

Design and analysis of a fast, two-mirror soft-x-ray microscope

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ABSTRACT

During the past several years, a number of investigators have addressed the design, analysis, fabrication, and testing of spherical Schwarzschild microscopes for soft-x-ray applications using multilayer coatings. Some of these systems have demonstrated diffraction limited resolution for small numerical apertures. Rigorously aplanatic, two-aspherical mirror Head microscopes can provide near diffraction limited resolution for very large numerical apertures. This paper summarizes the relationships between the numerical aperture, mirror radii and diameters, magnifications, and total system length for Schwarzschild microscope configurations. Also, an analysis of the characteristics of the Head-Schwarzschild surfaces will be reported. The numerical surface data predicted by the Head equations have been fit by a variety of functions and analyzed by conventional optical design codes. Efforts have been made to determine whether current optical substrate and multilayer coating technologies will permit construction of a very fast Head microscope which can provide resolution approaching that of the wavelength of the incident radiation.

1. INTRODUCTION

Due to the vacuum environment of a sample, conventional electron microscopes can not be used to investigate biological samples under natural conditions. X-ray microscopes provide a different way of studying samples with a resolution of several hundred angstroms.[1, 2, 3] Although diffractive zone plates[4] can be used to focus x-rays in a microscope with a resolution of about three hundred angstroms, there are some problems, such as, low diffraction efficiency and the high cost of making the zone plates, which seem to constrain zone plate x-ray microscopes from achieving resolutions of less than 100Å. The development of multilayer coatings[5, 6] provides the possibility of using multilayer coated mirrors for soft-x-ray microscopy studies with very high resolutions.

An important field for using high resolution soft-x-ray microscopy is cell biology. Many biological samples contain carbon based molecules in an aqueous environment. The water window[7] refers to the soft-x-ray wavelength region of 23 – 44Å in which water is relatively transparent and carbon is highly absorptive. This provides a possibility of studying the structure of DNA and macromolecules within living cells. In order to study microscopic features of biological objects, a multilayer coated, reflecting microscope has been proposed for use within the water window,[8, 9] where one would like to resolve features smaller than 100Å.[10] For a reflecting microscope, this

(NASA-CR-193035 DESIGN AND
 ANALYSIS OF A FAST, TWO-MIRROR
 SOFT-X-RAY MICROSCOPE Final Report,
 12 Aug. 1991 - 11 Aug. 1992
 (Alabama Univ.) 12 p

N93-20316

Unclas

G3/74 0149144

means that a numerical aperture of about 0.4 or greater is required to enable the system to achieve resolutions less than 100Å.

The Schwarzschild two-mirror system[11, 12] has been used for many microscopy and projection lithography applications over a wide range of the electromagnetic spectrum. Recently, the spherical Schwarzschild optics coated with multilayers have been used in soft-x-ray microscopy applications[8, 9, 13, 14, 15] and for projection lithography[16, 17] where linewidths of 500Å have been written on photoresist by AT&T Bell Labs. While operating within the 100 – 200Å region, diffraction limited performance has been obtained for a small numerical aperture ($NA \leq 0.15$) and over a small field of view.

In an effort to provide capabilities for using alternate configurations of two-mirror microscopes while only using third-order designs, Hannan[18] has presented a general analysis of a two conical mirror relay system which corrects third-order spherical aberration, coma, and astigmatism. The concentric, spherical Schwarzschild system is a special case of Hannan's formulation. Hannan's approach enables one to construct a two-mirror microscope where the two conical mirrors are used to overcome the constraint of concentric, spherical mirrors required in the conventional Schwarzschild system. However, the Hannan system does not provide for any higher order correction of aberrations and would likely not function well with a large NA . In order to increase the resolution, one can decrease the operating wavelength and/or increase the NA . To increase the NA and to control aberrations such that diffraction limited performance can be achieved, the authors have proposed using the aspherical Head microscope design.[19, 20]

A. K. Head[21] has used the aplanatism conditions to set up differential equations for the surfaces in a two-mirror imaging system such that all orders of spherical aberration and coma are zero. This means that the Head microscope should provide near diffraction limited performance for very large NAs over a small field of view. Analytical solutions of these two differential equations have been obtained but can not readily be used by conventional optical design codes to determine the performance of a Head microscope.

