

X-Ray Optics in the BMAD Beam Dynamics Computer Code

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The BMAD framework is currently employed at Cornell University for computer simulations of the CESR and ERL beam pipes. As the present implementation mainly deals with charged particle optics, we wish to extend the framework to include X-Ray optics. The mirror was the main optic that I developed; with various features ranging from offsets to curvature to orientation errors, mirrors can now be simulated in experiments involving photon sources. This paper details the calculations and geometry entailed in the framework extension and comments regarding the corresponding BMAD code.

I. INTRODUCTION

Two software components are used in accelerator simulation at Cornell: the Tool for Accelerator Optics (Tao) and BMAD. The former presents a front end interface in which users may specify lattice files and accelerator properties. Features such as drawing accelerator components and graphing accelerator functions over distance have also been implemented. Calculations and bookkeeping are taken care of by BMAD, a library of accelerator subroutines. The current BMAD libraries contain implementations for most accelerator optics and track most conventional accelerator properties. This project dealt with developing a mirror optic for BMAD to simulate X-Ray optics. Mirrors have a set of parameters which can be modified to specify placement, orientation, and shape. Users may also specify various errors to ensure that experimental error bounds are acceptable. Mirror parameters are listed as follows:

Mirror Parameters	
Graze Angle	ϕ
Tilt	τ
Tilt Error	τ_e
Graze Angle Error	ϕ_e
x-offset	x_0
y-offset	y_0
s-offset	s_0
x-pitch	θ_x
y-pitch	θ_y

We will now provide an introduction to the coordinate systems employed by BMAD.

II. BMAD COORDINATE SYSTEMS

A. Spatial and Angular Coordinates

Incoming beams are specified using a 6-vector, \vec{v} , where $v(1)$, $v(3)$, and $v(5)$ describe the beam's x , y , and z spatial coordinates, respectively, $v(2)$ and $v(4)$ describe the beam's x and y canonical momenta (from now on referred to as x' and y' , and $v(6)$ describes the beam's energy. For a diagram of the spatial coordinates, please refer to Figure 2.

The canonical momenta are normalized as follows:

$$x' = P_x/P_0 \quad (1)$$

$$y' = y'/P_0 \quad (2)$$

For practical purposes, $p_x, y' \ll 1$, so using the small-angle (paraxial) approximation, and assuming that the particles involved are highly relativistic, we find that

$$x' \approx dx/ds \quad (3)$$

$$y' \approx dy/ds \quad (4)$$

This project deals with photons whose trajectories are very close to the reference orbit, so the above approximations are justified.

B. Z Coordinates

For information regarding z-coordinates, canonical and spatial, please refer to pg. 21 in the BMAD Manual [1].

III. MIRROR PARAMETERS AND COORDINATE SYSTEMS

Mirrors in BMAD have a variety of parameters, each of which may be adjusted to simulate orientation and placement. These parameters are illustrated in Figure 1. Tilts, offsets, and pitches are illustrated in Figures 3 and 4.

A melange of four coordinate systems and three steps were used in the transfer calculations; this transfer system not only provides a methodical way of obtaining the result, but

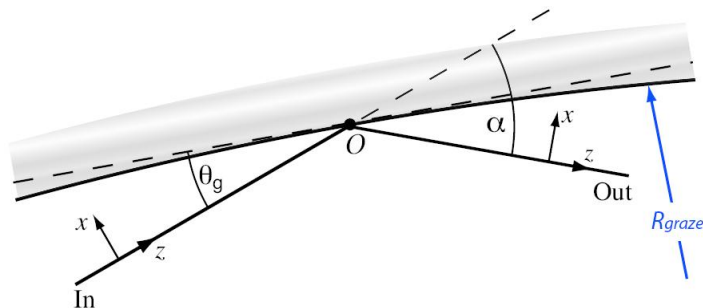


FIG. 1: A Sample Mirror in BMAD [1]

also allows for extension to curved and user-defined mirror geometries. These four coordinate systems are illustrated in Figure 5.

The idea is to first transfer the beam coordinates from the "lab in" (LI) frame to the "element in" (EI) frame, to next perform the reflection across the mirror, yielding coordinates in the "element out" (EO) frame, and to finally transfer these coordinates to the "lab out" (LO) frame. Within each of the steps, we will derive respective formulae which relate to each of the mirror parameters.

