## Lawrence Berkeley National Laboratory

LBL Publications

Title
Analytical expressions of the surface shape of 'diaboloid' mirrors
Permalink
https://escholarship.org/uc/item/9zp9d0wd
ISBN
978-1-5106-3792-4

Authors
Yashchuk, Valeriy V
Lacey, Ian
del Rio, Manuel Sanchez

Publication Date
2020-08-21

DOI
10.1117/12.2568332

Peer reviewed

# Analytical expressions of the surface shape of 'diaboloid' mirrors 

Valeriy V. Yashchuk*, Ian Lacey, and Manuel Sanchez del Rio ${ }^{\text {a }}$<br>Advanced Light Source, Lawrence Berkeley National Laboratory, 1 Cyclotron Rd., Berkeley, CA 94720, USA


#### Abstract

Modern deterministic polishing processes allow fabrication of x-ray optics with almost any arbitrary aspherical surface shape. Among these optics, the so called "diaboloid" mirror is of special interest. The diaboloid mirror that converts a cylindrical wave to a spherical wave would improve focusing in x-ray beamlines implementing a diffraction element between a parabolic cylinder and a toroidal mirror. The replacement of the toroidal mirror in existing beamlines by the diaboloid mirror would mitigate aberrations. The shape of the diaboloid mirror is usually calculated numerically based on a truncated polynomial solution of the optical path problem. Here, we present an exact analytical solution for the shape of a diaboloid mirror as a function of the conjugate parameters of the mirror placed in a beamline. The derived analytical expressions for the diaboloid mirror in both the canonical and mirror-based coordinate systems are implemented in ray-tracing simulations to verify the beamline performances.


Keywords: synchrotron radiation, x-ray optics, diaboloid mirror, analytical solution, aspherical optics, aberrations, monochromator, spectral resolution

## 1. INTRODUCTION

Modern deterministic polishing processes allow fabrication of x-ray optics with almost any arbitrary aspherical surface shape. Among these optics, the so called "diaboloid" mirror is of special interest [1-4]. The major distinguishing functionality of a diaboloid mirror consists in the transformation (focusing) of a divergent x-ray beam from a point source (assuming that the beam coming from the source is divergent in the solid angle) to a line beam, divergent in a plane orthogonal to the focal line, and without divergence in any plane containing the focal line - Fig. 1a. That is a conversion of a spherical wave to a cylindrical wave. This formulation is convenient for the analytical derivations discussed in this paper, and can be easily related by reversing the beam propagation direction to the diaboloid mirror definition and application in Refs. [1-4] - Fig. 1b.

The diaboloid mirror would improve x-ray beamlines that implement an optical scheme with a diffraction element between parabolic cylinder and toroidal mirrors. The replacement of the toroidal mirror by the diaboloid mirror would mitigate aberrations improving focusing and maximizing the resolving power of a spectrometer (see, for example, Refs. [2,3]).


Figure 1. (a) Optical schematic of the diaboloid mirror arrangement as considered in the present work, and (b) diaboloid mirror definition and application in Refs. [1-4].

[^0]To the best of our knowledge, so far the diaboloid mirror is calculated numerically based on a truncated polynomial solution of the optical path problem [1-4]. Here, we present an exact analytical solution for the shape of a diaboloid mirror as a function of the conjugate parameters of the mirror placed in a beamline. The analytical expressions for the diaboloid mirror shape are derived in both the canonical and mirror based coordinate systems. The shape expressions are implemented in ray-tracing simulations to verify the beamline performances with the diaboloid mirror.

Because of the lack of space, it is difficult if not impossible, to present in a single conference paper all the details of the derivations. Instead, this work just summarizes the results of a series of Advanced Light Source (ALS) Light Source Beam Line (LSBL) reports [5-7] that provide a chain of the logical and algebraic transformations used to derive the analytical equations for the shape of a diaboloid mirror in the canonical, shifted-canonical (with the origin at the mirror surface center) [5], and laboratory (mirror-related) coordinate systems (originated at the mirror center and additionally rotated to ensure the zero tangent to the surface at the mirror center) [6,7]. The validity of the analytical results is verified via raytracing calculations in Ref. [8]. The last report uses a Mathematica ${ }^{\mathrm{TM}}$ notebook to numerically generate the diaboloid mirror surface with the given data mesh based on the desired conjugate parameters and clear aperture of the mirror. We should also mention the report [9] where some approximations of the exact diaboloid shape potentially useful for practical realizations are also discussed.

## 2. OUTLINE OF THE SOLUTION IDEA

Intuitively, the shape of a diaboloid mirror should be a combination of parabolic and elliptical surfaces. Indeed, in the planes orthogonal to the focal line, a diaboloid mirror transforms the beam from point to point. This is similar to an elliptical mirror. However, in any plane containing the focal line, it forms a parallel beam, analogous to a parabolic mirror. We are exploiting this intuitive guess in the derivation in this paper.
Our approach to deriving an analytical equation, describing the surface shape of a diaboloid mirror, is a "purely geometrical" rather than classical geometrical optics. Thus, we do not start from a priori requirement for the equal optical path length for the focused rays. However, this condition arises "automatically" in the course of the geometrical consideration.

