at $\mathrm{n}=191$ having a size of 51 sites. For (B)-(D), the blue and green curves differ only in the illumination position, which is centered at $n=220$ and 180 , respectively (with a fixed illumination size of 240 sites and sharp edges, $\sigma_{\mathrm{n}}<1$ ). The grey curves have an illumination center of $n=220$, an illumination size of 240 , and a rms width of the illumination edges of $\sigma_{n}=25$ sites.

Figure 5: The two islands are located with their centers at $\mathrm{n}=191$ and 271 , with sizes of 51 and 31 sites, respectively, with an illumination centered at $\mathrm{n}=220$ with an illumination size of 240 sites, with either sharp edges, $\sigma_{\mathrm{n}}<1$, or soft edges, $\sigma_{\mathrm{n}}=25$.

## 2) Sorting the Second Order Patterson Function, $P_{2}(\Delta x)$, to Reveal the Topography:

Here it is assumed that the scattering occurs at the anti-Bragg condition, $L=1 / 2$, so that the effective scattering factor is $\exp (\mathrm{i} \pi h(\mathrm{n}))$ which takes on values of $\pm 1$. The observed spacings and contrasts obtained directly from the second order Patterson function, $\mathrm{P}_{2}(\Delta x)$ are sorted in decreasing order of :

$$
\begin{aligned}
\Delta X_{\mathrm{i}} & =[75,72,57,50,40,35,32,25,22,18,17,15,10,7,3] \\
\Delta \mathrm{F}_{\mathrm{i}} & =[-4,4,-4,4,-4,4,-4,-4,4,4,4,-4,-4,-4,-4]
\end{aligned}
$$

The number of observed spacings is 15 . Since a profile with $N$ steps has $N(N-1) / 2$ Fourier components corresponding to the individual step spacings, $\Delta x_{\mathrm{ij}}=x_{\mathrm{j}}-x_{\mathrm{i}}$, the observation of 15 Fourier components suggest that the structure consists of 6 steps and that there are no degeneracies in the observed step spacings. Therefore each spacing appears only once in the extended Patterson map. (Strictly speaking, the observation of 15 spacings requires that $\mathrm{N} \geq 6$. The possibility of a structure with $\mathrm{N}=7$ would require that there are exactly 6 degeneracies in the observed spacings. This and other possibilities can be tested using the same process described here, especially if no solutions are found for $\mathrm{N}=6$ ).
The challenge is to arrange these spacings and contrasts into extended Patterson maps to reveal the $x_{\mathrm{i}}$ and $\mathrm{f}_{\mathrm{i}}$, corresponding to the step locations that define a unique topographic profile (to within a constant positional offset which is not determined).

$$
\begin{aligned}
& \Delta \mathrm{x}_{1,6} \\
& \Delta x_{1,5} \quad \Delta x_{2,6} \\
& \Delta x_{1,4} \quad \Delta x_{2,5} \quad \Delta x_{3,6} \\
& \Delta \mathrm{x}_{1,3} \quad \Delta \mathrm{x}_{2,4} \quad \Delta \mathrm{x}_{3,5} \Delta \mathrm{x}_{4,6} \\
& \begin{array}{c}
\Delta \mathrm{x}_{1,2}
\end{array} \quad \Delta \mathrm{x}_{2,3} \quad \Delta \mathrm{x}_{3,4} \quad \Delta \mathrm{x}_{4,5} \Delta \mathrm{x}_{5,6},
\end{aligned}
$$

$$
\begin{gathered}
\Delta f_{1} \Delta f_{6} \\
\Delta f_{1} \Delta f_{5} \Delta f_{2} \Delta f_{6} \\
\Delta f_{1} \Delta f_{4} \Delta f_{2} \Delta f_{5} \Delta f_{3} \Delta f_{6} \\
\Delta f_{1} \Delta f_{3} \Delta f_{2} \Delta f_{4} \quad \Delta f_{3} \Delta f_{5} \Delta f_{4} \Delta f_{6} \\
\Delta f_{1} \Delta f_{2} \Delta f_{2} \Delta f_{3} \Delta f_{3} \Delta f_{4} \Delta f_{4} \Delta f_{5} \Delta f_{5} \Delta f_{6} \\
\hdashline \Delta f_{1} \quad \Delta f_{2} \quad \Delta f_{3} \quad \Delta f_{4} \quad \Delta f_{5} \quad \Delta f_{6}
\end{gathered}
$$

The first step is to sort the spacings through a decision tree that generates multiple generations of seed structures that tests potential structures.

