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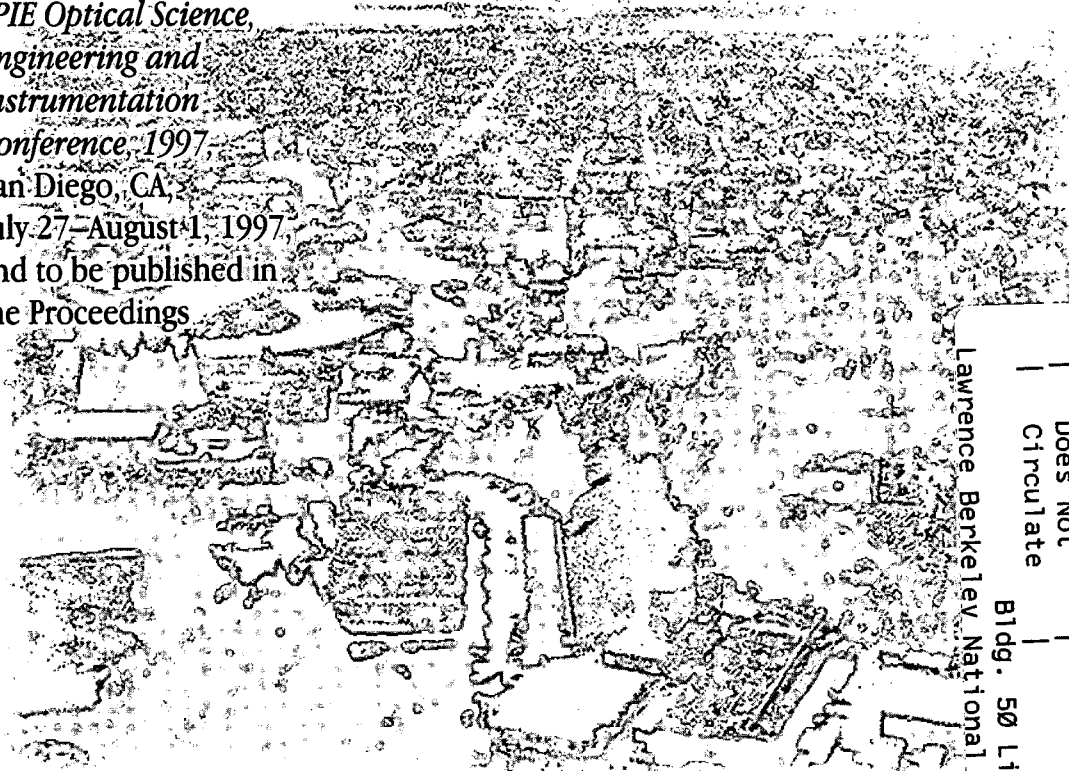
# ERNEST ORLANDO LAWRENCE BERKELEY NATIONAL LABORATORY

## Derivation of Aberration Coefficients for Single-Element Plane-Symmetric Reflecting Systems Using Mathematica™

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**DERIVATION OF ABERRATION COEFFICIENTS  
FOR SINGLE-ELEMENT PLANE-SYMMETRIC  
REFLECTING SYSTEMS USING MATHEMATICA™**

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## Derivation of Aberration Coefficients for Single-Element Plane-Symmetric Reflecting Systems using Mathematica™

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### ABSTRACT

The definition of the generalized optical path function for a grating or mirror with a single plane of symmetry is reviewed. The generalized optical path function is then expanded in a series of wavefront aberration terms using only a few lines of code in the Mathematica™ scientific programming environment. The use of the algebraic capabilities of the Mathematica™ environment allows straightforward calculation of aberration coefficients that would normally require considerable effort if undertaken by paper and pencil. In addition, the derivation can be carried out to higher order aberration terms, limited only by the capabilities of the computer platform used.

**Keywords:** gratings, aberrations, Mathematica™

### 1. INTRODUCTION

Many designers of grazing-incidence optical systems use specialized, non-axially-symmetric aberration coefficients to model the imaging properties of the system. For many years these aberration coefficients were taken from the scientific literature and could not be readily confirmed without extensive, laborious calculation by hand. With the development of software for symbolic algebraic manipulation, it is now relatively straightforward to check the results in the literature. Moreover, symbolic algebra programs can be readily adapted to derive aberration coefficients for higher orders and for other geometries.