In this paper, a parametric study for a spherical Schwarzschild microscope has evaluated the relationships between NA , mirror radii and diameters, magnifications, and the total system length. Also, an analysis of the characteristics of the aspherical surfaces of a Head-Schwarzschild microscope will be presented, including a discussion of fitting several different functions to the mirror surface data. Then, the optical performance of a fast Head microscope has been analyzed by conventional optical design codes. Analyses of the Head surface shapes and variation of the angles of incidence over the mirror surfaces have been conducted to determine whether current optical substrate and multilayer coating technologies will permit construction of a very fast Head microscope which may provide resolution approaching that of the wavelength of the incident radiation.

2. SPHERICAL SCHWARZSCHILD MICROSCOPE

A third-order aplanatic design for a reflecting microscope can be made from two concentric spherical mirrors as shown in Fig. 1, if the mirror radii satisfy the Schwarzschild condition:

$$\frac{R_2}{R_1} = \frac{3}{2} - \frac{R_2}{Z_0} \pm \sqrt{\frac{5}{4} - \frac{R_2}{Z_0}} \quad (1)$$

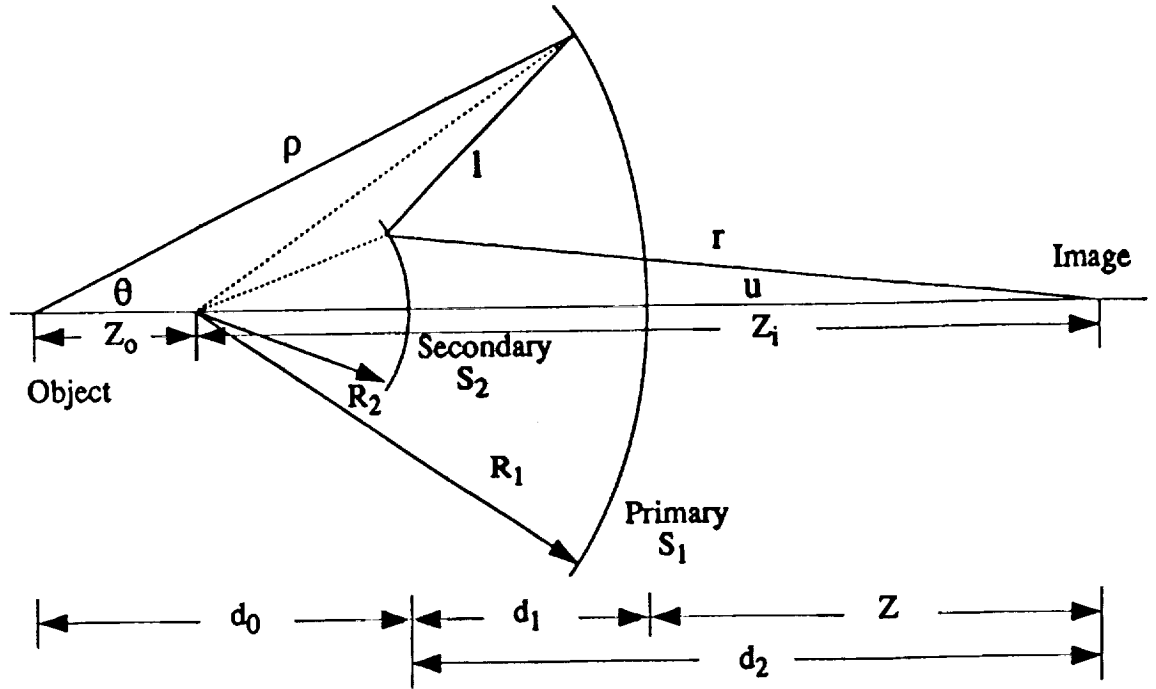


Figure 1: Geometrical configuration of a Head-Schwarzschild microscope.

where R_1 and R_2 are the radii of curvature of the primary and secondary mirrors, Z_0 is the distance from the object point to the center of curvature of the two mirrors, and the + sign in Eq. 1 is used when the magnification is greater than 5. Using paraxial optics relationships, the magnification of a spherical Schwarzschild microscope can be written as

$$m = \frac{-R_1 R_2}{(2R_1 Z_0 - R_1 R_2 - 2R_2 Z_0)} \quad (2)$$

For a derivation and more discussion of the Schwarzschild condition, Eq. 2, and some ray tracing analyses, see Ref. [12]. It has also been shown[22] that a spherical Schwarzschild microscope does not have any third-order astigmatism while also satisfying the third-order aplanatism conditions.

