Mosaic crystals in SHADOW: an update

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March 22, 2013

Abstract

This document explains an update of the SHADOW model for mosaic crystals. The model is described in [1]. This update corrects some problems with the model and fix some bugs that prevent to use this mosaic crystal option in SHADOW3.

1 The mosaic model

Since version 3 of SHADOW, the mosaic model is not working properly because it produces beam images that are not symmetric but lacking of a part of the image. It is due to the random number generator used does not update the random seed. This is easily fixed with this code (routine `MOSAIC` in file `shadow_kernel.F90`):

```
! *next lines give the random direction (ccw or acw) for the rotation
!
! note that random seed initialization is useless, as now WRAN only
    initializes
! once at the beginning of the run. Thus, MOSAIC_SEED is not considered.
        IPP = MOSAIC_SEED
        DUMM = WRAN (IPP)
!       IF (IPP.LT.0) XXX=-XXX
        IF (DUMM.LT.0.5) THEN
           xxx1 = -xxx1
        END IF
```

A simplification can be made using the following expression for ϕ as a function of β, obtained by some manipulation of Eqs. (2) and (3) in Ref. [1]:

$$\cos\phi = \cos\alpha\cos\theta_D + \cos\beta\sin\alpha\sin\theta_D \tag{1}$$

Therefore, the new code to calculate β is:

```
        !HH2 = ABS(TAN_VAL - TAN_B)
        !HHH = SQRT(COS_B**(-2)+COS_VAL**(-2)-2*COS(XX)/COS_B/COS_VAL)
        !COS_XXX = (HHH**2-TAN_VAL**2-TAN_B**2)/(-2*TAN_VAL*TAN_B)
        !IF (ABS(COS_XXX).GT.1) CALL MSSG('Error in MOSAIC','cos>1',
            izero)
        !XXX = ACOS(COS_XXX)
        !XXX = ABS(XXX)
        xxx1 = (cos(xx) - cos_val*cos_b) / (sin_val*sin_b)
        xxx1 = acos(xxx1)
```

Moreover, the Eqs. (6) and (7) in [1] are incorrect, and should say:

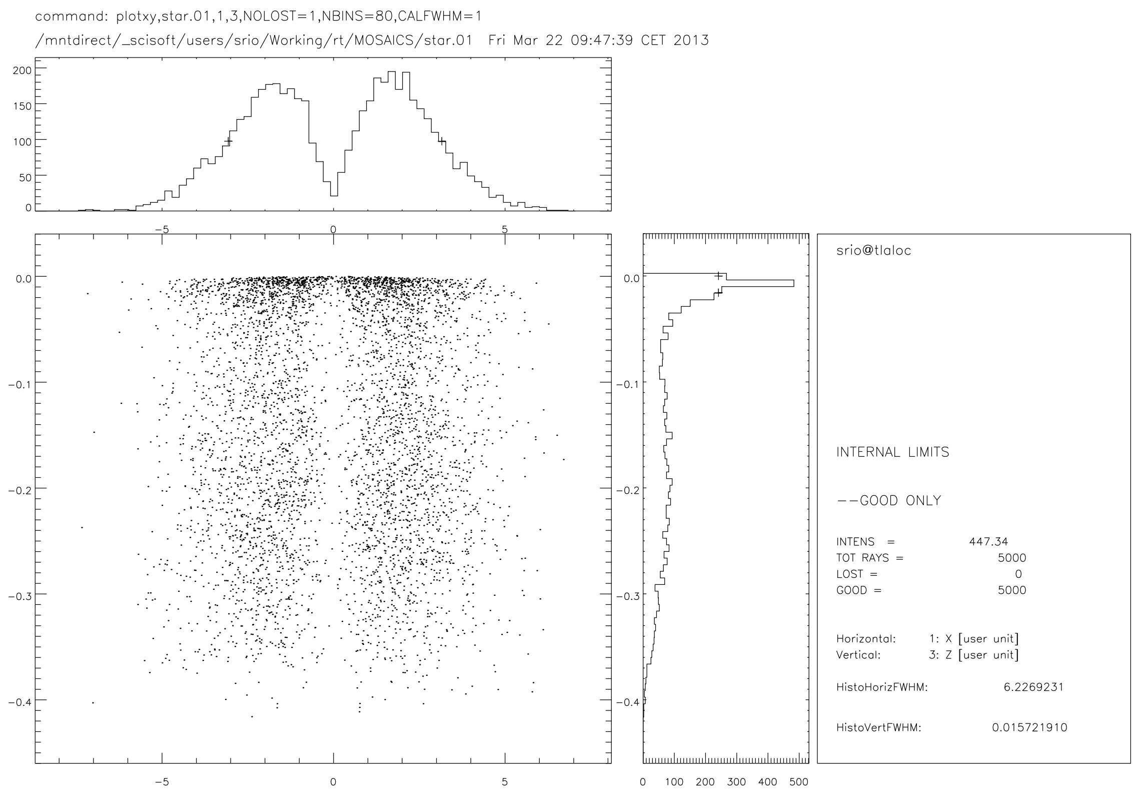

Figure 1: ray tracing of a HOPG 002 crystal , using a point source at 3 keV with vertical divergence 0.02 rad and zero horizontal divergence. The crystal is placed at 10 m from the source and the image is taken at 20 m from the source. Workspace file `mymosaic_v1.ws`

$$Q_s = \left(\frac{e^2}{mc^2} \frac{1}{v_0} \right)^2 \frac{|F_H|^2 \lambda^3}{\sin 2\theta_B} \tag{2}$$

$$Q_p = Q_s (\cos 2\theta_B)^2 \tag{3}$$

.

This model presents two problems, although they do not prevent of using SHADOW for most cases:

- it fails to obtain the output ray direction when a ray arrives far from the Bragg angle
- it produces some “holes” in the ray distribution around the center. It can be appreciated looking carefully at the Fig.(6) in [1]: there is some “lack: of points around the zero. This can be better appreciated in Fig. 1.

2 The corrected mosaic model: solutions for the problems

The reason of the problems mentioned in the previous section is that in the calculation we first obtain a random number ϕ in the interval $[\alpha - \theta_D, \alpha + \theta_D]$ and then we "force" the ray to have this ϕ but verifying the Bragg law. Instead, we should first calculate the new probability density as a function of the β angle, matching the possible crystallite normals that fit the Bragg law, and then sample a number following this new probablity distribution. We start with the Gaussian distribution of crystallites (Eq. (1) in [1]):

$$w(\phi) \propto e^{-\frac{\phi^2}{2\tau}} \tag{4}$$

The new probability distribution as a function of β is just obtained expressing $w(\phi)$ as a function of β :

$$w(\beta) \propto e^{-\frac{[\phi(\beta)]^2}{2\tau}} \tag{5}$$

This can be expanded using Eq. 1, giving a complicated expression. However, numerical calculations of several cases ranging from grazing to normal incidence showed that the resulting probability distribution $w(\beta)$ is Gaussian in a very good approximation. Therefore, instead of working with the complicated new probability distribution we can obtain the approximated Gaussian distribution. Sampling a number from this distribution is easy and already implemented in SHADOW. Expanding in power series ϕ^2 around $\beta = 0$:

$$\phi^2(\beta) = s_0 + s_1\beta^2 + o(\beta^4) \tag{6}$$

The s_0 coefficient will give a multiplying constant when introducing Eq. 6 in 4, and the s_1 will give the standard deviation of the new Gaussian distribution:

$$w(\beta) \propto e^{-\frac{\beta^2}{2\tau'}} \tag{7}$$

$$\tau' = \frac{\tau}{\sqrt{s_1}} \tag{8}$$

The value of s_1 is (see Appendix):

$$s_1 = \frac{\sin\theta_D \sin\alpha \cos^{-1}(\sin\theta_D \sin\alpha + \cos\theta_D \cos\alpha)}{\sqrt{1 - (\sin\theta_D \sin\alpha + \cos\theta_D \cos\alpha)^2}} \tag{9}$$

These equations have been written in the new version of the `MOSAIC` routine and now give correct results (see Figs. 2 and 2).