IV. FROM LI TO EI

In this procedure, we transfer from the lab-in reference frame to the element-in reference frame. When doing so, we operate on the displacements and errors in the following order: offsets, pitches, tilts, graze angle error. It is essential to note that the final beam coordinates will not be computed using all parameters simultaneously, but will be computed using each parameter individually in a multistep fashion. By using the above order, we repeatedly shift the reference frame and finally arrive at the appropriate element-in frame after resolving the graze angle error. This method increases code readability, extends flexibility, and facilitates debugging.

A. Offsets

We first deal with mirror offsets given an input 6-vector. Note that without any tilts or mirror pitches, the y -component doesn't affect the output. In Figure 6, we must solve for $O'Y$ to find x in the EI reference frame. Looking at quadrilateral $WAO'Y$, we find that

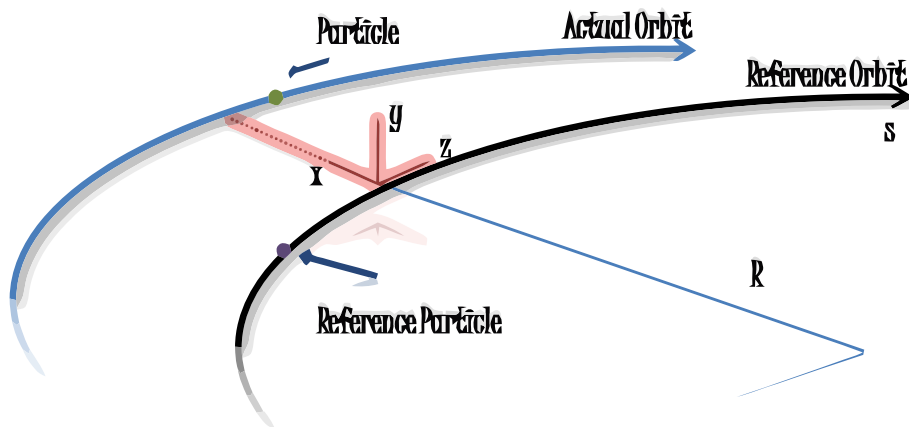


FIG. 2: BMAD Coordinate Systems

$$x_{EI} = O'Y = \frac{\cos x'(x - x_0) + s_0 \sin x'}{\cos x'} = x - x_0 + s_0 \tan x', \quad (5)$$

which is our x in the EI reference frame. We can also deduce from the figure that x' is invariant since lines $O'I$ and XO are parallel. By symmetry, coordinate y is identical to the above if we replace x' with y' and x with y ; the y' coordinate is invariant. We next compute the z canonical component of the offsets. From Figure 6, we observe that the particle travels an extra distance, equal to the length from the LI z plane to the EI z plane, compared to the reference particle. This corresponds to the length of segment WY . Again, considering quadrilateral $WAO'Y$, we find that

$$\Delta z_{can} = -WY = \frac{s_0}{\cos x'} \quad (6)$$

Since the particle falls behind by travelling this distance, the distance for WY is negative, as illustrated above. At this point, we add Δz_{can} to the z_{can} value to receive our z_{can} value in the EI frame.

B. Pitches

Because we have broken down the procedure into manipulating parameters separately, we can, in fact, treat x-pitches the same way we treat the graze angle error. When in the EI reference frame, x-pitches and graze angle errors operate in the same manner, excepting that they rotate in opposite directions. It turns out that y-pitches are very similar as well; this is because of the inherent symmetry in the transformations. Particularly, transformations involving x-pitches and y-pitches are identical, including signs, excepting for one small detail. When using y-pitches, we have to make use of the z' -spatial coordinate, since a y-pitch involves a positive rotation about the negative x-axis (in contrast to x-pitches, which involve positive rotations about the positive y-axis). To compute this change in the z' -spatial