When configuring a reflecting microscope system, the magnification is normally determined by object and detector resolutions. Therefore, Eqs. 1 and 2 are not in a convenient form for determining system parameters for a specific microscope. However, R_1 can be eliminated by combining Eqs. 1 and 2 to obtain:

$$\frac{R_2}{Z_0} = \frac{-m(m-1) + m\sqrt{(m-1)^2 + 4(m+1)^2}}{(m+1)^2} \quad (3)$$

where R_1 can now be evaluated as a function of m , using Eqs. 1 and 3. Using the mirror equation and Eqs. 1 - 3, one can evaluate the data in Table 1, which gives the Schwarzschild system parameters for a range of magnifications where $L(= Z_0 + Z_i)$ is the total length of a microscope and $Z(= Z_i - R_1)$ is the distance from the vertex of the primary mirror to the image plane. The data in Table 1 can be scaled linearly. For example, to obtain the system parameters for a

$M(x)$	$R_1(cm)$	$Z_0(cm)$	$Z(cm)$	$L(cm)$
10	31.7929	8.023756	48.4446	88.2613
20	28.7361	8.052073	132.3053	169.0935
30	27.8342	8.063728	214.0777	249.9756
40	27.4027	8.069952	295.3954	330.8680
50	27.1497	8.073812	376.5409	411.7644

Table 1: Schwarzschild Microscope Parameters for $R_2 = 10cm$.

microscope with a secondary radius of curvature of 5cm, then multiply the data in Table 1 by 0.5 to obtain the systems parameters for such a microscope.

While configuring a Schwarzschild microscope for a specific application, it is desirable to understand the relationship between the numerical aperture (NA) of the microscope, the magnification (m), the diameter of the primary mirror ($D_{1,apt}$), and the radius of curvature of the secondary mirror (R_2). For a spherical Schwarzschild microscope, it follows from the definition $NA = \sin \theta_{max}$ and Fig. 1:

$$NA = \frac{(D_{1,apt}/2)}{\sqrt{(D_{1,apt}/2)^2 + (Z_0 + R_1 - z_{1,max})^2}} \quad (4)$$

where from the equation of the primary mirror surface

$$z_{1,max} = \frac{(D_{1,apt}/2)^2}{R_1 + \sqrt{R_1^2 - (D_{1,apt}/2)^2}} \quad (5)$$

Using Eq. 4 for the calculations, Fig. 2 displays the relationship between NA , m , and the ratio ($D_{1,apt}/R_2$). One notes from Fig. 2 that NA is a much stronger function of ($D_{1,apt}/R_2$) than of the magnification of the system. For a practical example of the usefulness of the data presented in Fig. 2, consider that based on the object and detector resolutions, one seeks to build a 30x microscope with a NA within the range of 0.3 – 0.4. Then, from Fig. 2, it follows that ($D_{1,apt}/R_2$) would need to be within the range of 2.05 – 2.70. It is generally recognized[20] that a spherical Schwarzschild microscope can not perform with diffraction limited resolution for $NA \geq 0.15$, but the aspherical Head microscope, which will be discussed in the next section, will be able to operate with diffraction limited resolution for a very large NA .

Figure 3 presents a plot of the object space NA versus R_2 for different values of $D_{1,apt}$. The relationships between these parameters should be considered before building a specific configuration of a two-mirror microscope. After a determination of m and NA , then substrate fabrication, polishing, and multilayer coating technologies will drive a determination of R_2 and $D_{1,apt}$. Also, it should be noted that a determination of first-order system parameters is required before the aspherical mirror shapes can be evaluated for a Head-Schwarzschild microscope that can provide diffraction limited performance for very large NAs . For example, if one wishes to build a 30x microscope with a 12.5cm diameter primary, then Fig. 3 predicts that R_2 would decrease from

