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Nested mirrors for X-rays and Neutrons

Gene E. Ice[*a], Rozaliya I. Barabash[a,b], Ali Khounsary[c]
[a]Materials Science and Technology Division, ORNL, Oak Ridge TN 37831-6118;
[b]Center for Materials Processing, U. of Tenn. Knoxville, Knoxville,TN 37902
[c]Advanced Photon Source, Argonne National Laboratory, Argonne IL 60439

ABSTRACT

Montel (nested) Kirkpatrick-Baez mirrors can focus X-ray and neutron beams with larger divergences into small beams than is possible with standard (sequential) Kirkpatrick-Baez optics. They also provide for a more compact focusing system and higher fluxes into small beams than with current alternatives. These attributes make Montel optics critically important for both achromatic neutron and X-ray focusing. Here we describe design rules that optimize mirror performance under various constraints, including diffraction-limited, and flux-limited focusing. We also describe first tests of optical designs that employ nesting as a way to improve neutron microfocusing optics and suggest future directions for X-ray nanofocusing optics.

Keywords: Montel mirrors, Kirkpatrick-Baez mirrors, X-ray microfocus, neutron microfocus, nanofocus

1. INTRODUCTION

Modern mirror optics can focus to state-of-the-art small x-ray and neutron beams [1,2]. To go beyond current performance however, new approaches are required that can collect more divergence than with standard sequential Kirkpatrick-Baez (KB) x-ray mirrors and that can collect the greatest possible intensity into small beams for neutron optics. Indeed, the quality of x-ray mirrors has now reached the diffraction limit, and simply more perfect KB mirrors cannot decrease spot size. Efforts in Japan, Europe and America have concentrated on the use of multilayer coatings to increase the critical angle of reflection of x-rays. This increases the numerical aperture (amount of radiation collected, which allows for a lower diffraction limit [3-5]. However multilayer x-ray mirrors typically have a restricted bandpass. As a result, total-external-reflection X-ray mirrors are still needed to preserve achromatic performance over a bandpass suitable for diffraction experiments or for extended x-ray absorption fine-structure measurements.

Similarly, with neutron microfocusing, mirror perfection is not the limiting factor. With neutron mirrors, supermirror coatings increase the divergence that can be collected onto the image plane by a factor of 3 or more but even so, the low source brilliance of even the most powerful neutron sources means that as beam sizes are reduced, there are simply not enough neutrons to make measurements in a reasonable amount of time. This is a case where the beam size is determined by the geometrical demagnification of an intermediate object slit placed between the source and the sample. The source flux is determined by the efficiency of the focusing optics and the total beam emittance (size x divergence) focused onto the sample. The essential challenge is to preserve source brilliance at the image plane, while maximizing the divergence of the focused microbeam for a given spot size.

2. OPTIMIZED DESIGNS FOR KB FOCUSING

2.1 Diffraction limit of Montel (Nested) KB Optics compared to Sequential KB optics

The focal spot size for x-ray reflective optics is determined by the geometrical magnification of the optics, by aberrations /mirror imperfections, by sample and/or mirror vibrations and by the diffraction limit. For elliptical Kirkpatrick-Baez (KB) mirrors, the demonstrated perfection of mirror surfaces and the geometrical demagnification for ultra-brilliant sources has improved so much over the past decade that the achievable beam size is sometimes limited primarily by

*IceGE@ornl.gov; phone 865 574-2744; fax 865 574-7659

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diffraction and mechanical/environmental factors. The diffraction limit is determined by the X-ray wavelength and the divergence on the sample. To understand the design constraints on KB mirror optics, we consider a simple elliptical mirror as shown in Fig. 1. Typically mirrors are discussed in terms of the object distance F_1, the image distance F_2, the mirror angle at the center of the mirror, θ, and the mirror length, L. However for the discussions of this paper where the divergences that can be accepted are pushed to the extreme limits achievable, it is convenient to

describe glancing-angle elliptical micro and nanofocusing mirrors in terms of the clearance distance, F_D, from the downstream end of the mirror to the image plane, the distance, x, upstream from the downstream end of the mirror, the divergence focused onto the image plane θ_i, the reflection angle at the downstream edge of the mirror, θ_D and the source divergence intercepted by the mirror θ_O. These parameters are illustrated in Fig. 2.

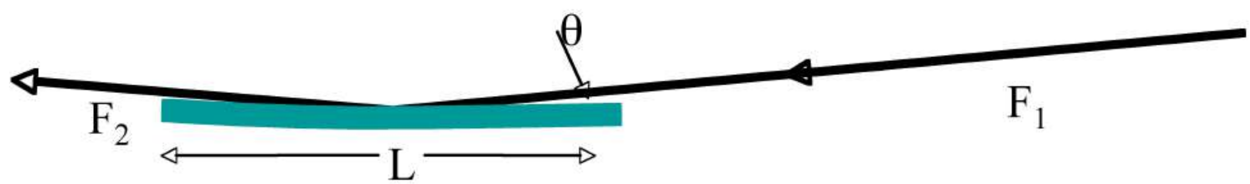

Fig. 1. Standard parameters for an elliptical focusing mirror with object distance F_1, image distance F_2, mirror length L, and glancing angle at the mirror center of θ.