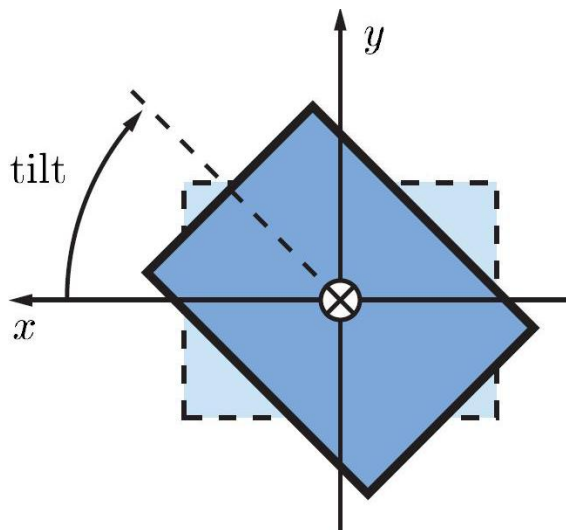


FIG. 3: Tilts [1]

coordinate, we apply the appropriate rotation matrix to the input canonical momentum vector. It turns out that the new z' value may be expressed as $y' \sin \theta_y + \cos \theta_y$.

C. Tilts and Tilt Errors

A tilt is a rotation about the incoming lab reference frame in the positive direction; this parameter is special in that it also rotates the outgoing lab reference frame about this axis. When a tilt has been performed, the mirror, and therefore the EI frame, rotates about the incoming lab reference frame by τ , the tilt angle. Since the incoming beam doesn't rotate about the axis, transferring the coordinates is equivalent to rotating the coordinates about the negative incoming lab reference frame; in other words, this is a change of basis, whose basis vectors are rotated by the tilt around the axis mentioned. We thus have

$$x_{EI} = x \cos \tau + y \sin \tau \quad (7)$$

$$y_{EI} = -x \sin \tau + y \cos \tau \quad (8)$$

Similarly, the x' and y' coordinates transform as above, so we have

$$x'_{EI} = x' \cos \tau + y' \sin \tau \quad (9)$$

$$y'_{EI} = -x' \sin \tau + y' \cos \tau \quad (10)$$

As we will see, inverting this tilt when going from the EO frame to the LO frame is similar to the above; we simply rotate in the opposite direction, but about the positive EO reference frame instead of the negative LI reference frame. In BMAD, the subroutine `tilt_coords` is used to work with tilts since the above action is common.

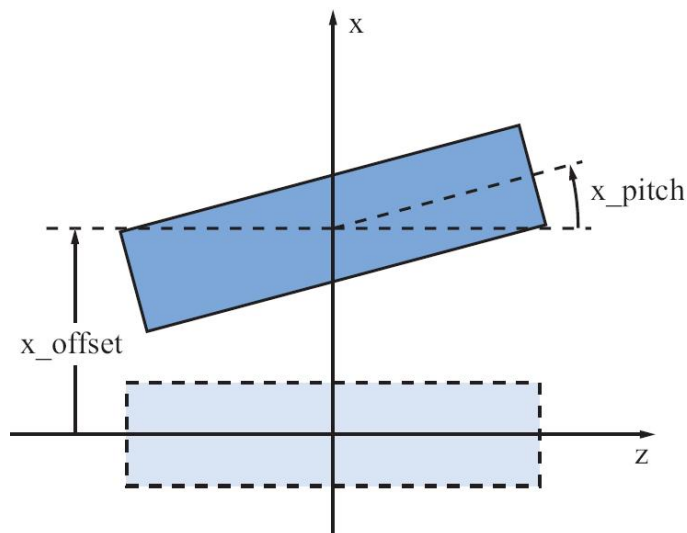


FIG. 4: Pitches and Offsets [1]

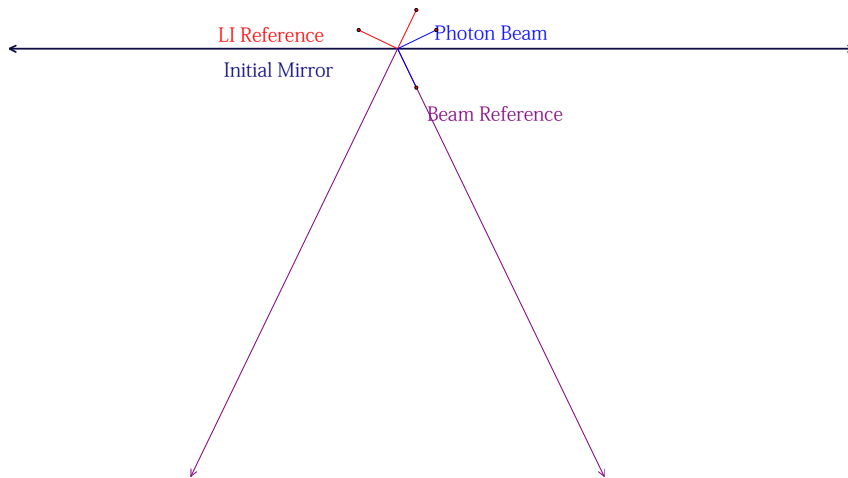


FIG. 5: Mirror Coordinate Systems

D. Graze Angle Error

In deriving the formulae for graze angle errors, we use Figure 7. We observe that we need to find OB . Considering $\triangle OAB$, we find that