Generally, aberration coefficients found in the literature are available only to fourth order in the aperture and field variables. The increasing use of sharply curved aspheric mirror figures for adaptive optical elements requires terms higher than fourth order for modeling in wavefront aberration theory (as opposed to raytrace analysis), particularly for bendable mirrors in the tangential direction.<sup>1</sup>

## 2. WAVEFRONT ABERRATIONS & GRATING SYSTEM GEOMETRY

The most often used set of off-axis aberration coefficients is that presented in 1974 by Noda, Namioka and Seya.<sup>2</sup> Noda *et al.* extended the earlier work by Beutler<sup>3</sup> and Haber<sup>4</sup>. We used the coordinate system used by Noda *et al.* in our calculations below.

For demonstration purposes we have chosen to derive one part of the optical path function for a curved Rowland diffraction grating with a plane of symmetry. Figure 1 shows the basic geometry. The "path" consists of three terms: (a) the two geometrical lengths  $\overline{AP}$  and  $\overline{PB}$  which (in air or vacuum) are the distances from the source point to an arbitrary point on the grating surface and the distance from that same point to the image point, and (b) the diffraction term:

$$F = \overline{AP} + \overline{PB} + Nm\lambda. \quad (1)$$

The third term allows for the fact that the outgoing wavefront is really a combination of wavefronts which left the source point at different times. We will limit our discussion to the first term,  $\overline{AP}$ . The second term  $\overline{PB}$  can be easily generated using the functional dependence of the first with the proper substitution of variables, and attention to signs.

The term  $\overline{AP}$  is the optical distance from point  $A(x_a, y_a, z_a)$  to point  $P(x, y, z)$ ; in air or vacuum, this equals the geometric distance between the two points, which can be expressed in the familiar way:

$$\overline{AP} = \sqrt{(x_a - x)^2 + (y_a - y)^2 + (z_a - z)^2}. \quad (2)$$

Converting  $x_a$  and  $y_a$  to cylindrical coordinate form yields

$$\overline{AP} = \sqrt{(r \cos \alpha - x)^2 + (r \sin \alpha - y)^2 + (z_a - z)^2}. \quad (3)$$

The term  $\overline{PB}$  can be obtained by replacing  $r$  with  $r'$  and  $\alpha$  with  $\beta$  in Eq. (3).

There are only two degrees of freedom in the position of point P, since it must lie on the grating surface; the coordinate  $x$ , therefore, is represented in terms of  $y$  and  $z$ :

$$x = \sum_{i=0}^{\infty} \sum_{j=0}^{\infty} a_{ij} y^i z^j. \quad (4)$$

The coefficients  $a_{ij}$  determine the shape of the grating surface. For systems with a plane of symmetry,  $a_{ij} = 0$  if  $j$  is odd. Gratings whose surfaces are planar, cylindrical, spherical, toroidal, etc., can be represented by Eq. (4) with the correct choice of  $a_{ij}$  coefficients.<sup>5</sup>