Let us consider a vertically deflecting diaboloid mirror in the face-up orientation (Fig. 1a) with the center of the clear aperture in point $P_{0}$. The mirror is supposed to be used with a grazing incidence x-ray beam from a point source $S$. The vertical cross-section of the geometry of the mirror beamline application is schematically shown in Fig. 2 in the canonical coordinate system.


Figure 2. Vertical cross-section of beamline application geometry of a vertically deflecting diaboloid mirror in the face-up orientation (for notations, see the text). Axes refer to the canonical coordinate system.

Depicted by the cross-section in Fig. 2, the central meridional ( $x=0$ ) surface of the mirror has a parabolic shape (the bold solid line). In this case, if the point source $S$ is placed in the focus of the generating parabola. The x-rays emitted
in the cross-section plane after being reflected by the mirror parabolic area are parallel to the tangential axis $\vec{Z}$. That is required for a diaboloid mirror.

In Fig. 2, the mirror parabolic cross-section is shown in its canonical orientation defined by the generating parabola. The x-ray point source $S$ is in the focus of the generating parabola; $f$ is the distance between $S$ and the vertex of the parabola. $F$ is the focal line orthogonal to the axis $\vec{Z} ; z_{F}$ is the distance between the focal line and the axis $\vec{Y}$. The position of the diaboloid mirror center is marked as the point $P_{0} \equiv\left(x_{0}=0, z_{0}, y_{0}\right)$. The rays incident to and reflected from the mirror center $P_{0}$ are noted as $r_{01}$ and $r_{02}$, respectively; $\phi_{0}$ is the position on the focal line of the central ray with the vertical coordinate $y_{0}$.

Let us now consider the same application geometry of the diaboloid mirror as in Fig. 2, but with accounting the reflected beam divergent in the horizontal plane, defined by the condition

$$
\begin{equation*}
y=\text { const }=y_{0} \tag{1}
\end{equation*}
$$

containing the point $P_{0}$ - see Fig. 3. The horizontal plane is coming out of the page. As mentioned above, the diaboloid mirror cross-section defined by this plane has to have an elliptical shape that is also a cross-section of an ellipsoid-ofrotation that focuses the x-rays from the source $S$ to the point $\phi_{0}$ of the focal line. This enveloping ellipsoid-ofrotation, corresponding to the ray reflected by the center point $P_{0}$ of the diaboloid mirror, is depicted in Fig. 3 with its vertical cross-section shown with the dotted line.


Figure 3. Vertical cross-section of the beamline application geometry of a vertically deflecting diaboloid mirror in the faceup orientation with additional sketch of the corresponding cross-section of the enveloping ellipsoid-of-rotation surface (see discussion in the text).

Thus, a surface segment of the ellipsoid-of-rotation mirror corresponding to the cross-section of the ellipsoid surface and the central horizontal plane given by condition (1) focuses the beam rays (with the sagittal coordinates $x \neq 0$ ) in the central horizontal plane to the same point of the focal line with position $\phi_{0}$, and with diversion only in the plane.

A consideration similar to the one depicted in Fig. 3 for the rays focused in the central horizontal plane, can be applied to any other point of the focal line with coordinate $\phi$. For each focal-line point, we can determine the corresponding enveloping ellipsoid-of-rotation and find the segment of its cross-section with the assigned horizontal plane given by $y=\phi=$ const . Correspondingly, the rays reflected by the ellipsoid segment that includes the point $P=(x=0, y, z)$ on the parabolic central trace of the diaboloid mirror, are focused in the focal-line point $\phi$ without diversion in the vertical direction.

Based on the above consideration, we can now formulate the idea of our approach to the problem of the analytical description of the surface shape of a diaboloid mirror. We suggest presenting the diaboloid mirror surface as a set of the cross-section segments of the ellipsoids corresponding to all points of the focal-line interval, characteristic for the mirror. In this paper, we are realizing this "purely geometrical" approach.