## First Generation Solution (Seed 1.0):

The longest spacing is 75 , which must be assigned to $\Delta x_{1,6}$. The next longest spacing of 72 can be assigned to $\Delta x_{1,5}$, without any loss of generality (assigning this value to $\Delta x_{5,6}$ will lead to the mirror image of the structure generated by this assignment). Since $\Delta x_{1,6}=\Delta x_{1,5}+\Delta x_{5,6}$, the value of $\Delta x_{5,6}=75-72=3$. Therefore the $1^{\text {st }}$ generation solution (Seed 1.0) is:

$$
\begin{aligned}
& 75 \\
& 72 \Delta x_{2,6} \\
& \Delta x_{1,4} \quad \Delta x_{2,5} \quad \Delta x_{3,6} \\
& \Delta \mathrm{x}_{1,3} \quad \Delta \mathrm{x}_{2,4} \quad \Delta \mathrm{x}_{3,5} \Delta \mathrm{x}_{4,6} \\
& \Delta x_{1,2} \quad \Delta x_{2,3} \quad \Delta x_{3,4} \quad \Delta x_{4,5} \quad 3 \\
& \mathrm{x}_{1} \quad \mathrm{x}_{2} \quad \mathrm{x}_{3} \quad \mathrm{x}_{4} \quad \mathrm{x}_{5} \quad \mathrm{x}_{6}
\end{aligned}
$$

The possible solutions are explored through a decision tree, in which assignments for each generation (i.e., Seed 1.1 and 1.2 are the two second generation structures that are considered, and Seed 1.1.M will be the $\mathrm{M}^{\text {th }}$ seed structures generated from Seed 1.1). At each new generation, assignments in the proposed solutions are shown in blue, and values that are inferred from those assignments, using the many relationships between spacings, are shown in red. Current and past assignments that are not yet confirmed are labelled "?", but those where contradictions are identified are crossed-out, indicating that the structure is inconsistent with one or more observations (e.g., either because the value of a spacing is inconsistent with the observed spacings, or because different relationships reveal contradictory values for that spacing). The label for seed structures are shown as strike-through when they are ruled out and no subsequent seed structures are generated. The full decision tree for this example is:


This shows that only one structure (Seed 1.2.2.1) is consistent with the observed spacings in $\mathrm{P}_{2}(\Delta x)$. Assembling the contrast factors, using the locations determined above, confirms that this arrangement of spacings is consistent with the observed contrasts and therefore this result is fully consistent with the observations in the second order Patterson function and the measured intensities.

The specific process of sorting through these structures is shown, below, through four generations of possible solutions.

## Second Generation Seeds (1.X):

The possible second generation solutions are obtained by assigning the next largest observed spacing (57) to all possible locations within the Patterson map (noted in blue). Since this is the next largest unassigned spacing, it can only be in one of two places, $\Delta x_{2,6}$ or $\Delta x_{1,4}$. All other locations are lower in the extended Patterson map, and therefore will have smaller inter-step spacings. This leads to two second generation seed structures.

Seed 1.1 (with $\Delta x_{2,6}=57$ ):


Seed 1.2 (with $\Delta x_{1,4}=57$ ):

| 75 |
| :---: |
| $72 \Delta \mathrm{x}_{2,6}$ |
| 57? $\quad \Delta \mathrm{x}_{2,5} \quad \Delta \mathrm{x}_{3,6}$ |
| $\Delta \mathrm{x}_{1,3} \quad \Delta \mathrm{x}_{2,4} \quad \Delta \mathrm{x}_{3,5} 18$ ? |
| $\Delta \mathrm{x}_{1,2} \quad \Delta \mathrm{x}_{2,3} \quad \Delta \mathrm{x}_{3,4} \quad 15$ ? 3 |
| $\begin{array}{llll}\mathrm{x}_{2} & \mathrm{x}_{3} & \mathrm{x}_{4} & \mathrm{x}_{5}\end{array}$ |