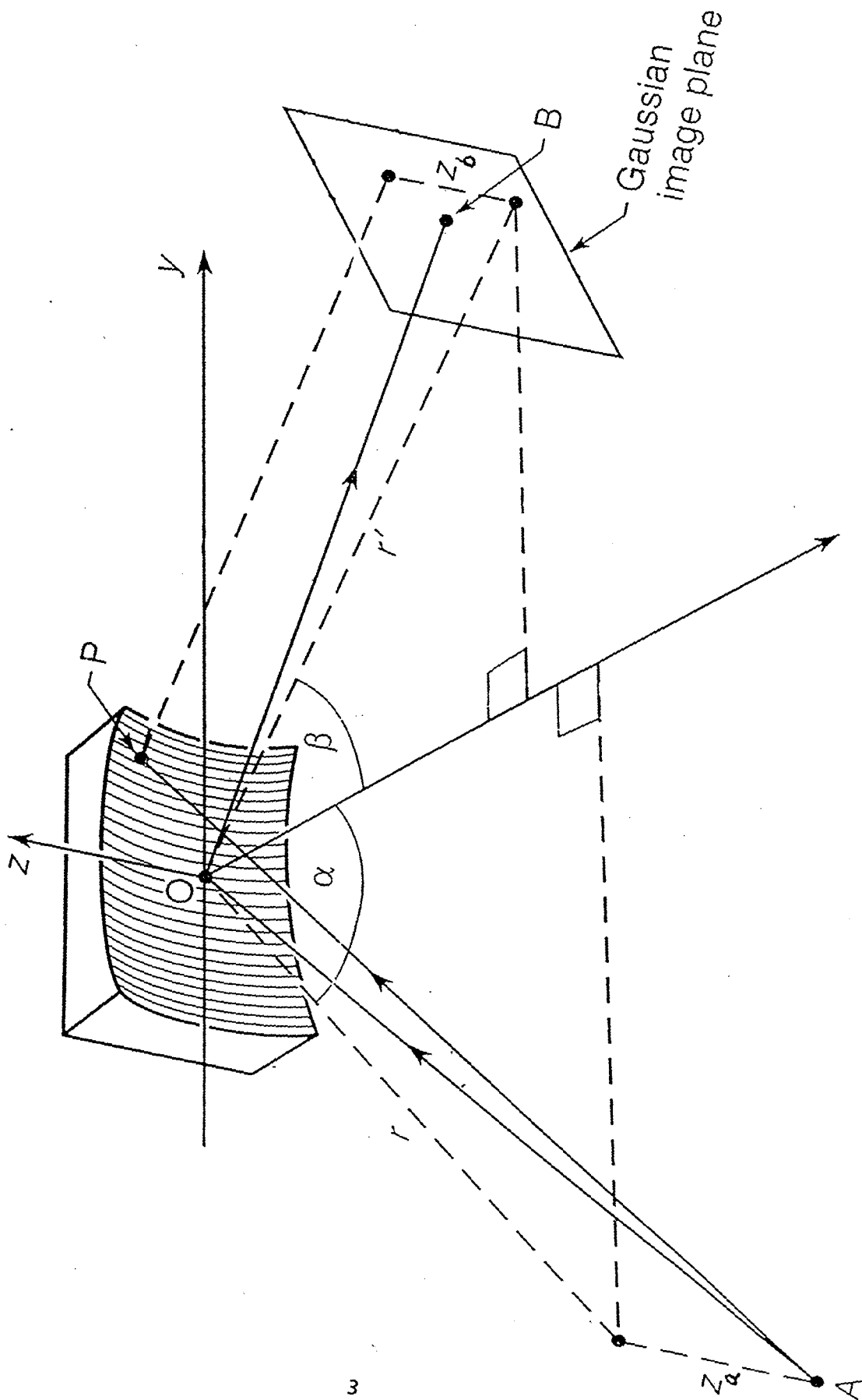


Figure 1 - Grating Geometry

With the help of Eqs. (3) and (4), the optical path difference  $F$  given by Eq. (1) can be expressed as a power series whose independent variables are  $y$  and  $z$  on the grating surface (the "aperture" variables) and the coordinate  $z_a$  of the object point (the "field" variable):

$$F = \sum_{i=0}^{\infty} \sum_{j=0}^{\infty} \sum_{k=0}^{\infty} F_{ijk} y^i z^j z_a^k \quad (5)$$

The coefficients  $F_{ijk}$  are independent of  $y$ ,  $z$  and  $z_a$ , and depend only on the characteristics of the grating and the optical system (e.g.,  $r$ ,  $r'$ ,  $\alpha$ ,  $\beta$ , and the groove pattern). The coefficients describe the aberrations of the grating system; the Mathematica™ code we present below derives the  $\overline{AP}$  part of these coefficients (i.e., that part containing  $r$  and  $\alpha$ ), from which the part for  $\overline{PB}$  can be easily determined.

To simplify the program output, we will use where possible the terms  $s$  and  $t$  introduced by Noda *et al.*; their  $\overline{AP}$  parts are given below, and their  $\overline{PB}$  parts can be found above:

$$t = \frac{\cos^2 \alpha}{r} - 2a_{20} \cos \alpha, \quad s = \frac{1}{r} - 2a_{02} \cos \alpha. \quad (6)$$

### 3. COMPUTER SYSTEM

The hardware used for the derivation of the aberration terms was an Apple Macintosh Power PC computer model 7500 with 112 MB of RAM and a 132 MHz processor card. It was running system 7.6 and Mathematica™ version 2.2 for Macintosh. The "front end" for the program was allotted 10 Mb of memory, and the kernel was allotted 90 Mb. Mathematica™ has a considerable software overhead, necessitating several Mb of memory just to properly run the basic program. The use of Mathematica™ to do intensive symbolic calculation in a reasonable time requires even more RAM.