For a doubly focused Kirkpatrick-Baez mirror system the full-width-at-half-maximum (FWHM) diffraction limit in each plane is given by,

$$D_{FWHM} \sim \frac{0.88\lambda}{\theta_i} \tag{1}$$

Here λ is the x-ray wavelength and θ_i is the divergence focused onto the image plane. For total-external reflection x-ray mirrors, the divergence that can be collected is limited by the critical angle, θ_C for efficient reflectivity from a dense surface,

$$\theta_c \sim \sqrt{\rho\delta} = 6.7\times10^{-2}\,\lambda(nm) = \frac{8.4\times10^{-2}}{E(keV)}. \tag{2}$$

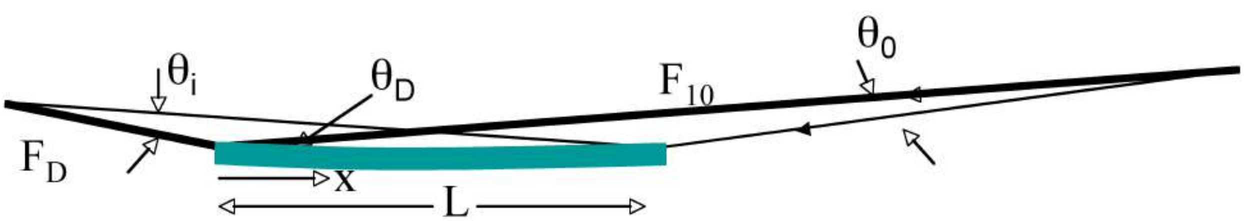

Fig. 2. Parameters useful for describing the ultimate limits to focusing with an elliptical mirror. These include the distance upstream from the downstream end of the mirror, x, the clearance from the downstream end of the mirror to the image plane, F_D, the glancing angle at the downstream end of the mirror θ_D, the divergence focused onto the image plane, θ_i, and the divergence collected from the object θ_O.

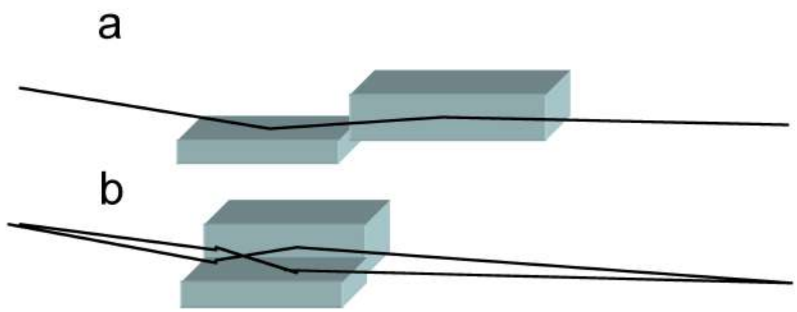

Fig. 3. (a) Sequential Kirkpatrick-Baez mirrors; (b) Nested (Montel) Kirkpatrick-Baez mirrors.

In principle, a simple 1-D focusing mirror surface can collect up to $2\theta_c$ and a figure of revolution can collect up to $4\theta_c$. In practice however, geometrical constraints on sequential KB mirrors limit the divergence that can be collected in each plane to about $0.84\theta_c$.

To understand the ultimate limit to KB diffraction limited mirrors, we study the theoretical limits of elliptical microfocusing mirrors depending on the choices of geometrical mirror parameters. Consider for example the elliptical mirror as shown in Fig. 2. At glancing angles, the image and object divergences, θ_i and θ_O, of an elliptical microfocusing