## 3. ANALYTICAL EXPRESSION FOR THE SHAPE OF A DIABOLOID MIRROR IN THE CANONICAL COORDINATE SYSTEM

In the normal coordinate system $\left(x^{\prime}, y^{\prime}, z^{\prime}\right)$ of the enveloping ellipsoid-of-rotation, when the axis $z^{\prime}$ is directed along the major axis and $x^{\prime}=0, y^{\prime}=0$, and $z^{\prime}=0$ at the center of the ellipsoid, the ellipsoid shape is defined in the normal form (see, for example, Ref. [7]):

$$
\begin{equation*}
\frac{x^{\prime 2}}{b^{2}}+\frac{y^{\prime 2}}{b^{2}}+\frac{z^{\prime 2}}{a^{2}}=1 \tag{2}
\end{equation*}
$$

In the notation of Fig. 3, the squared parameters of the major and minor semiaxes $a^{2}$ and $b^{2}$ are [5]

$$
\begin{equation*}
a^{2}=\frac{1}{4}\left(z_{F}+1 /(2 A)\right)^{2} \quad \text { and } \quad b^{2}=\frac{1}{4}\left(z_{F} / A+1 /\left(4 A^{2}\right)+\phi^{2}\right) \tag{3}
\end{equation*}
$$

where $A$ is the power coefficient of the generating parabola (see Fig. 3):

$$
\begin{equation*}
z=A \cdot y^{2}-f, \quad f=(4 A)^{-1} \tag{4}
\end{equation*}
$$

The normal coordinate system $\left(x^{\prime}, y^{\prime}, z^{\prime}\right)$ of the enveloping ellipsoid is rotated and shifted with respect to the canonical coordinate system $(x, y, z)$ of the generating parabola (Fig. 2). The rotation is around the axis $\vec{X}$ by the angle $\alpha$ (see Fig. 3), defined with

$$
\begin{equation*}
\sin \alpha=\phi /(2 c) \quad \text { or } \quad \cos \alpha=z_{F} /(2 c) \tag{5}
\end{equation*}
$$

where the parameter $c$ is a half of the distance between the foci of the ellipsoid (Fig. 3) equal

$$
\begin{equation*}
2 c=\sqrt{z_{F}^{2}+\phi^{2}} \tag{6}
\end{equation*}
$$

In order to express the ellipsoid (2) in the coordinate system $(x, y, z)$, the rotation is accounted with the corresponding matrix of rotation $R_{x}(\alpha)$ (see, for example, Ref. [7]) applied to the coordinate system $(x, y, z)$ :

$$
\left(\begin{array}{c}
\tilde{x}  \tag{7}\\
\tilde{y} \\
\tilde{z}
\end{array}\right)=R_{x}(\alpha)\left(\begin{array}{l}
x \\
y \\
z
\end{array}\right)=\left(\begin{array}{ccc}
1 & 0 & 0 \\
0 & \cos \alpha & -\sin \alpha \\
0 & \sin \alpha & \cos \alpha
\end{array}\right)\left(\begin{array}{l}
x \\
y \\
z
\end{array}\right)=\left(\begin{array}{c}
x \\
y \cdot z_{F} / \sqrt{z_{F}^{2}+\phi^{2}}-z \cdot \phi / \sqrt{z_{F}^{2}+\phi^{2}} \\
z \cdot z_{F} / \sqrt{z_{F}^{2}+\phi^{2}}+y \cdot \phi / \sqrt{z_{F}^{2}+\phi^{2}}
\end{array}\right)
$$

Additionally, the rotated coordinate system $(\tilde{x}, \tilde{y}, \tilde{z})$ has to be shifted along $\tilde{Z}$ axis by $c$ to place the ellipsoid focus to the point of the source $S$ and finally, to superpose the ellipsoid with the generating parabola in the joint reflection point $P$ in the vertical cross-section:

$$
\left(\begin{array}{c}
x^{\prime}  \tag{8}\\
y^{\prime} \\
z^{\prime}
\end{array}\right)=\left(\begin{array}{c}
\tilde{x} \\
\tilde{y} \\
\tilde{z}-c
\end{array}\right)=\left(\begin{array}{c}
x \\
y \cdot z_{F} / \sqrt{z_{F}^{2}+\phi^{2}}-z \cdot \phi / \sqrt{z_{F}^{2}+\phi^{2}} \\
z \cdot z_{F} / \sqrt{z_{F}^{2}+\phi^{2}}+y \cdot \phi / \sqrt{z_{F}^{2}+\phi^{2}}-c
\end{array}\right)
$$

The equation for the rotated and shifted enveloping ellipsoid as a function of the coordinates $(x, y, z)$ is obtained by substitutions to Eq. (2) the expressions for coordinates $x^{\prime}, y^{\prime}$, and $z^{\prime}$ given by Eq. (8) and accounting Eq. (6) for $c$ :

$$
\begin{align*}
f(x, y, z) & =\frac{x^{2}}{b^{2}}+\frac{\left[y \cdot z_{F} / \sqrt{z_{F}^{2}+\phi^{2}}-z \cdot \phi / \sqrt{z_{F}^{2}+\phi^{2}}\right]^{2}}{b^{2}}  \tag{9}\\
& +\frac{\left[z \cdot z_{F} / \sqrt{z_{F}^{2}+\phi^{2}}+y \cdot \phi / \sqrt{z_{F}^{2}+\phi^{2}}-\sqrt{z_{F}^{2}+\phi^{2}} / 2\right]^{2}}{a^{2}}-1=0 .
\end{align*}
$$