$$OB = \frac{x \cos(\phi_e + x')}{\cos(2\phi_e + x')}, \quad (11)$$

which is our x in the element frame. We also observe that our x' is $\angle AX'O = \phi_e + x'$. Coordinates y and y' do not change in this procedure. Using Figure 7, we find that

$$\Delta z_{can} = -GH = \frac{x \sin \phi_e}{\cos(x' + \phi_e)} \quad (12)$$

V. FROM EI TO EO

Another advantage to using this three step process supplemented with modifying parameters in succession is that the set and unset procedures are invariant with respect to mirror shape; the only part which changes is this step. Fortunately, we can safely ignore the offsets and errors mentioned above, as the set method has placed us within the element's frame of reference. In this paper, we will discuss only reflections about flat mirrors.

A. Flat Mirrors

Reflections with flat mirrors are relatively simple to deal with. Looking at Figure 9, it is clear that

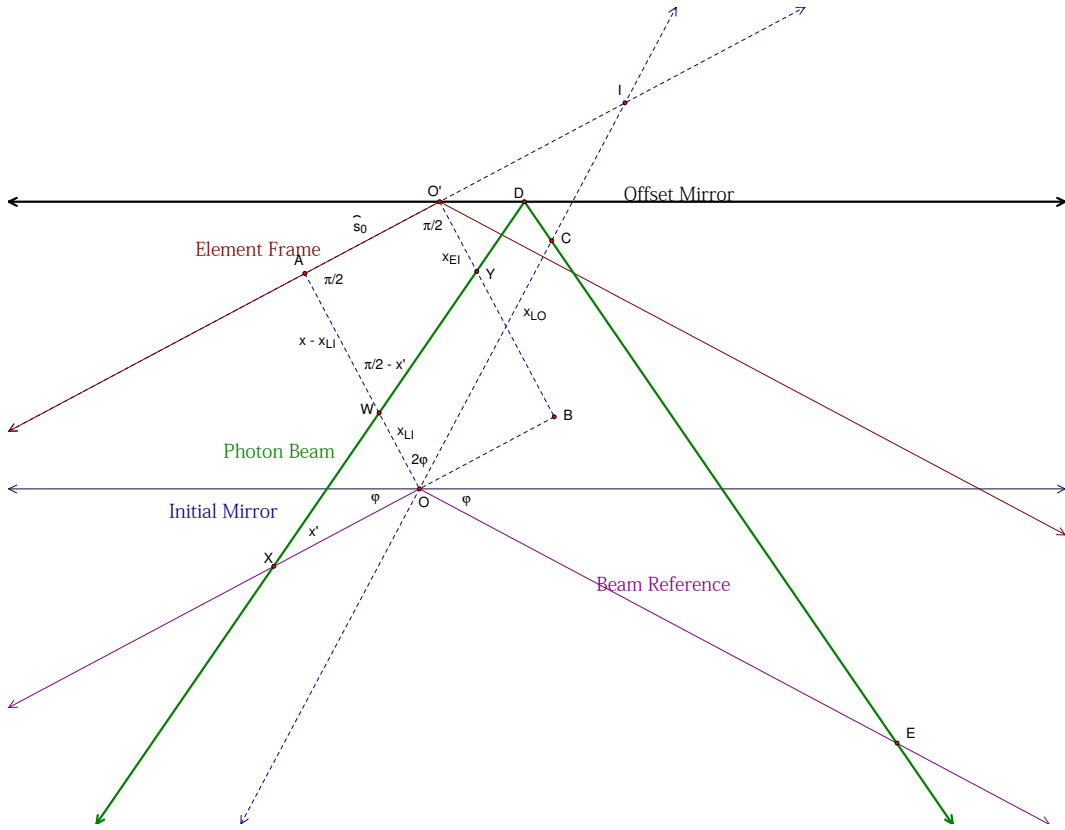


FIG. 6: Offsets: LI to EI

$$x_{EO} = -x_{EI}, x'_{EO} = -x'_{EI}, y_{EO} = -y_{EI}, y'_{EO} = -y'_{EI} \quad (13)$$

To see why, reflect all lines about the mirror. If A's image is A' and B's image is B', we find that points A' and B are concurrent as are points A and B'. Since OA and OB can be obtained by reflection about the mirror, they have the same length. Similar arguments may be made for the other coordinates.