In each case, additional spacings can be inferred from this assignment: for Seed 1.1 it can inferred that $\Delta x_{1,2}$ $=18$, and in Seed $1.2 \Delta x_{4,5}=15$, and $\Delta x_{4,6}=18$ (these inferences are shown in red). These are derived from the implicit relationships of the inter-step spacings in the extended Patterson map (e.g., for Seed 1.1: $\Delta x_{1,2}$ $+\Delta x_{2,6}=\Delta x_{1,6} ;$ for Seed 1.2: $\Delta x_{1,4}+\Delta x_{4,5}=\Delta x_{1,5}$ revealing that $\Delta x_{4,5}=15$, and then $\Delta x_{4,5}+\Delta x_{5,6}=\Delta x_{4,6}$ revealing that $\Delta x_{4,6}=18$ ). All of these inferred spacings are consistent with the observations (i.e., they are all observed values seen in $\left\{\Delta X_{\mathrm{i}}\right\}$ ). Consequently both of these Seeds remain possible and next generation Seeds need to be explored.

## Third Generation Seeds (e.g., 1.1.X):

Initially focus on using Solution 1.1 to generate next generation seeds. The next largest spacing observed, 50 , can be located in three places.

Seed 1.1.1: $\left(\Delta x_{1,4}=50\right)$ :

| 75 |
| :---: |
| 72 57? |
| 50? $\quad \Delta x_{2,5} \quad \Delta x_{3,6}$ |
| $\Delta \mathrm{x}_{1,3} \quad \Delta \mathrm{x}_{2,4} \quad \Delta \mathrm{x}_{3,5} \quad 15$ ? |
| 18? $\quad \Delta \mathrm{x}_{2,3} \quad \Delta \mathrm{x}_{3,4} \quad 12 ? 3$ |
| $\begin{array}{llll}\mathrm{x}_{2} & \mathrm{x}_{3} & \mathrm{x}_{4} & \mathrm{x}_{5}\end{array}$ |

This assignment implies that $\Delta x_{4,5}=12$, but that spacing is not observed (indicated by the cross-out). This seed is ruled out.

Seed 1.1.2: $\left(\Delta x_{2,5}=50\right)$

| 75 |
| :---: |
| 72 57? |
|  |
| $\Delta \mathrm{x}_{1,3} \quad \Delta \mathrm{x}_{2,4} \quad \Delta \mathrm{x}_{3,5} \quad \Delta \mathrm{x}_{4,6}$ |
| 18? $\quad \Delta \mathrm{x}_{2,3} \quad \Delta \mathrm{x}_{3,4} \quad \Delta \mathrm{x}_{4,5} 3$ |
| $\begin{array}{llll}\mathrm{x}_{2} & \mathrm{x}_{3} & \mathrm{x}_{4} & \mathrm{x}_{5}\end{array}$ |

This assignment is inconsistent with previously assigned values since $\Delta x_{2,5}+\Delta x_{5,6}=\Delta x_{2,6}$, but $50+3 \neq 57$.
This seed is ruled out.
Seed 1.1.3: $\left(\Delta x_{3,6}=50\right)$ :


This implies that $\Delta x_{2,3}=7$ and also that $\Delta x_{3,5}=47$. From these we can also infer that $\Delta x_{1,3}=25$. The assignment $\Delta x_{3,5}=47$ is inconsistent with the observations since it is not obsreved. This seed is ruled out. Therefore, no solutions deriving from Seed 1.1 are consistent with the observations.