From Eq. (9), the cross-section $f(x, z ; \phi)$ of the ellipsoid with the plane $y=\phi=$ const is

$$
\begin{equation*}
f(x, y=\phi, z)=\frac{x^{2}}{b^{2}}+\frac{\phi^{2}}{b^{2}} \frac{\left(z_{F}-z\right)^{2}}{\left(z_{F}^{2}+\phi^{2}\right)}+\frac{\left[2 z \cdot z_{F}+\phi^{2}-z_{F}^{2}\right]^{2}}{4 a^{2}\left(z_{F}^{2}+\phi^{2}\right)}-1=0 \tag{10}
\end{equation*}
$$

Additionally to the spatial variables $x, \phi$, and $z$, the ellipsoid minor axis $b$ is also a variable because of its dependence on $\phi$, given with Eq. (3). In order to explicitly deduce this dependence, we substitute in Eq. (10) the expression [compare with Eqs. (3) and (6)]

$$
\begin{equation*}
b^{2}=a^{2}-c^{2}=\left[a^{2}-\left(z_{F}^{2}+\phi^{2}\right) / 4\right] \tag{11}
\end{equation*}
$$

Finally, we obtain the analytical expression for the shape of a diaboloid mirror expressed as a function of the mirror height on the tangential and sagittal positions in the canonical coordinate system with the origin in the parabola focus $S$, as depicted in Figs. 2 and 3:

$$
\begin{equation*}
y(x, z)=\sqrt{\frac{1}{4 A^{2}}-2 z \cdot z_{F}+\left(\frac{1}{A}+2 z_{F}\right)\left(z_{F}-\sqrt{x^{2}+\left(z_{F}-z\right)^{2}}\right)} . \tag{12}
\end{equation*}
$$

## 4. TRANSFORMATION OF THE SHAPE EQUATION FOR A DIABOLOID MIRROR TO THE MIRROR-RELATED COORDINATE SYSTEM

In this section, we transfer Eq. (12) to the laboratory (mirror-related) coordinate system ( $s, h, t$ ) and express the diaboloid mirror shape via the parameters of the beamline application of the mirror (the mirror conjugate parameters). These are: the distance $p \equiv r_{01}$ from the point focus $S$ to the mirror center $P_{0}$, the distance $q \equiv r_{02}$ from the focal line $F$ to the mirror center $P_{0}$, and the grazing incidence angle $\theta$.

In the mirror related coordinate system $(s, h, t)$, the tangent to the mirror center is at zero angle with respect to the tangential axis $t$. Therefore, the transformation incorporates a shift of the canonical coordinate system to the mirror center and, after that, a rotation of the mirror surface counterclockwise by the angle $\theta$.

Let us first express the parameters of the generating parabola $A$ and $z_{F}$ as the functions of the mirror conjugate parameters $r_{1}, r_{2}$, and $\theta$. Referring to Fig. 1, one can see that the coordinates $x_{0}, y_{0}, z_{0}$ of the mirror center in the canonical coordinate system and the position $z_{F}$ of the focal line $F$ can be expressed via the conjugate parameters as:

$$
\begin{equation*}
x_{0}=0, y_{0}=p \sin 2 \theta, \quad z_{0}=p \cos 2 \theta, \text { and } z_{F}=p \cos 2 \theta+q \tag{13}
\end{equation*}
$$

The coefficient $A$ can be found from the differential of the generated parabola (4) at $z_{0}$ :

$$
\begin{equation*}
A=\left(4 p \sin ^{2} \theta\right)^{-1} \tag{14}
\end{equation*}
$$

By substituting $A$ and $z_{F}$ given with Eqs. (13) and (14) to Eq. (12) and shifting the coordinates to the mirror center:

$$
\begin{equation*}
y=y_{0}-v \text { and } z=z_{0}+\zeta \tag{15}
\end{equation*}
$$

we express the shape of the diaboloid mirror as a function of the flipped sagittal coordinate $\xi=-x$, the shifted vertical coordinate $v$, and the shifted tangential coordinate $\zeta$ in the shifted canonical coordinate system:

$$
\begin{align*}
v & =p \sin 2 \theta \\
& -\sqrt{4 p^{2} \sin ^{4} \theta-2(p \cos 2 \theta+q) \cdot(\zeta+p \cos 2 \theta)+2(p,+q)\left(p \cos 2 \theta+q-\sqrt{\xi^{2}+(q-\zeta)^{2}}\right)} \tag{16}
\end{align*}
$$

The corresponding expression for the generating parabola is obtained from Eq. (16) by substitution of $\xi=0$ :

$$
\begin{equation*}
v=p \sin 2 \theta-2 \sin \theta \sqrt{p\left(\zeta+p \cos ^{2} \theta\right)} \tag{17}
\end{equation*}
$$

