quite well in many cases. In his model, roughness is parameterized with β which is a occupation probability of the first layer on top of the perfectly terminated crystal. Then, the probability of the second layer, the third layer and so on are given by β^2, β^3 ... . Therefore, the CTR including surface roughness can be calculated as in Eq.(9), where $\mathrm{I_{ctr}}(\mathbf{q}\cdot\mathbf{a_3}) = 1/4\sin^2(\mathbf{q}\cdot\mathbf{a}_3/2)$. The dotted curve in Fig. 2 is a example of surface with a roughness of $\beta = 0.2$. However, this derivation is only true for a rough surface with unit cell high steps. In other words, if the unit cell consists of two atomic layers and the step is not a unit cell in height but an atomic layer, then the formula will not be a simple expression like Eq.(9).

$$\begin{aligned}\mathrm{I_{ctr,rough}}(\mathbf{q}\cdot\mathbf{a_3}) &\propto \left|\sum_{\mathrm{j}=-\infty}^{0}\exp(i\mathbf{q}\cdot\mathrm{j}\mathbf{a}_3)+\sum_{\mathrm{j}=1}^{\infty}\beta^j\exp(i\mathbf{q}\cdot\mathrm{j}\mathbf{a}_3)\right|^2 \\ &= \left|\frac{1}{1-\exp(-i\mathbf{q}\cdot\mathbf{a}_3)}+\frac{\beta\exp(i\mathbf{q}\cdot\mathbf{a}_3)}{1-\beta\exp(i\mathbf{q}\cdot\mathbf{a}_3)}\right|^2 \\ &= \mathrm{I_{ctr}}(\mathbf{q}\cdot\mathbf{a_3})\frac{(1-\beta)^2}{1+\beta^2-2\beta\cos(\mathbf{q}\cdot\mathbf{a}_3)} \qquad (9)\end{aligned}$$

An alternative roughness model has been proposed,[5] using a Poisson distribution with parameter λ rather than geometric. In that case, the intensity is given by

$$\mathrm{I_{ctr,rough}}(\mathbf{q}\cdot\mathbf{a_3}) \propto \mathrm{I_{ctr}}(\mathbf{q}\cdot\mathbf{a_3})\exp\Big(-4\lambda\sin^2(\frac{\mathbf{q}\cdot\mathbf{a_3}}{2})\Big) \qquad (10)$$

where a standard deviation of roughness is $\sigma = \sqrt{\lambda}$.

2.1.3 Algebra of orientation matrix

In this section, we briefly show how a least-squares fit works to construct the best reciprocal lattice from multiple Bragg peaks measurement. In order to make the explanation easier and since it is true that it is always possible to convert diffractometer angles to Cartesian coordinates, here we use Cartesian coordinates to locate Bragg peaks in the reciprocal space. Now consider we have n Bragg peaks which have indices (usually integers) of y_{ij}, where i runs from 1 to 3 and j from 1 to n.

These form a matrix, **Y**. Their Cartesian coordinates in the reciprocal space are x_{ij}, where i and j run from 1 to 3 and n, respectively. Note that we fix and use some reference coordinate system to locate the Bragg peaks from the beginning, which is defined relative to the zero's of the diffractometer angles by Busing and Levy[6]. If n is 3, there exists a unique 3×3 matrix **A** so that **Y=AX**. **A** is a transformation matrix which relates our reference coordinate system and the one we would like to define. In other words, it transforms the unit vectors from one coordinate system to those of the other. If n is larger than 3, there will not usually exist a matrix which satisfies **Y=AX**. So, our goal is to find a matrix **A** with known matrices **X, Y** which minimizes

$$\Lambda = \sum_{j=1}^{n} \sum_{i=1}^{3} (\sum_{k=1}^{3} a_{ik} x_{kj} - y_{ij})^2 \tag{11}$$

So,

$$\frac{\partial \Lambda}{\partial a_{pq}} = 2 \sum_{j=1}^{n} \sum_{i=1}^{3} (\sum_{k=1}^{3} a_{ik} x_{kj} - y_{ij}) \delta_{ip} x_{qj} = 2 \sum_{j=1}^{n} (\sum_{k=1}^{3} a_{pk} x_{kj} - y_{pj}) x_{qj} = 0 \tag{12}$$

which is in a matrix notation

$$\mathbf{A}\mathbf{X}\mathbf{X}^{\mathrm{T}} = \mathbf{Y}\mathbf{X}^{\mathrm{T}}. \tag{13}$$

Therefore,

$$\mathbf{A} = \mathbf{Y}\mathbf{X}^{\mathrm{T}}(\mathbf{X}\mathbf{X}^{\mathrm{T}})^{-1}. \tag{14}$$

Note that an inverse of **X** has no meaning since **X** is a 3×n matrix. We can calculate the lattice constants from a transformation matrix **A** because unit vectors of a reciprocal space have one-to-one correspondence with those of a real space. More details can be found in reference[6].

2.1.4 X-ray diffraction geometry

In our x-ray diffraction experiments, four angles, $2\theta, \theta, \chi$ and ϕ, are used to control the sample orientation and detector position. Since only three Eulerian angles are