Mathematica™ is an interpreted language. Because of the intense software overhead, it is slow, but it is extremely powerful and convenient. To sixth order in the field and aperture variables the longest calculation with the above configuration took 5 to 6 hours. With less memory, using virtual memory swapping, full sixth-order calculations took approximately 24 hours.

### 4. MATHEMATICA™ DEVELOPMENT

In this section, the Mathematica™ code used to derive the aberration terms is presented. The flow of the program is sequential, and below we have divided the program into six sequential steps. We have used  $\alpha$  for  $\alpha$ ; all other variable names are self-explanatory. Comments are contained within the symbols (\* and \*).



- 4.1. Define the sag  $x$  in terms of the  $a_{ij}$  coefficients and the aperture variables. This statement contains the non-zero terms in Eq. (4):

```
x = a20 y^2 + a02 z^2 (* 2nd order terms *)
    + a30 y^3 + a12 y z^2 (* 3rd order *)
    + a40 y^4 + a22 y^2 z^2 + a04 z^4 (* 4th order *)
    + a50 y^5 + a32 y^3 z^2 + a14 y z^4 (* 5th order *)
    + a60 y^6 + a42 y^4 z^2 + a24 y^2 z^4 (* 6th order *)
    + a06 z^6
```

- 4.2. Expand  $AP^2$  to order  $ord$  in  $y$ ,  $z$  and  $z_a$ . Using the statement above for the sag  $x$ , the optical path  $\overline{AP}$  given by Eq. (3) can be expanded in a power series in  $y$ ,  $z$  and  $z_a$  as in Eq. (5). The "rules" in the third and fourth statements impose trigonometric simplification that may not be automatically noticed by Mathematica™.

```
ord = 6;
f = Normal[Series[
    Expand[(r Cos[a] - x)^2 + (r Sin[a] - y)^2 + (za - z)^2],
    {y, 0, ord}, {z, 0, ord}, {za, 0, ord}]];
f = Normal[f /. (r^2 Cos[a]^2 + r^2 Sin[a]^2 -> r^2);
f = f /. (Sqrt[r^2 Cos[a]^2 + r^2 Sin[a]^2 -> r);
f = PowerExpand[f];
f = Cancel[f];
```

- 4.3. Create a table of coefficients of  $y$ ,  $z$  and  $z_a$  and define a function to relate to aberration terms. These two statements simply collect the coefficients of the power series of  $f$  ( $= AP^2$ ) determined above.

```
m[i_, j_, k_] := list[[i+1, j+1, k+1]];
list = CoefficientList[f, {y, z, za}];
```

- 4.4. Expand the series of  $AP^2$  and substitute in the quantities  $rs$  and  $rt$  where possible. These statements introduce the terms  $s$  and  $t$  given in Eqs. (6).

```
t = Cos[a]^2/r - 2 a20 Cos[a]
s = 1/r - 2 a02 Cos[a]
cf = ExpandAll[f];
cf = cf
    - z^2 + 2 a02 r Cos[a] z^2 + r s z^2
    - y^2 + y^2 Sin[a]^2 + 2 a20 r Cos[a] y^2 + r t y^2;
```

4.5. Take the square root in a series of the same order. For simplicity we have manipulated  $AP^2$ , but it is the quantity  $\overline{AP}$  whose power series terms provide the aberration expressions. The statements below are analogous to those in section 4.2.

```
fs = Normal[Series[Sqrt[Expand[cf]],
  {y, 0, ord}, {z, 0, ord}, {za, 0, ord}]];
fs = Normal[fs /. (r^2 Cos[a]^2 + r^2 Sin[a]^2 -> r^2)];
fs = fs /. (Sqrt[r^2 Cos[a]^2 + r^2 Sin[a]^2 -> r);
fs = PowerExpand[fs];
fs = Cancel[fs];
fs = ExpandAll[fs];
```