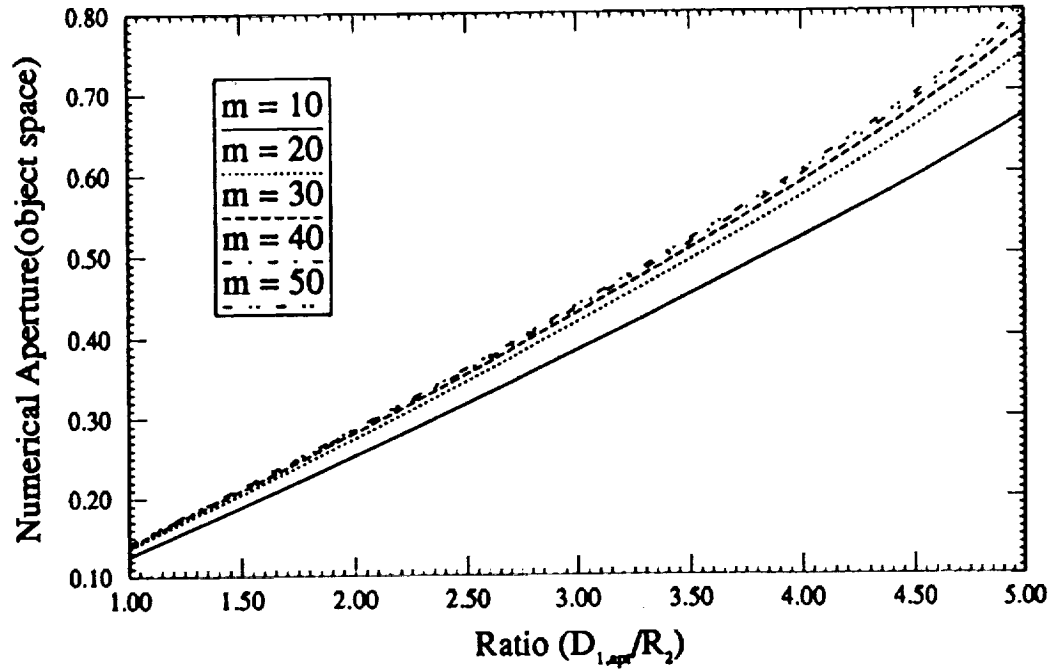


Figure 2: Numerical aperture of spherical Schwarzschild microscope versus the normalized primary mirror diameter($D_{1,apt}/R_2$) for different magnifications.

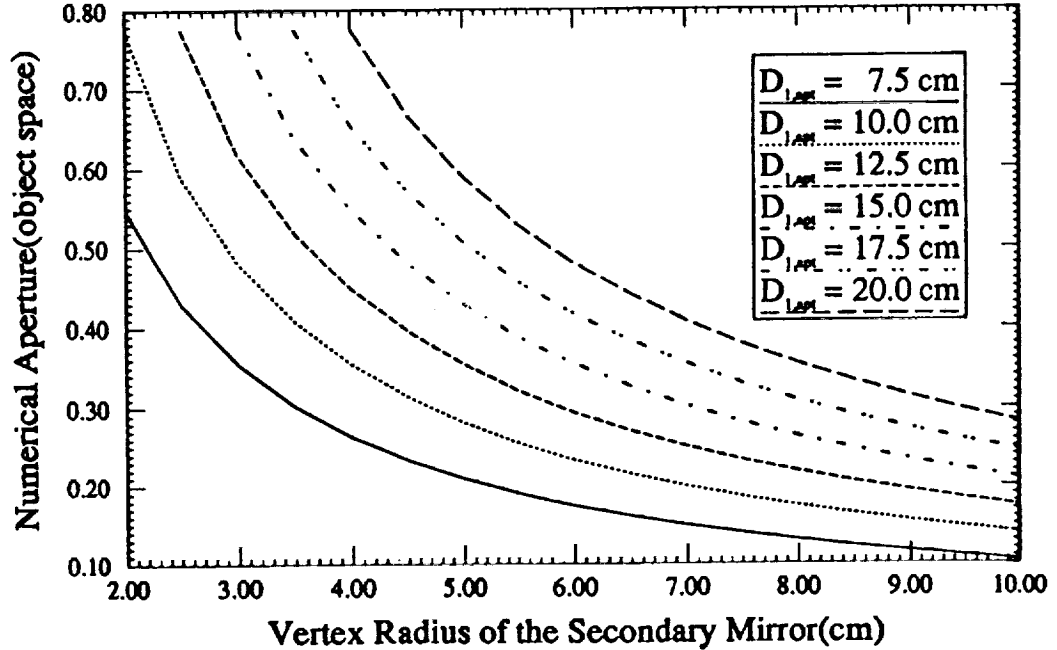


Figure 3: Numerical aperture of a 30x spherical Schwarzschild microscope versus the secondary radius of curvature(R_2) for different diameters of the primary mirror($D_{1,apt}$).