The last step of the transformation of the equation (16) for the diaboloid mirror shape to the mirror-related coordinate system is to express it in the coordinate system $(s, h, t)$ that is rotated around the sagittal axis $\vec{\xi}$ by the angle of $\theta$ with respect to the shifted coordinate system $(\xi, v, \zeta)$. The transformation performed analogously to the rotation of the enveloping ellipse given by Eq. (7), leads to the diaboloid mirror shape equation in the mirror based (shifted and rotated canonical) coordinate system (the details of the transformation can be found in Ref. [6]):

$$
\begin{align*}
F(s, h, t)= & \sin \theta \cdot t-\cos \theta \cdot h+p \sin 2 \theta \\
& -\binom{4 p^{2} \sin ^{4} \theta-2(p \cos 2 \theta+q) \cdot(\cos \theta \cdot t+\sin \theta \cdot h+p \cos 2 \theta)}{+2(p+q)\left(p \cos 2 \theta+q-\sqrt{s^{2}+(q-\cos \theta \cdot t-\sin \theta \cdot h)^{2}}\right)}^{1 / 2}=0 . \tag{18}
\end{align*}
$$

Equation (18) was first solved [6] and coded [8] in the form of a normal analytical surface shape function $h=f(s, t)$ in Mathematica ${ }^{\mathrm{TM}}$ that allows numerical calculations of the desired diaboloid three-dimensional surface profiles applicable, in particular, for Shadow ray tracing simulations. Unfortunately, the exact analytical expression derived with help of Mathematica ${ }^{\mathrm{TM}}$ in report [6], is rather cumbersome. It is presented in Appendix of Ref. [6] in 17 pages. The cumbersome appearance of the exact expression can discourage a potential user from its application for simulations using other than Mathemaica ${ }^{\mathrm{TM}}$ software.

The presentation of the solution is improved in the work [7], where a chain of algebraic transformations that lead to the exact shape of a diaboloid mirror in the form of a function $h=f(s, t)$ is presented. The expressions obtained in Ref. [7] are significantly more compact compared to the 17-page long expression obtained in Mathamatica ${ }^{\mathrm{TM}}$. This solution provides a possibility for straightforward coding of the exact analytical expression for the shape of a diaboloid mirror practically in any software used for data processing and optical ray-tracing simulations. However, the reproduction of the solution obtained in the report [7] is out of the scope of the present work and will be published elsewhere. Instead, below we discuss a verification via ray-tracing optical simulations of the analytical expression for the diaboloid mirror shape in the laboratory mirror-based coordinate system given by Eq. (18) and its transformation to the form $h=f(s, t)$ found and coded in Mathematica ${ }^{\mathrm{TM}}$.

## 5. MATHEMATICA ${ }^{T M}$ CODE FOR GENERATION OF SHAPE DATA OF A DIABOLOID MIRROR

The ray-tracing simulations (see Sec. 6) are performed using Shadow software in the OASYS environment [11]. As the input data on surface height shape of a diaboloid mirror under evaluation, we use model data numerically calculated in a specially developed code in Mathematica ${ }^{\mathrm{TM}}$. The code utilizes the analytical expressions derived in reports [6,7] for the shape of a diaboloid mirror in the laboratory (mirror based) coordinate system.
In this section, we overview the structure and the major functions of the Mathematica ${ }^{\mathrm{TM}}$ code developed for generation of shape data of a diaboloid mirror in the form and format that is acceptable for ray-tracing simulations with the Shadow software.

The Mathematica ${ }^{\mathrm{TM}}$ notebook 'diaboloidDesignModelling.cdf' defines the surface height as a multivariate function of the sagittal $x$ and the tangential $z$ coordinates of the shape of a diaboloid mirror with the coordinates in the mirrorrelated coordinate system. The notebook consists of three sections as depicted in Fig. 4.
$-\frac{\square}{-\quad \times}$

Figure 4. Structure of the Mathematica ${ }^{\mathrm{TM}}$ notebook 'diaboloidDesignModelling.cdf' defining the multivariate CDF of the diaboloid mirror shape in the mirror-related coordinate system.

The initialization block should be run first - Fig. 5a. Then, the user defined parameters for the mirror shape calculation has to be entered to the Calculation and Display block - Fig. 5b.