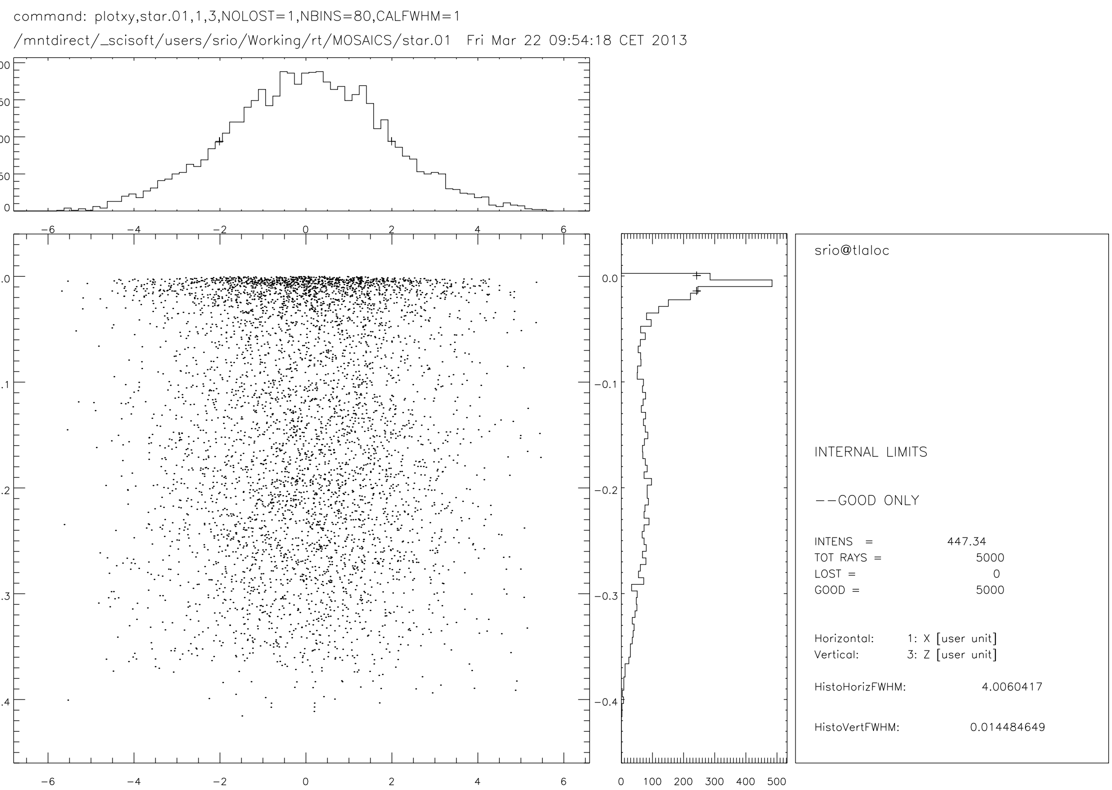

Figure 2: The same as in Fig. 1 but using the upgraded mosaic model.