5.9cm to 4.5cm as NA is increased from 0.3 to 0.4. More specifically, Table 1 and Fig. 3 predict the following system first-order system parameters

$$m = 30x, NA = 0.35, L = 124.88cm, R_1 = 13.917cm, D_{1,opt} = 12.5cm, R_2 = 5cm. \quad (6)$$

A microscope with these system parameters can be fabricated with current technology. However, one must examine the aspherical surfaces required of this system to provide diffraction limited resolution with $NA = 0.35$ and a resolution of $Res = \lambda / (2NA) = 1.4\lambda$. Also, one must evaluate the variation of the angle of incidence over both mirrors to determine the nature of the multilayer coatings which will be required.

3. ASPHERICAL HEAD MICROSCOPE

In order to improve the optical performance of a third-order design, such as the spherical Schwarzschild microscope[12] or the conical microscope of Hannan[18], one often seeks an optical system which rigorously satisfies the Abbé Sine Condition for all rays:

$$\sin \theta = m \sin u \quad (7)$$

and the constant optical path length condition:

$$\rho + r + l = \rho_0 + r_0 + l_0 \quad (8)$$

where m is the microscope magnification, and the variables (ρ, r, l) are defined in Fig. 1. The constants (ρ_0, r_0, l_0) are the paraxial values of the corresponding variables. An optical system which satisfies Eqs. 7 and 8 is called an aplanat, which is free of all orders of spherical aberration and coma. In 1957, Head[21] presented an analytical solution in closed form for a two-mirror aplanat with finite object and image points, that is, a microscope or projection system. The primary and secondary mirror surfaces are specified by the following equations[19]:

Primary Microscope Mirror

$$\begin{aligned} \frac{l_0}{\rho} &= \frac{(1 + \kappa)}{2\kappa} + \frac{(1 - \kappa)}{2\kappa} \cos \theta + \left(\frac{l_0}{\rho_0} - \frac{1}{\kappa} \right) \left(\frac{\gamma}{1 + m} \right)^{-1} \\ &* \left[\frac{\gamma - (1 - m)}{2m} \right]^\alpha \left[\frac{\gamma - (m - 1)}{2} \right]^\beta \left| \frac{(\kappa + 1)\gamma}{2(m + 1)} - \frac{(\kappa - 1)}{2} \right|^{2 - \alpha - \beta} \end{aligned} \quad (9)$$

where $\kappa = (\rho_0 + r_0)/l_0$, $\alpha = m\kappa/(m\kappa - 1)$, $\beta = m/(m - \kappa)$, and $\gamma = \cos \theta + \sqrt{m^2 - \sin^2 \theta}$.

Secondary Microscope Mirror

$$\begin{aligned} \frac{l_0}{r} &= \frac{(1 + \kappa)}{2\kappa} + \frac{(1 - \kappa)}{2\kappa} \cos u + \left(\frac{l_0}{r_0} - \frac{1}{\kappa} \right) \left(\frac{\delta}{1 + M} \right)^{-1} \\ &* \left[\frac{\delta - (1 - M)}{2M} \right]^{\alpha'} \left[\frac{\delta - (M - 1)}{2} \right]^{\beta'} \left| \frac{(\kappa + 1)\delta}{2(M + 1)} - \frac{(\kappa - 1)}{2} \right|^{2 - \alpha' - \beta'} \end{aligned} \quad (10)$$

where $M = 1/m$, $\alpha' = M\kappa/(M\kappa - 1)$, $\beta' = M/(M - \kappa)$, and $\delta = \cos u + \sqrt{M^2 - \sin^2 u} = M\gamma$.

It is straight forward to evaluate the mirror profiles of a Head microscope from Eqs. 9 and 10 for given input parameters (m, r_0, l_0 , and ρ_0), which follow from Fig. 1 and Table 1 using the following correspondence between Schwarzschild and Head parameters:

$$(L - Z) \Rightarrow \rho_0, \quad (R_1 - R_2) \Rightarrow l_0, \quad (L - Z_0 - R_2) \Rightarrow r_0.$$

In order to use a conventional optical design program to analyze the performance of a Head microscope, it is necessary to fit an equation to the numerical surface data representing the primary and secondary mirror surfaces.