- Initialization
(a)

> Left click to select the section block, then "Shift" + "Enter" to evaluate

## - Calculation and Display

- Establishing the conjugate parameters
- User Input of conjugate parameters here

```
\operatorname{ln}[34]:= sourceD = 29300 (* millimeters *);
```

        targetD \(=19530\) ( \(*\) millimeters *) ;
        grazingAng \(=0.0045\) (* radians *);
    $\ln [235]$ : $=$ clearTangAperture $=200$ (* millimeters *);
clearSagAperture $=20 \quad$ ( $*$ millimeters *);
tangStepResolution $=\boldsymbol{\theta} .2$ (* millimeters *); (* this defines the mesh, or effecive pixel size *)
sagStepResolution $=\boldsymbol{t a n g S t e p R e s o l u t i o n ~ ( * ~ s q u a r e ~ f o r ~ t h i s ~ c a s e ~ * ) ; ~}$

- defining a diaboloid with those parameters
(b)

Figure 5. Structure of the Mathematica ${ }^{\mathrm{TM}}$ notebook 'diaboloidDesignModelling.cdf' defining the multivariate function of the diaboloid mirror shape in the mirror-related coordinate system.

In the latter block, the diaboloid shape is specified via the mirror conjugate parameters: the source to the mirror center distance sourceD, the mirror center distance to the focus distance targetD, and the grazing incidence angle at the mirror center grazingAng. Note that the model calculation, based on the analytic expression, assumes a point source and line focus for the sourceD and targetD parameters (in the Saving Data to Disk section, the defined surface may be 'flipped' to match beamline use to focus a line source to a point). The mirror clear aperture is specified with the sizes in the tangential and the sagittal directions clearTangAperture and clearSagAperture, respectively. The mesh of the output shape data is defined with parameters tangStepResolution and sagStepResolution of the effective pixel size in the tangential and in the sagittal directions, respectively. All spatial parameters are defined in millimeters, while the grazing incidence angle in radians.

There are a few options for graphical presentation of the output data. These are the isometric plot of the mirror clear aperture with the cross-section traces highlighted (Fig. 6a) and 2D plots of how the cross-sections differ from the central sagittal (Fig. 6b) and tangential (Fig. 6c) cross-sections.


Figure 6: Optional displays of the calculated diaboloid mirror shape: (a) the isometric plot of the mirror clear aperture with the cross-section traces highlighted, and planar plots of the differences of the highlighted cross-sections from the central cross-section for (b) the sagittal and (c) tangential cross-sections.

The cross section traces highlighted in Fig. 6 (a) are primarily for diagnosis and a visual reality check of the defined shape. Given the extreme sagittal curvature, where for typical conjugate parameters, the total sagittal height variation is
on the order of 1-2 mm, Fig. 6 (b) and (c), shows the difference of the sagittal cross-sections from the central cross sections (in the tangential and sagittal directions).

In the Saving Data to Disk section of the 'diaboloidDesignModelling.cdf' notebook, the path of the directory to save the files with the calculated data is defined - Fig. 7. Here, the filename with the mirror conjugate parameters used in the calculations are inserted automatically. Note that because of the Shadow convention, the spatial dimensions of the output data are given in the same units, typically in meters. In addition to the Shadow format, currently, the data can also be saved in the typical $* . x y z$ format. Figure 7 a depicts the file format of the output data table of the mirror surface heights as the function of the sagittal and tangential coordinates. The format is dictated by the application of the data in raytracing simulations with the Shadow software. The structure of the output table file in more general xyz data-file format is illustrated with Fig. 7b.


Figure 7: The output data file (a) of the format useful for ray-tracing simulations with the Shadow software, and (b) of the more general xyz data-file format that can be used for data processing with different software.

Concluding the overview of the Mathematica ${ }^{\mathrm{TM}}$ notebook, where the function that describes the diaboloid is defined using a point source and vertical line-segment focus, in the "Saving Data to Disk" section there is a Boolean flag, flippedQQ, that when True effectively rotates the surface height data about the vertical y-axis. In this way the saved data is for a surface that point focuses from a line source.

## 6. VERIFICATION OF DIABOLOID MIRROR SHAPE GENERATED IN MATHEMATICA ${ }^{\text {TM }}$ VIA RAY-TRACING SIMULATIONS WITH THE SHADOW SOFTWARE

In this section, we present the results of the ray-tracing simulation with the Shadow software performed to verify the correctness of the analytical solution and its realization in the Mathematica ${ }^{\mathrm{TM}}$ code discussed in Sec. 5, for the diaboloid mirror shape in the mirror-based coordinate system with the sagittal, vertical and tangential coordinates $x, z$, and $y$, respectively, as defined in the Shadow.

For the Shadow simulation, a diaboloid profile defined with the conjugate parameters

$$
\begin{equation*}
p=29.300 \mathrm{~m}, q=9.530 \mathrm{~m}, \text { and } \theta=0.0045 \mathrm{rad} \tag{3}
\end{equation*}
$$

was calculated with the 'diaboloidDesignModelling.cdf' notebook (see Sec. 5).
Note that for the ray-tracing simulation, the mirror was used in the reversed (flipped) orientation compared to the one shown in Figs. 2 and 3 and used for the analytical derivations throughout this paper. This means that the light image has a vertical line-segment shape as shown in Fig. 8a.