4.6. Display the non-zero aberration terms. These Do loops determine those aberration terms that equal zero, so that only non-zero ones will be printed.

```
Clear[ia, ja, ka, la, ib, jb, kb]; printlist = {};

Do[
  If[
    EvenQ[ja+ka] == True && 0 <= ia+ja+ka <= ord,
    AppendTo[printlist, {ia,ja,ka}]; ],
  {ia, 0, ord, 1}, {ja, 0, ord, 1}, {ka, 0, ord, 1}}

Do[
  ib = printlist[[la,1]];
  jb = printlist[[la,2]];
  kb = printlist[[la,3]];
  Print[ib, jb, kb, " ", InputForm[ma[ib,jb,kb]]],
  {la, 1, Length[printlist]}}
```

This completes the Mathematica™ notebook.

## 5. MATHEMATICA™ RESULTS

The output of the above code is the set of non-zero aberration terms, up to and including sixth order in  $y, z$  and  $z_a$ , given in Figure 2. The terms from order zero through order four match those in the literature. Note again that only the  $\overline{AP}$  part of the aberration terms is presented.

## 6. CONCLUSIONS

We have calculated the aberration terms  $F_{ijk}$  for a plane-symmetric grating system using a few dozen lines of Mathematica™ code. Terms up to sixth order have been presented. These expansions are readily calculable with modern software to higher order in the aperture and field