There are many ways to describe optical surfaces. Normally, optical surfaces are described by an equation with a conic term plus some aspherical deformation terms:

$$z = \frac{ch^2}{1 + \sqrt{1 - (1 + \kappa)c^2h^2}} + \sum_{i=2}^n A_{2i}h^{2i} \quad (11)$$

where h is the radial distance of a point on the surface from the symmetry axis, $c (= 1/R)$ is the curvature of the vertex of the mirror, κ is the conic constant, and A_{2i} are the aspherical deformation coefficients. If κ and A_{2i} are zero, then Eq. 11 specifies that the surface is a sphere. If κ is not zero, but all A_{2i} are zero, then Eq. 11 represents a conical surface.

After evaluating the surface data for the primary and secondary mirrors in a Head microscope from Eqs. 9 - 10, then we have used both linear and nonlinear least squares fitting algorithms to determine the surface parameters of Eq. 11 such that the Head microscope can be very consistently modeled to satisfy the aplanatism conditions and to yield diffraction limited resolution for the desired NA . For a specific set of surface data, it is not clear initially how many aspherical deformation terms will be required or whether the conic constant is zero. Experience has shown that it is desirable to determine an approximate shape of the Head surfaces before doing extensive nonlinear least squares fitting. As a result of the initial values used in this work, the Head surfaces can be approximated by spherical Schwarzschild microscope surfaces with the corresponding surface parameters. Good representations for Head surfaces have been determined to have a small conic constant and one to two aspherical deformation terms or to have zero conic constant with four to eight aspherical deformation terms. It has been found that there are no unique representations for the fitting of a Head microscope surface, but all well behaved solutions have the same diffraction limited optical performance.

For example, using a nonlinear least squared fitting algorithm, a set of Head surface parameters is given in Table 2 for a 30x microscope with $NA = 0.35$ where the following axial spacings have been used

$$d_0 = 90.318625mm, \quad d_1 = 89.1710mm, \quad d_2 = 1159.5595mm. \quad (12)$$

The aspherical surfaces described in Table 2 represent surfaces which differ from a spherical surface by approximately one micron for a primary aperture radius of 70mm, which corresponds to a $NA = 0.35$. Current substrate fabrication technologies should be able to make the mirror surfaces defined by Table 2. Figure 4 presents the MTF for the system given in Table 2 and Eq.12, which shows that this representation of the 30x Head microscope is diffraction limited.

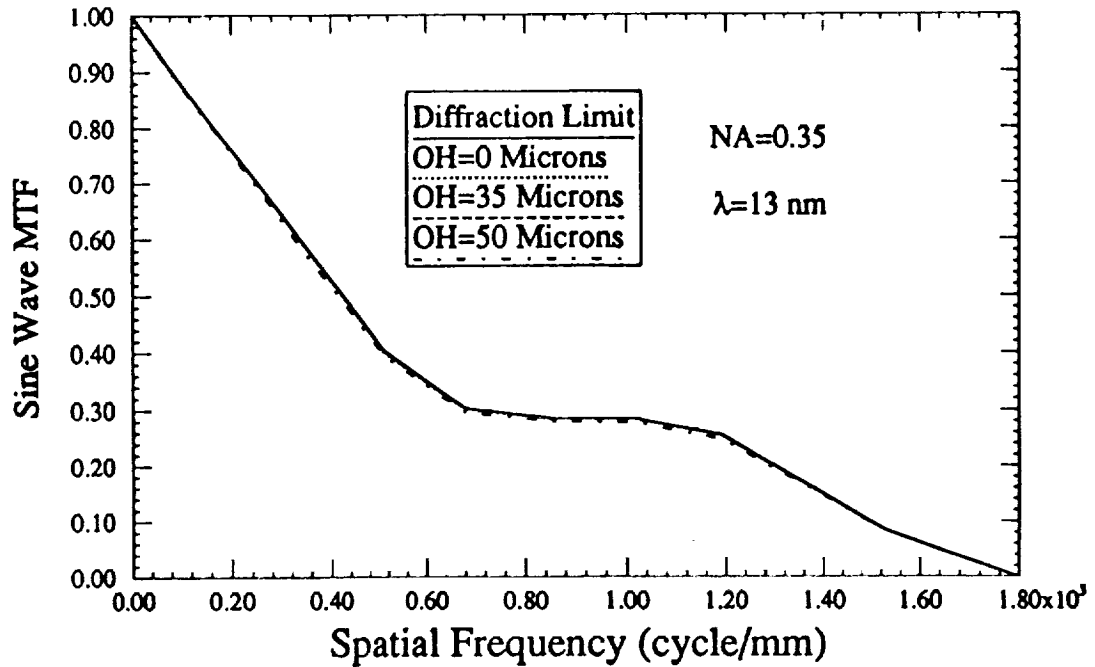


Figure 4: MTF vs the spatial frequency for 30x Head microscope where OH is the object height.