VI. FROM EO TO LO

We now proceed with inverting the changes made above to transform to the lab out frame. Most of the following procedures are relatively simple to follow. However, results for tilt errors and pitches can be difficult to derive analytically. Because of this, we follow this general algorithm:

1. Find the transformation that converts the lab-in displacement vectors to the lab-out displacement vectors.
2. Apply this transformation to the displacement vector involved (rotation, offset) in the lab-in reference frame to transform this displacement vector to the equivalent lab-out displacement.
3. Apply the lab-out displacement vector to the input coordinates.

4. Propagate the above beam coordinates until the z component is 0; these beam coordinates are the final beam coordinates in the lab-out frame.

Using first order approximations, the above algorithm provides accurate data providing that the parameters involved are very small. The BMAD code follows the above algorithm; the `xrot`, `xrot`, and `zrot` variables form the displacement vectors involving rotations, while the `xdisp`, `xdisp`, and `zdisp` variables form the displacement vectors involving translations. These vectors have already been transformed from LI to LO using the transformation denoted by Eq. 20 [1]. Next, the code performs the above displacements about the respective axes. For z -rotations, the `tilt_coords` method is called, as this is essentially a tilt. Finally, propagations are coded.

A. Graze Angle Error

Our first step will be to invert the graze angle error; to do so, we use Figure 8. For simplicity, the EI reference frame has been omitted. Now, note that the x received is $-OA$, since the step from EI to EO inverts x . Repeatedly using the law of sines, we find that

$$OY = -\frac{OA \cos(x' - \phi_e)}{\cos(x' + \phi_e)} = \frac{x \cos(x' - \phi_e)}{\cos(x' + \phi_e)}, \quad (14)$$

which gives us x in the LO reference frame. From the diagram, we find that $\angle BYC = -(2\phi_e + x')$, which is our x' in the LO reference frame. Note that in both formulae, signs