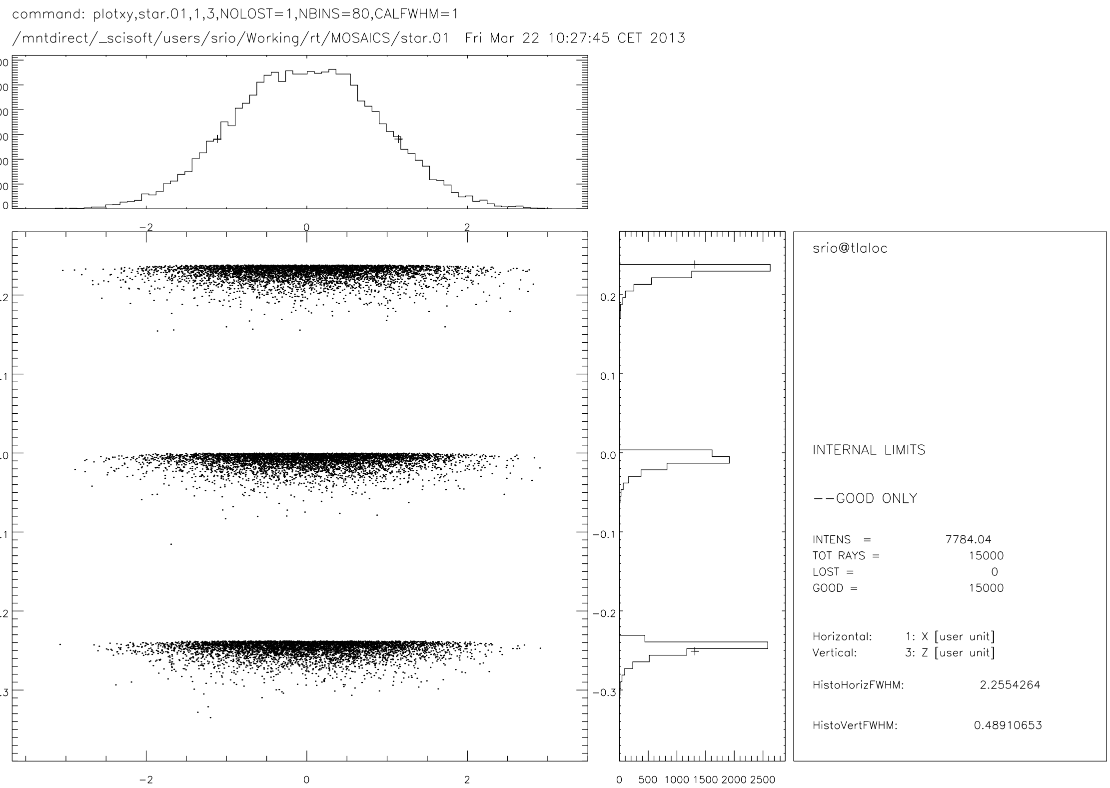

Figure 3: The same as in Fig. (6) in Ref. [1] but using the upgraded mosaic model.

A Series expansion of ϕ as a function of β

The Eqs. 1 and 9 have been obtained with the following Mathematica piece of code:

```
In[3]:= f3 = (Tan[thetaD]^2 + Tan[alpha]^2 - 2 Tan[thetaD] Tan[alpha]
      Cos[beta] -
     Cos[thetaD]^(-2) - Cos[alpha]^(-2)) (-1/2) Cos[thetaD] Cos[alpha]

Out[3]= -(1/2) Cos[alpha] Cos[
  thetaD] (-Sec[alpha]^2 - Sec[thetaD]^2 + Tan[alpha]^2 -
   2 Cos[beta] Tan[alpha] Tan[thetaD] + Tan[thetaD]^2)

In[4]:= f4 = FullSimplify[f3]

Out[4]= Cos[alpha] Cos[thetaD] + Cos[beta] Sin[alpha] Sin[thetaD]

In[8]:=
newphi2 = Series[(ArcCos[f4])^2, {beta, 0, 3}]

Out[8]= SeriesData[beta, 0, {
 ArcCos[Cos[alpha] Cos[thetaD] + Sin[alpha] Sin[thetaD]]^2, 0,
  ArcCos[Cos[alpha] Cos[thetaD] + Sin[alpha] Sin[thetaD]] Sin[alpha] Sin
      [
   thetaD] (1 - (
     Cos[alpha] Cos[thetaD] + Sin[alpha] Sin[thetaD])^2)^Rational[-1,
     2]}, 0, 4, 1]

In[9]:= cl = CoefficientList[newphi2, beta]

Out[9]= {ArcCos[Cos[alpha] Cos[thetaD] +
   Sin[alpha] Sin[thetaD]]^2, 0, (ArcCos[
     Cos[alpha] Cos[thetaD] + Sin[alpha] Sin[thetaD]] Sin[alpha] Sin[
     thetaD])/(Sqrt[1 - (Cos[alpha] Cos[thetaD] + Sin[alpha] Sin[thetaD
         ])^2])}

In[10]:= FortranForm[cl[[3]]]

Out[10]//FortranForm=
        (ArcCos(Cos(alpha)*Cos(thetaD) +
     -        Sin(alpha)*Sin(thetaD))*Sin(alpha)*Sin(thetaD))/
     -    Sqrt(1 - (Cos(alpha)*Cos(thetaD) +
     -         Sin(alpha)*Sin(thetaD))**2)
```

References

[1] M. Sanchez del Rio, S. Bernstorff, A. Savoia, and F. Cerrina. A conceptual model for ray tracing calculations with mosaic crystals. *Review of Scientific Instruments*, 63(1):932–935, 1992.