Variable	Primary	Secondary
Diameter(mm)	140.0	29.0
Hole Dia. (mm)	30.0	none
Vertex Radius (mm)	139.170963	49.999915
Conic Constant	0.0029751487	-0.002862214
A4 (mm-3)	1.405927D-10	-1.826711D-9
A6 (mm-5)	0	-4.739086D-11

Table 2: Nonlinear least squares technique has been used to fit the numerical surface data of a Head microscope to a formula with a conic surface term plus 6th order polynomial representing the aspherical and non-conic deformation terms.

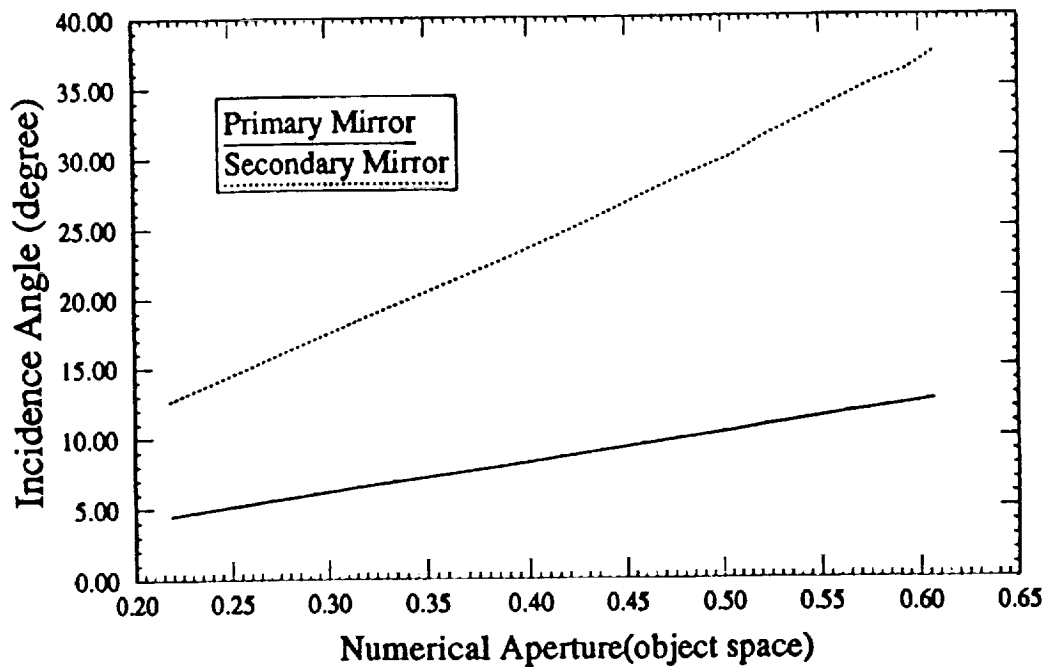


Figure 5: Variation of the angle of incidence over the Head surfaces of a 30x microscope versus the numerical aperture.

Next, it is important to determine whether it is possible to deposit multilayer coatings on these fast mirror surfaces. Figure 5 presents the variation of the angle of incidence on both the primary and secondary Head mirrors as a function of the microscope NA for the 30x Head microscope which is defined by Table 2 and Eq.12, where the diameter of the primary was increased to achieve larger NAs . It is evident from Fig. 5 that the angle of incidence varies more rapidly over the secondary than the primary. This strong variation of the angle of incidence over the secondary mirror has significant implications for the design and fabrication of multilayer coatings of a fast Head microscope.

Depending on how a multilayer is designed, peak reflectivities may only be maintained for a $5 - 10^\circ$ variation in the angle of incidence over the multilayer. Therefore, conventional multilayer coatings can not be used for a very fast Head microscope. However, graded or segmented multilayer coatings may be used to coat the secondary mirror such that operation with acceptable reflectivity may be achieved for a wide range of NAs . To illustrate this concept, consider designing off-axis multilayers to work with a peak reflectivity for segments of the primary and secondary mirrors corresponding to the aperture of $NA = 0.45$ for a water window microscope using Ni/Ca multilayers.[23] Figure 6 illustrates this concept where the multilayer coatings on the primary have been optimized for a 8° angle of incidence with a d-spacing period of 20.3\AA and ratio $(\frac{d_{Ni}}{d_{Ca}}) = 0.414$, and the multilayers on the secondary have been optimized for a 27° angle of incidence with a d-spacing period of 22.5\AA and ratio $(\frac{d_{Ni}}{d_{Ca}}) = 0.32$. The multilayer optical constants for Ni [$n=0.988225$, $k=0.004120$] and Ca [$n=0.999145$, $k=0.000278$] were evaluated from the Henke Tables.[24] It is interesting to note that for these segments of the mirror surfaces and for this configuration of multilayer coatings, this water window Head microscope would have a net reflectivity