Because the beam from the source is divergent only in the horizontal plane, the beam expands only in the sagittal direction $x$ and the size in the vertical direction $y$ does not change. This is apparent in Fig. 8b where the image of the light beam propagated 10 m downstream of the source is shown.


Figure 8. (a) The image of a line-segment like source at the focal point of the Figs. 2 and 3, used in the ray-tracing simulations with the Shadow software. (b) The image of the light beam propagated 10 m downstream the vertical linesegment like source.

The horizontal and the vertical light intensity distributions in the diaboloid mirror focus (corresponding to the position of the point source $S$ in Figs. 2 and 3), resulted in the Shadow ray-tracing simulations, are shown in Figs. 9 and 10.

The calculated full-width-half-maximum (FWHM) size of the beam focused by the diaboloid mirror is 0.1 nm in the horizontal (see Fig. 9) and the divergence in the vertical directions is 1 nrad (see Fig. 10). The fact that these values are not zero, having an additional defocus of the vertical beam is probably due to the limited numerical calculation accuracy. It may originate with writing the Mathematica ${ }^{\mathrm{TM}}$ file, and/or due to the numerical error of the Shadow software raytracing (where the surface is digitized to discrete points, and accurate interpolation between points, given the complex shape is likely not perfect). The Shadow method for dealing with a surface expressed as a numerical mesh, as done here, uses an iterative approximation to get the intersect coordinates, with a small, but non zero error.


Figure 9. The light intensity distribution as a function of the horizontal coordinate in the diaboloid mirror focus as calculated in the Shadow ray-tracing simulations.


Figure 10. The light intensity distribution versus the vertical angle in the diaboloid mirror focus as calculated in the Shadow ray-tracing simulations.

It is worth to mention that an approximated and simple method to obtain numerically the rotated surface consisting in using Eq. (12) to evaluate the diaboloid surface in the shifted canonical (mirror-centered but rotated) coordinate system and then subtract a plane tangent to the mirror center can lead a significant error. For example, in the case, considered in this section, this approximation gives the values of the residual variations of 13 nrad in vertical and 200 nm in horizontal direction, much larger than those obtained when the diaboloid surface is rotated correctly as presented here. This is a similar problem as appeared in aspherical shape calculations when the plane subtraction is used instead of the exact matrix rotation (see, for example, the related discussion in Ref. [12].

## 7. SUMMARY AND CONCLUSIONS

We have outlined the derivation of analytical expressions for the shape of a diaboloid mirror in the different coordinate systems, including the canonical, shifted-canonical (with the origin at the mirror surface center), and laboratory (mirrorrelated) coordinate systems (originated at the mirror center and additionally rotated to ensure the zero tangent to the surface at the mirror center).

An explicit chain of the logical and algebraic transformations used for the derivation constitutes a subject of a series of Advanced Light Source (ALS) Light Source Beam Line (LSBL) reports [5-7] and cannot be reproduced in this publication due to its limited size. Nevertheless, the reports are available upon request.

We have described the structure and the major feature of the 'diaboloidDesignModelling.cdf' Mathematica ${ }^{\mathrm{TM}}$ program for the generation of shape data of a diaboloid mirror in the laboratory (mirror based) coordinate system. The program is based on an analytical diaboloid mirror shape function given as a dependence of the mirror height on the sagittal and tangential coordinates. The shape equation is a result of a straightforward application of the Mathematica ${ }^{\mathrm{TM}}$ to solve the derived general surface equation. Unfortunately, the shape function is rather cumbersome and we cannot reproduce it here. It is presented in Appendix of Ref. [6] in 17 pages. Nevertheless, our Mathematica ${ }^{\mathrm{TM}}$ program allows numerical calculations of the desired diaboloid three-dimensional surface profiles by utilizing the derived analytical expression. In particular, the program provides the mirror shape data in the form and format that is acceptable for ray-tracing simulations with the Shadow software.

We have also presented the results of ray-trace simulation with the Shadow software of the light beam propagation in the case of a diaboloid mirror with the conjugate parameters typical for potential applications of diaboloid mirrors. The Shadow simulations have confirmed the correctness of the analytical solution and its realization in the Mathematica ${ }^{\mathrm{TM}}$ code on the level of the accuracy of the numerical calculations with Mathematica ${ }^{\mathrm{TM}}$ and Shadow software.

The cumbersome appearance of the exact diaboloid shape expression, mentioned above, can discourage a potential user from its application for simulations using other than Mathemaica ${ }^{\mathrm{TM}}$ software.

This inconvenient is fixed in the work [7], where a chain of algebraic transformations that lead to the exact shape of a diaboloid mirror in the form of a surface height function of the mirror coordinate in the laboratory coordinate system is presented. The expressions obtained in Ref. [7] are significantly more compact compared to the 17-page long expression obtained in Mathamatica ${ }^{\mathrm{TM}}$. This solution provides a possibility for straightforward coding of the exact analytical expression for the shape of a diaboloid mirror practically in any software used for data processing and optical ray-tracing simulations. However, the reproduction of the solution [7] is out of the scope of the present work. It will be published elsewhere.

