Bohr *et al.* Respond: The preceding Comment by Yang and Zhao[1] raises the interesting question of the significance of a fractional Patterson function. In this reply we will show that a fractional Patterson function has a straightforward meaning which allows the standard interpretation of its peaks: The set of positive peaks corresponds to a subset of the interatomic vectors.

The Patterson function $P(x,y)$ is the pair-correlation function of the electronic density. Thus $P(x,y) \geqslant 0$ and its peaks are signatures of interatomic vectors. In crystallography of reconstructed surfaces it is customary to define Miller indices which are fractions of those of the "primal" (unreconstructed) unit cell. We now define the "fractional Patterson function" $F(x,y)$ as

$$F(x,y) = \sum_{\text{Fract. } h,k} |F_{hk}|^2 \cos 2\pi(hx+ky),$$

where F_{hk} are the structure factors and where the sum is over only noninteger h,k. We seek to determine the relation of this function $F(x,y)$ to $P(x,y)$,

$$P(x,y) = \sum_{\text{All } h,k} |F_{hk}|^2 \cos 2\pi(hx+ky),$$

where the sum is over all fractional and integer h,k. We can write $F(x,y) = P(x,y) - I(x,y)$, where

$$I(x,y) = \sum_{\text{Int. } h,k} |F_{hk}|^2 \cos 2\pi(hx+ky),$$

where the sum is over only integer h,k. The integer-order F_{hk}'s are the complete set of Fourier components of the electronic density of a hypothetical structure, constructed by dividing the bigger reconstructed unit cell into primal-sized regions and superimposing the electronic densities. Therefore $I(x,y)$ is itself a Patterson function and thus never negative. *Consequently all positive peaks (above zero) in $F(x,y) = P(x,y) - I(x,y)$ must also be peaks in $P(x,y)$.*

In a diffraction experiment one is limited to measuring a finite set of structure factors. The truncated Patterson sum, calculated from a set of experimental data, is a map of the pair correlation of the electronic density with limited resolution. Under these circumstances, it is possible for a peak in $P(x,y)$ to be annihilated by a strong peak in $I(x,y)$ nearby. Also a peak in $F(x,y)$ could be shifted in position as a result of a nearby peak in $I(x,y)$. This, however, does not change the conclusion that $F(x,y)$ can have no false positive peaks.

Fractional Patterson functions have been successfully applied in several other studies. The x-ray diffraction study of Au(110)2×1[2] and the transmission electron diffraction study of Si(111)7×7[3] are notable examples. In our InSb(111)2×2[4] study, we calculated $F(x,y)$ and found a structure to explain all the interatomic vectors therein. For reasons given above, this was not the complete structure. Subsequently, the remaining atom was revealed in a difference Fourier map. Finally, least-squares refinement confirmed the consistency of the derived structure. We believe that we have defended our claim of a model-independent structure determination.

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