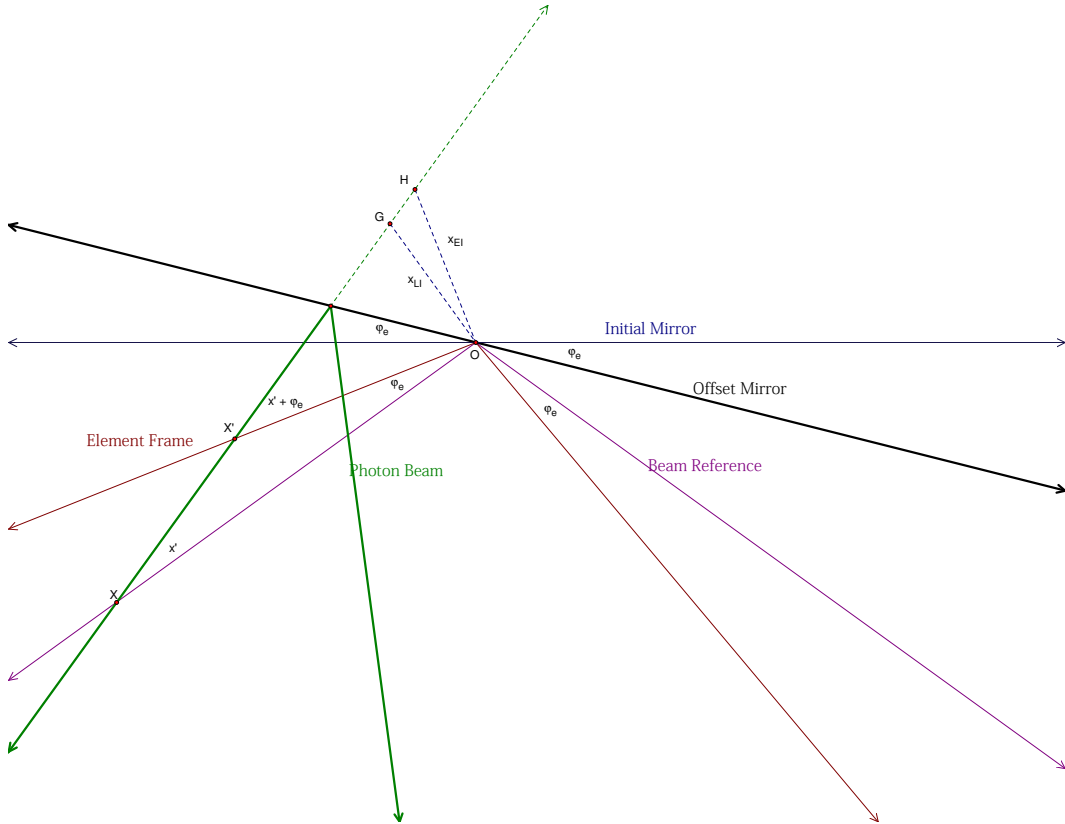


FIG. 7: Graze Angle Error: LI to EI

play an important role in orientation. The y, y' coordinates aren't affected here. In the BMAD code, x' isn't replaced with $-(2\phi_e + x')$, but is instead replaced with $x' - \phi_e$. To see why, remember that in the previous steps, we first added ϕ_e to x' (in the LI to EI step) and inverted this value (in the reflection step), to arrive at the starting x' coordinate in the EO to LO step. However, the formula derived above uses the value of x' in the LI frame, ignoring all other mirror parameters; the original value of x' , expressed in terms of the x' value in the EO frame, is $-x' - \phi_e$. Since we need the final x' to be $-(2\phi_e + x')$, we simply subtract x' from this quantity.

To find how z canonical is affected, we use Figure 8. Using standard trigonometry, we find that

$$\Delta z_{can} = \frac{x_0 \sin \phi_e}{\cos(y' + 2\phi_e)} \quad (15)$$

This distance is to be subtracted from the canonical z at this point, since the particle has to cover this extra distance when travelling through space.

B. Tilts

To transfer from the EO to the LO frame given an initial tilt, we simply tilt back about the lab out reference frame. To see why, consider the rotation made in the EI frame; construct an equivalent transformation in the LO frame. If we apply the inverse of this equivalent