000	r	002	1/(2*r)	004	-1/(8*r^3)
006	1/(16*r^5)	011	-r^(-1)	013	1/(2*r^3)
015	-3/(8*r^5)	020	s/2	022	-1/(2*r^3) - s/(4*r^2)
024	3/(4*r^5) + (3*s)/(16*r^4)	031	s/(2*r^2)	033	-1/(2*r^5) - (3*s)/(4*r^4)
040	a02^2/(2*r) - s^2/(8*r) - a04*cos[a]				
042	-a02^2/(4*r^3) + (3*s)/(4*r^4) + (3*s^2)/(16*r^3) + (a04*cos[a])/(2*r^2)				
051	a02^2/(2*r^3) - (3*s^2)/(8*r^3) - (a04*cos[a])/r^2				
060	(a02*a04)/r - (a02^2*s)/(4*r^2) + s^3/(16*r^2) - a06*cos[a] + (a04*s*cos[a])/(2*r)				
100	-Sin[a]				
102	Sin[a]/(2*r^2)				
104	(-3*sin[a])/(8*r^4)				
111	-(sin[a]/r^2)				
113	(3*sin[a])/(2*r^4)				
120	-(a12*cos[a]) + (s*sin[a])/(2*r)				
122	(a12*cos[a])/(2*r^2) - (3*sin[a])/(2*r^4) - (3*s*sin[a])/(4*r^3)				
131	-((a12*cos[a])/r^2) + (3*s*sin[a])/(2*r^3)				
140	(a02*a12)/r - a14*cos[a] + (a12*s*cos[a])/(2*r) + (a02^2*sin[a])/(2*r^2) - (3*s^2*sin[a])/(8*r^2) - (a04*cos[a]*sin[a])/r				
200	t/2				
202	-t/(4*r^2) + sin[a]^2/(2*r^3)				
204	(3*t)/(16*r^4) - (3*sin[a]^2)/(4*r^5)				
211	t/(2*r^2) - sin[a]^2/r^3				
213	(-3*t)/(4*r^4) + (3*sin[a]^2)/r^5				
220	(a02*a20)/r - (s*t)/(4*r) - a22*cos[a] - (a12*cos[a]*sin[a])/r + (s*sin[a]^2)/(2*r^2)				
222	-(a02*a20)/(2*r^3) + (3*t)/(4*r^4) + (3*s*t)/(8*r^3) + (a22*cos[a])/(2*r^2) + (3*a12*cos[a]*sin[a])/(2*r^3) - (3*sin[a]^2)/r^5				
	-(3*s*sin[a]^2)/(2*r^4)				
231	(a02*a20)/r^3 - (3*s*t)/(4*r^3) - (a22*cos[a])/r^2 - (3*a12*cos[a]*sin[a])/r^3 + (3*s*sin[a]^2)/r^4				
240	a12^2/(2*r) + (a04*a20)/r + (a02*a22)/r - (a02*a20*s)/(2*r^2) - (a02^2*t)/(4*r^2) + (3*s^2*t)/(16*r^2) - a24*cos[a] + (a22*s*cos[a])/(2*r) + (a04*t*cos[a])/(2*r) - (a12^2*cos[a]^2)/(2*r) + (a02*a12*sin[a])/r^2 - (a14*cos[a]*sin[a])/r + (3*a12*s*cos[a]*sin[a])/(2*r^2) + (a02^2*sin[a]^2)/(2*r^3) - (3*s^2*sin[a]^2)/(4*r^3) - (a04*cos[a]*sin[a]^2)/r^2				
300	-(a30*cos[a]) + (t*sin[a])/(2*r)				
302	(a30*cos[a])/(2*r^2) - (3*t*sin[a])/(4*r^3) + sin[a]^3/(2*r^4)				
311	-((a30*cos[a])/r^2) + (3*t*sin[a])/(2*r^3) - sin[a]^3/r^4				
320	(a12*a20)/r + (a02*a30)/r - a32*cos[a] + (a30*s*cos[a])/(2*r) + (a12*t*cos[a])/(2*r) + (a02*a20*sin[a])/r^2 - (3*s*t*sin[a])/(4*r^2) - (a22*cos[a]*sin[a])/r - (a12*cos[a]*sin[a]^2)/r^2 + (s*sin[a]^3)/(2*r^3)				
400	a20^2/(2*r) - t^2/(8*r) - a40*cos[a] - (a30*cos[a]*sin[a])/r + (t*sin[a]^2)/(2*r^2)				
402	-a20^2/(4*r^3) + (3*t^2)/(16*r^3) + (a40*cos[a])/(2*r^2) + (3*a30*cos[a]*sin[a])/(2*r^3) - (3*t*sin[a]^2)/(2*r^4) + sin[a]^4/(2*r^5)				
411	a20^2/(2*r^3) - (3*t^2)/(8*r^3) - (a40*cos[a])/r^2 - (3*a30*cos[a]*sin[a])/r^3 + (3*t*sin[a]^2)/r^4 - sin[a]^4/r^5				
420	(a20*a22)/r + (a12*a30)/r + (a02*a40)/r - (a20^2*s)/(4*r^2) - (a02*a20*t)/(2*r^2) + (3*s*t^2)/(16*r^2) - a42*cos[a] + (a40*s*cos[a])/(2*r) + (a22*t*cos[a])/(2*r) - (a12*a30*cos[a]^2)/r + (a12*a20*sin[a])/r^2 + (a02*a30*sin[a])/r^2 - (a32*cos[a]*sin[a])/r + (3*a30*s*cos[a]*sin[a])/(2*r^2) + (3*a12*t*cos[a]*sin[a])/(2*r^2) + (a02*a20*sin[a]^2)/r^3 - (3*s*t*sin[a]^2)/(2*r^3) - (a22*cos[a]*sin[a]^2)/r^2 - (a12*cos[a]*sin[a]^3)/r^3 + (s*sin[a]^4)/(2*r^4)				
500	(a20*a30)/r - a50*cos[a] + (a30*t*cos[a])/(2*r) + (a20^2*sin[a])/(2*r^2) - (3*t^2*sin[a])/(8*r^2) - (a40*cos[a]*sin[a])/r - (a30*cos[a]*sin[a]^2)/r^2 + (t*sin[a]^3)/(2*r^3)				
600	a30^2/(2*r) + (a20*a40)/r - (a20^2*t)/(4*r^2) + t^3/(16*r^2) - a60*cos[a] + (a40*t*cos[a])/(2*r) - (a30^2*cos[a]^2)/(2*r) + (a20*a30*sin[a])/r^2 - (a50*cos[a]*sin[a])/r + (3*a30*t*cos[a]*sin[a])/(2*r^2) + (a20^2*sin[a]^2)/(2*r^3) - (3*t^2*sin[a]^2)/(4*r^3) - (a40*cos[a]*sin[a]^2)/r^2 - (a30*cos[a]*sin[a]^3)/r^3 + (t*sin[a]^4)/(2*r^4)				

Figure 2 The Aberration Terms

variables, as required for adaptive optical systems. Higher orders are possible by changing the value of the variable  $\alpha$ , but this requires considerable computing power and computing time.

Except for known errata, the power series expansions of the generalized optical path functions for reflective grating systems as given in the literature are correct.

## 7. ACKNOWLEDGEMENT

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