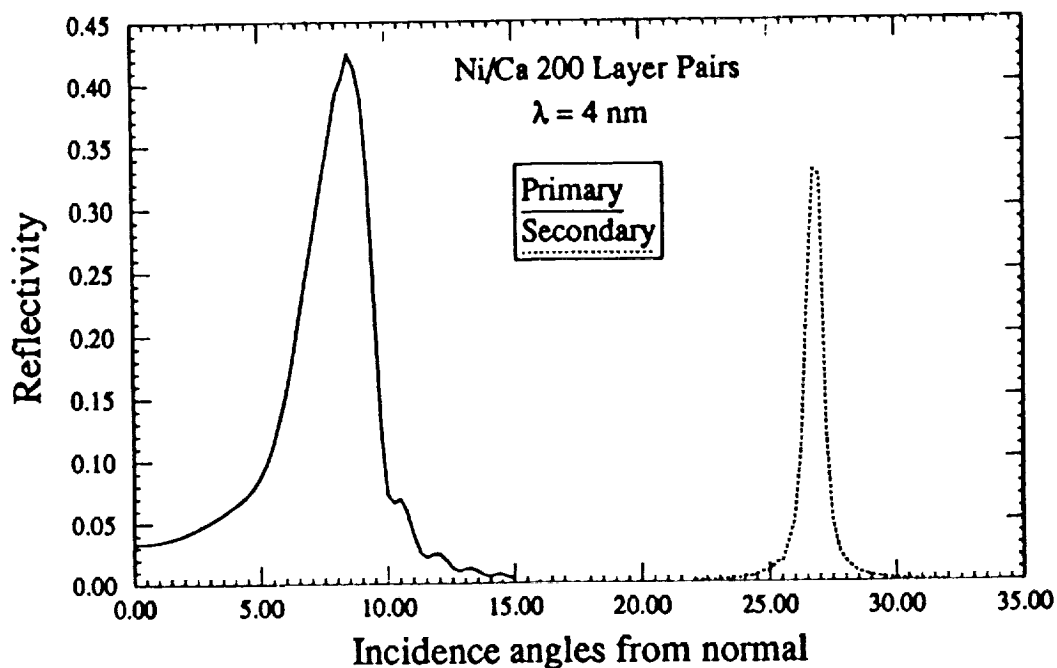


Figure 6: Reflectivity of proposed water window Head microscope versus the angle of incidence of radiation on mirror surfaces.

varying from a peak value of 14% to the full-width half-maximum value of 2.4%. By further optimizing the multilayers, one may be able to broaden the reflectivity versus angle of incidence peaks and to increase the system throughput. Efforts are also underway to identify different microscope configurations for which the angle of incidence does not vary as strongly over the secondary mirror surface as indicated in Fig. 5.

4. CONCLUSIONS

This work has summarized some useful relationships between NA , magnification, diameter of the primary mirror, radius of curvature of the secondary mirror, and the total length of the Schwarzschild configurations of a microscope. To achieve resolutions better than about 3λ , it is necessary to use aspherical Head surfaces to control higher-order aberrations. For a NA of 0.35, the aspherical Head microscope could provide diffraction limited resolution of 1.4λ where the aspherical surfaces would differ from the best fit sphere by approximately 1 micron. However, the angle of incidence would vary by about 6° over the secondary and 3° over the primary, which may require graded multilayer coatings to operate near peak reflectivities. For higher NA s, the variation of the angle of incidence over the secondary mirror surface becomes a serious problem which must be solved before multilayer coatings can seriously be considered for this application.

5. ACKNOWLEDGEMENTS

The authors would like to express gratitude to the NASA/MSFC Center Director's Discretionary Fund, NASA/MSFC Technology Utilization Office, and to The University of Alabama at Birmingham for partial support of this research.

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