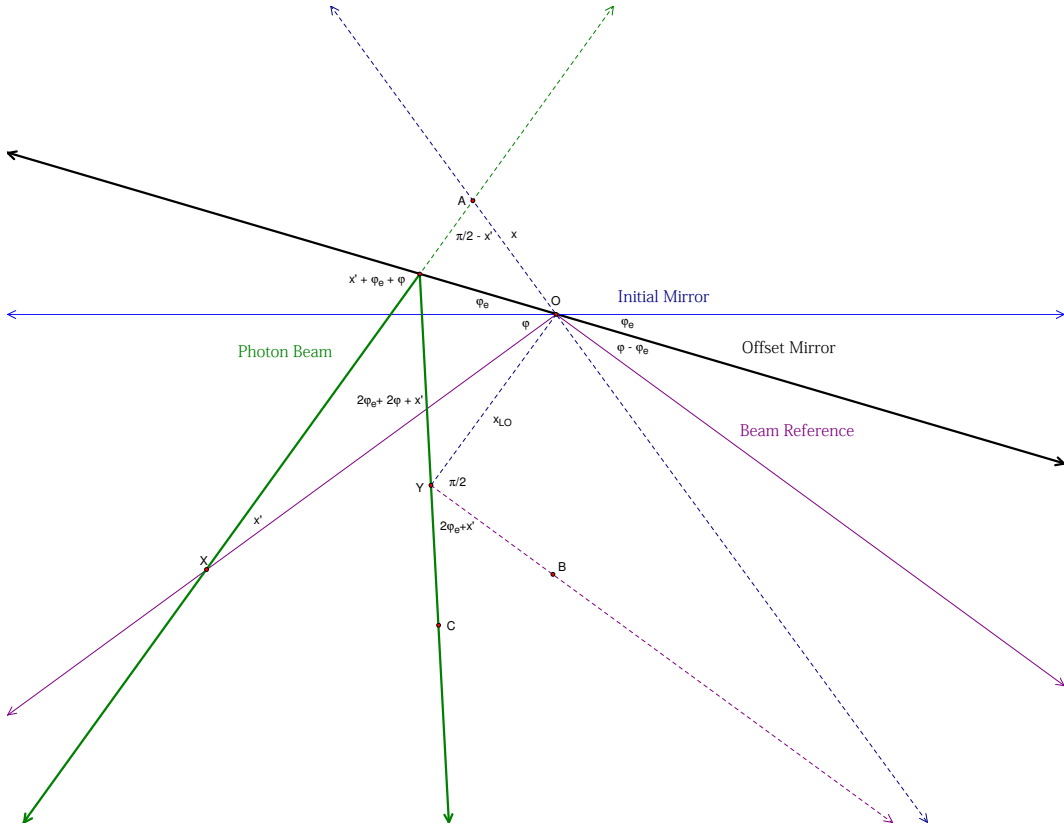


FIG. 8: Graze Angle Error: EO to LO

transformation, we proceed to the LO frame. That is,

$$x_{EI} = x \cos \tau - y \sin \tau \quad (16)$$

$$y_{EI} = x \sin \tau + y \cos \tau \quad (17)$$

$$x'_{EI} = x' \cos \tau - y' \sin \tau \quad (18)$$

$$y'_{EI} = x' \sin \tau + y' \cos \tau \quad (19)$$

Since tilts change the beam reference in the same way the particle reference is affected, tilts don't affect the z canonical component. The `tilt_coords` method is employed in BMAD here as well.

C. Tilt Errors

The BMAD Manual provides the transformation from the LI frame to the LO frame. A mirror is a bend of length 0 with bend angle 2ϕ . Given this information, we have this transformation, $S = TS_0T^{-1}$, where

$$T = \begin{pmatrix} \cos \tau & -\sin \tau & 0 \\ \sin \tau & \cos \tau & 0 \\ 0 & 0 & 1 \end{pmatrix}, S_0 = \begin{pmatrix} \cos 2\phi & 0 & -\sin 2\phi \\ 0 & 1 & 0 \\ \sin 2\phi & 0 & \cos 2\phi \end{pmatrix} \quad (20)$$

Now, a tilt error in the LI frame entails a positive rotation about the z axis. Therefore, this LI rotation vector, R , corresponds to the following LO rotation vector, \hat{R} :

$$\hat{R} = SR = \begin{pmatrix} -\tau_e \cos \tau \sin 2\phi \\ -\tau_e \sin \tau \sin 2\phi \\ \tau_e \cos 2\phi \end{pmatrix}, R = \begin{pmatrix} 0 \\ 0 \\ \tau_e \end{pmatrix} \quad (21)$$

We apply the opposite of this rotation vector (i.e. rotate around the x -axis by $-\hat{R}_x$, etc.) to the input 6-vector V_0 and get another vector V_1 . Next, we propagate this vector until the vector's z -component is 0. This gives us the vector in the LO frame, V_2 , which is

$$V_2 = \begin{pmatrix} x_{v_1} - x'_{v_1} z_{v_1} / z'_{v_1} \\ y_{v_1} - y'_{v_1} z_{v_1} / z'_{v_1} \\ 0 \end{pmatrix} \quad (22)$$

Finally, to compute the z canonical component for this vector, we find the distance of propagation and subtract this from Δz_{disp} , the total amount by which z_{v_1} changed through the rotations performed with Eq. 20. We thus add

$$\Delta z_{can} = -\sqrt{\left(\frac{x' z_{v_1}}{z'_{v_1}}\right)^2 + \left(\frac{y' z_{v_1}}{z'_{v_1}}\right)^2} + \Delta z_{disp} \quad (23)$$

from the z canonical component; note that we subtract Eq. 23 from the z canonical component instead of adding, since the particle travels a path longer than the reference particle.