Next, we also plan to investigate different approximations to the exact diaboloid mirror shape that would be useful from the point of view of simplification of the fabrication of diaboloid mirrors. This work has been already started in Ref. [9] where an approximation of the diaboloid shape with a sagittal conical cylinder bent to a tangential parabola is considered.

In conclusion, the 'LSBL1445_diaboloidDesignModelling.cdf' program presented here and developed for calculation of the diaboloid mirror height topography in the laboratory (mirror-related) coordinate system is available upon request.

## ACKNOWLEDGEMENTS

V.V.Y. dedicates this article to Viatcheslav Mikhailovich Kharlamov, Yury Josifovich Ionin, and Boris Mikhailovich Bekker, who were his mentors in advance geometry and algebra essential for the derivations discussed in this article.

The authors are very thankful to Kenneth Goldberg, Viatcheslav Mikhailovich Kharlamov, Wayne McKinney and Howard Padmore for useful discussions.

The Advanced Light Source is supported by the Director, Office of Science, Office of Basic Energy Sciences, Material Science Division, of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231 at Lawrence Berkeley National Laboratory.

## Disclaimer

This document was prepared as an account of work sponsored by the United States Government. While this document is believed to contain correct information, neither the United States Government nor any agency thereof, nor The Regents of the University of California, nor any of their employees, makes any warranty, express or implied, or assumes any legal responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by its trade name, trademark, manufacturer, or otherwise, does not necessarily
constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof, or The Regents of the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof or The Regents of the University of California.

## REFERENCES

[1] McKinney, W. R., and Howells, M. R., "Optical Path Function for Simple Incoming Cylindrical Wave," Light Source Beam Line Note LSBL-0644, Advanced Light Source, Berkeley (June 2003).
[2] Zeschke, T., "Surface Description for 'Diaboloid Mirror'," Bessy-II Technical Report, Berlin (January 2007).
[3] McKinney, W. R., "Generation of Surface Expansion Coefficients for the Ellipsoid and Paraboloid," Light Source Beam Line Note LSBL-0930, Advanced Light Source, Berkeley (December 2008).
[4] McKinney, W. R., Glossinger, J. M., Padmore, H. A., and Howells, M. R., "Optical path function calculation for an incoming cylindrical wave," Proc. SPIE. 7448, 744809/1-8 (2009); https://doi.org/10.1117/12.828490.
[5] Yashchuk, V. V., "An analytical solution for shape of diaboloid mirror," Light Source Beam Line Note LSBL-1436, Advanced Light Source, Berkeley (January 8, 2020).
[6] Yashchuk, V. V., "Shape of diaboloid mirror in laboratory coordinate system," Light Source Beam Line Note LSBL-1438, Advanced Light Source, Berkeley (January 13, 2020).
[7] Yashchuk, V. V., "Explicit algebraic derivation of an expression for the exact shape of diaboloid mirror in laboratory coordinate system," Light Source Beam Line Note LSBL-1462, Advanced Light Source, Berkeley (May 17, 2020).
[8] Lacey, I., Sanchez del Rio, M., and Yashchuk, V. V., "Analytical expression for the diaboloid shape in laboratory mirror coordinates verified by ray-tracing simulations," Light Source Beam Line Note LSBL-1445, Advanced Light Source, Berkeley (March 24, 2020).
[9] Yashchuk, V. V., "Diaboloid shape approximation with a sagittal conical cylinder bent to a tangential parabola: Analytical consideration," Light Source Beam Line Note LSBL-1451, Advanced Light Source, Berkeley (April 14, 2020).
[10] Bronshtain, L. N., Semindyayev, K. A., Musiol, G., and Muehlig, H., "Handbook of Mathematics," Firth Edition (Springer, 2007).
[11]Rebuffi, L. and Sanchez del Rio, M., "ShadowOui: a new visual environment for X-ray optics and synchrotron beamline simulations" J. Synchrotron Rad. 23, 1357-1367 (2016); https://doi.org/10.1107/S1600577516013837.
[12] Yashchuk, V. V., Lacey, I., Gevorkyan, G. S., McKinney, W. R., Smith, B. V., and Warwick, T., "Ex situ metrology of aspherical pre-shaped x-ray mirrors at the Advanced Light Source," Rev. Sci. Instrum. 90(2), 021711/1-13 (2019); doi: 10.1063/1.5057441.


[^0]:    *vvyashchuk@lbl.gov; phone 1510 495-2592; fax 1510 495-2591; https://als.lbl.gov
    ${ }^{\text {a }}$ Present address: ESRF, 71 Avenue des Martyrs, 38043 Grenoble, France