Next Generation Seeds from Seed 1.2.

$$
\begin{aligned}
& 75 \\
& 72 \Delta x_{2,6} \\
& \text { 57? } \Delta x_{2,5} \quad \Delta x_{3,6} \\
& \Delta x_{1,3} \quad \Delta x_{2,4} \quad \Delta x_{3,5} \quad 18 \text { ? } \\
& \Delta \mathrm{x}_{1,2} \quad \Delta \mathrm{x}_{2,3} \quad \Delta \mathrm{x}_{3,4} \quad 15 \text { ? } 3 \\
& \begin{array}{llllll}
\mathrm{x}_{1} & \mathrm{x}_{2} & \mathrm{x}_{3} & \mathrm{x}_{4} & \mathrm{x}_{5} & \mathrm{x}_{6}
\end{array}
\end{aligned}
$$

Third generation Seeds assign the spacing 50 to one of two locations:
Seed 1.2.1 $\left(\Delta x_{2,6}=50\right)$.


This assignment implies that $\Delta x_{2,5}=47$. But this spacing is not observed and this Seed is ruled out.
Seed 1.2.2 $\left(\Delta x_{1,3}=50\right)$ :

$$
\begin{aligned}
& 75 \\
& 72 \Delta x_{2,6} \\
& \text { 57? } \Delta x_{2,5} 25 \text { ? } \\
& \text { 50? } \Delta x_{2,4} \text { 22? 18? }
\end{aligned}
$$

This implies $\Delta x_{3,4}=7$, and therefore $\Delta x_{3,5}=22$, and $\Delta x_{3,6}=25$. These spacings are consistent with the observations.

## Fourth Generation Seeds (e.g., 1.2.2.X):

Seed 1.2.2 is the only viable $3^{\text {rd }}$ generation Seed, and it is used to generate a new generation of Seeds. The next largest spacing is 40 , which can be assigned in only two locations:

Solution 1.2.2.1: Assigning $\Delta x_{1,2}=40$.


Other spacings can be assigned, including $\Delta x_{2,3}=10, \Delta x_{2,4}=17, \Delta x_{2,5}=32$, and $\Delta x_{2,6}=35$. All spacings are observed and accounted for, there are no contradictions with the observed spacings, $\left\{X_{i}\right\}$, and therefore is consistent with the second order Patterson function.

Solution 1.2.2.2: Assigning $\Delta x_{2,6}=40$.


Other implied spacings include: $\Delta x_{1,2}=35, \Delta x_{1,3}=15, \Delta x_{2,4}=22$, and $\Delta x_{2,5}=37$. However, the spacing $\Delta x_{2,5}$ $=37$ is not observed and therefore this solution is ruled out.

Only one structure is consistent with the observed spacings:


Here, the step locations, $x_{\mathrm{i}}$, (indicated below the horizontal line) are derived based on the assumption that $x_{1}=0$ (the absolute location of the structure is not determined).

Finally, we can test the consistency of these assignments with the observed contrast factors.

$$
\begin{gathered}
\Delta f_{1} \Delta f_{6} \\
\Delta f_{1} \Delta f_{5} \Delta f_{2} \Delta f_{6} \\
\Delta f_{1} \Delta f_{4} \Delta f_{2} \Delta f_{5} \Delta f_{3} \Delta f_{6} \\
\Delta f_{1} \Delta f_{3} \Delta f_{2} \Delta f_{4} \quad \Delta f_{3} \Delta f_{5} \Delta f_{4} \Delta f_{6} \\
\Delta f_{1} \Delta f_{2} \Delta f_{2} \Delta f_{3} \Delta f_{3} \Delta f_{4} \Delta f_{4} \Delta f_{5} \Delta f_{5} \Delta f_{6} \\
\hline \Delta f_{1} \quad \Delta f_{2} \quad \Delta f_{3} \quad \Delta f_{4} \quad \Delta f_{5} \quad \Delta f_{6}
\end{gathered}
$$

The contrast factors have the same arrangement of the Patterson map of the spacings:


From this, we can infer the changes in the effective scattering factor at each step assuming that $\Delta f_{1}=-2$ (corresponding to a monoatomic step at $\mathrm{L}=1 / 2$ ):


This is consistent with the observation that 9 of the features have negative contrast and 6 have positive contrast. It also reproduced the original structure in which the effective contrast at each step alternates in sign. This derived structure is the only one consistent with the observations from both the spacings and the contract values. Therefore the solution is unique.