D. Pitches

To compute the final vector with mirror pitches, We follow a similar procedure as the one used with tilt errors. In this case, however, our rotation vector for an x-pitch is $(0, -\theta_y, 0)$ and that of a y-pitch is $(-\theta_x, 0, 0)$. These rotation vectors, converted to the LO frame, may be expressed as

$$\hat{R}_{xp} = SR_{xp} = \begin{pmatrix} \theta_x \sin \tau \\ -\theta_x \cos \tau \\ 0 \end{pmatrix} \quad (24)$$

$$\hat{R}_{yp} = SR_{yp} = \begin{pmatrix} -\theta_y (\cos 2\phi \cos^2 \tau + \sin^2 \tau) \\ 2\theta_y \cos \tau \sin^2 \phi \sin \tau \\ -\theta_y \cos \tau \sin 2\phi \end{pmatrix} \quad (25)$$

using Eq. 20. We apply the opposite of these rotation vectors to our input coordinates and propagate the vectors as was done using Eq. 22 to get the coordinates in the LO frame. Computing the change in z canonical is identical to the procedure employed with tilt errors; we compute Δz_{disp} and use Eq. 23 to compute Δz_{can} .

E. Offsets

To invert the offsets, we follow a similar procedure. However, in this case, our displacement vector isn't a rotation vector, but is instead a translation vector. We are to transform the vector

$$\begin{pmatrix} -x_0 + s_0 \tan x' \\ -y_0 + s_0 \tan y' \\ \frac{s_0}{\cos x'} \end{pmatrix} \quad (26)$$

into the LO frame. Using Eq. 20, we have the transformed vector to be

$$\begin{pmatrix} -\frac{s_0 \cos \tau \sin 2\phi}{\cos x'} + (\cos 2\phi \cos^2 \tau + \sin^2 \tau)(-x_0 + s_0 \tan x') + 2 \cos \tau \sin^2 \phi \sin \tau (y_0 - s_0 \tan y') \\ -\frac{s_0 \sin \tau \sin 2\phi}{\cos x'} + (\cos 2\phi \sin^2 \tau + \cos^2 \tau)(-y_0 + s_0 \tan y') + 2 \cos \tau \sin^2 \phi \sin \tau (x_0 - s_0 \tan x') \\ \frac{s_0 \cos 2\phi}{\cos x'} + \sin 2\phi (\cos \tau (-x_0 + s_0 \tan x') + \sin \tau (-y_0 + s_0 \tan y')) \end{pmatrix} \quad (27)$$

Since this is a translation vector, we add the opposite of this vector to the incoming vector instead of applying a rotation. We then use Eq. 22 to propagate this vector to get the coordinates in the LO frame. To compute z canonical, we follow the same procedure outlined in the tilt error and pitches sections. Once we complete this step, we have our final vector.

In the BMAD code, we actually perform the above steps, but instead transform the vector

$$\begin{pmatrix} -x_0 - s_0 \tan x' \\ -y_0 + s_0 \tan y' \\ \frac{s_0}{\cos x'} \end{pmatrix} \quad (28)$$

To see why, remember that the reflection component which took us from EI to EO inverted the value for x' . Since we need the value of x' employed in the LI frame, assuming only offsets exist, we have to invert the value of x' here.

VII. ZEROETH ORDER KICKS AND FIRST ORDER TRANSFER MATRICES

For all beam elements, BMAD displays the zeroth order kick and first order transfer matrix. To compute these terms, we first compute the transfer matrix by visiting each step and reducing all formulas to first order in the beam coordinates. After formulating each step's respective matrix (LI to EI, EI to EO, and EO to LO), the first order transfer matrix is $M_1 = M_{unset}M_{EI-EO}M_{set}$. Using the first order transfer matrix, we calculate the zeroth order kick as follows: $v_{kick} = v_{out} - M_1v_{in}$ where v_{in} represents the incoming beam coordinates and v_{out} represents the final vector in the LO frame.

VIII. CONCLUSION

The overall procedure is broken up into three steps: set, reflection, and unset. These three steps correspond to the LI-EI, EI-EO, and EO-LO steps, respectively. One advantage of using this method over computing one formula to convert the coordinates directly from LI to LO is that mirror parameters can be dealt with one at a time, as above. This procedure simplifies much of the work that has to be done through structuring the problem. Another advantage is that much of the above procedure can be extended to mirrors with curvature; the set and unset procedures are invariant, meaning that only the reflection portion changes. This method may also be extended to crystal simulations, as the unset and set procedures do not change here either. By isolating the problem to one small step, deriving the necessary formulas for curved mirrors and crystals has been simplified greatly.

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X. BIBLIOGRAPHY

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- [2] D. Sagan, J. Smith, *The Tao Manual*.