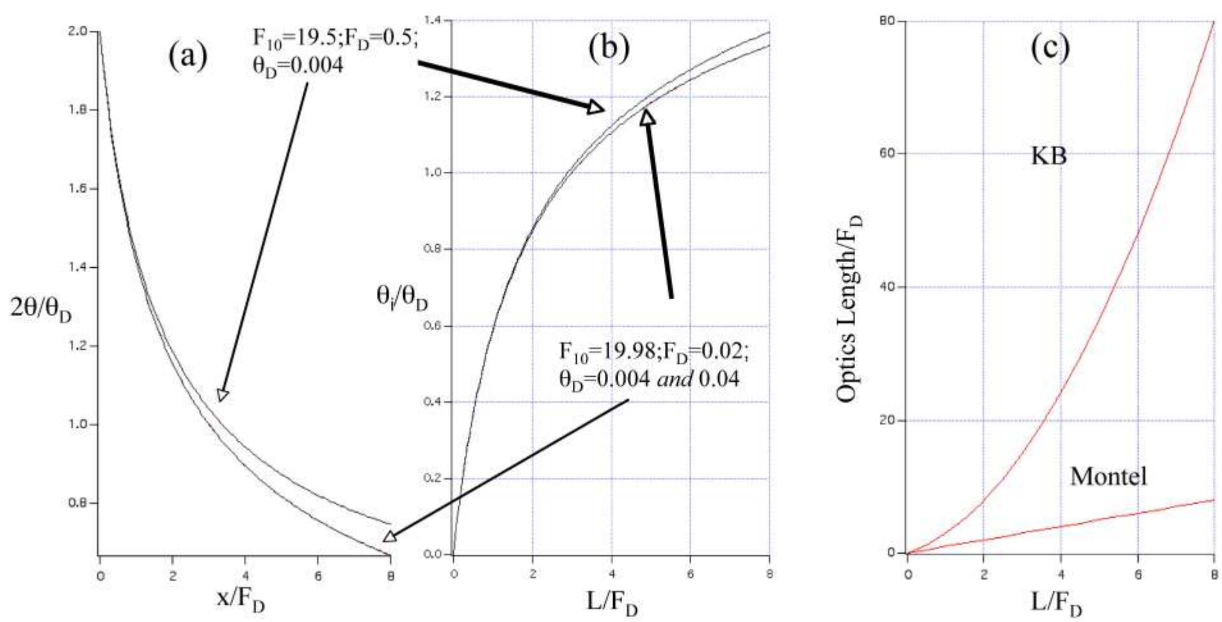

Fig. 4 (a) The 2θ reflection angle decreases with distance, x, from the downstream end of a microfocusing elliptical mirror. If the position along the mirror, x, is normalized to the downstream clearance, F_D, and the 2θ reflection angle is normalized to the downstream edge reflection angle, θ_D, then the curve is only weakly dependent on the absolute value of the clearance. (b) The divergence focused onto the image plane by a mirror with downstream glancing angle θ_D , and mirror length X is nearly a universal function when normalized to θ_D and the clearance distance, F_D. (c) The length of optics required grows rapidly for a Kirkpatrick Baez sequential pair as a function of the mirror length to downstream edge clearance to the image.

mirror, depend primarily on the mirror angle, θ_D and the ratio of the mirror length L to the image distance F_D. For example, the reflection angle at positions, x, upstream of the mirrors downstream edge are compared in Fig. 4a for three different mirror conditions. Because the numbers are normalized to the clearance distance, F_D and the downstream reflection angle, θ_D, the three curves lie very close together. Figure 4a can be used to estimate the fraction of the mirror that can reflect various wavelengths. For example, if the mirror is designed with $\theta_D = \theta_c$ for wavelength λ, then for wavelength $\lambda/2$, only the part of the mirror $x/F_D > 3.5$ will efficiently reflect. Similarly the divergence that can be collected onto the image plane can be estimated from a normalized curve (Fig. 4b). As can be seen, if the mirror length is normalized by the clearance distance, and the divergence collected onto the image plane is normalized by the angle of reflection at the downstream edge of the mirror (largest angle) then the normalized numbers again fall on an almost universal curve that changes only slightly for factors of 10-20 in distance and angle. With this curve it is possible to estimate the total divergence that can be collected by a KB mirror pair in either sequential or nested (Montel) geometries. For example, if L/F_D is n for each mirror of a sequential mirror pair, then the total length of the mirror pair is related to the clearance distance of the secondary mirror by,

$$L = \left(2n + n^2\right) F_D \tag{3}$$

On the other hand the length of a Montel mirror pair is only $x/F_D = n$. This behavior is illustrated in Fig. 4c. Clearly, sequential mirror systems become extremely large for n >2 and even an n=2 mirror system for sequential mirrors has about the same length as an n= 8 system for a Montel pair. Thus the diffraction limit for total-external-reflection optics with sequential KB mirrors is ~<u>16 nm,</u> whereas with a Montel pair the diffraction limit is ~<u>11 nm</u>.

Of course for broad bandpass reflective optics it is not possible to simultaneously optimize a mirror for all wavelengths. Depending on the strategy, the mirror can be optimized for shortest, longest or an intermediate wavelength. If the mirror is optimized for the *shortest* wavelength, then the divergence collected onto the sample is roughly independent of wavelength and the diffraction limit increases with wavelength according to Eq. 1. This effect is linear with wavelength. If however the mirror angle θ_D is optimized for the *longest* wavelength than only a fraction of the mirror reflects shorter wavelength radiation, and the diffraction limit for shorter wavelengths is compromised. For glancing angle elliptical mirrors, the loss of divergence with shorter wavelength grows faster than linear. In practice, a good compromise is to set the downstream mirror angle to the critical angle for an intermediate wavelength. Examples of these three strategies are shown in Fig. 5a for a case where the bandpass of 0.6-1.0 angstroms.

2.2 Flux limit of Montel (Nested) KB Optics compared to Sequential KB optics

If flux is the main limitation to the use of small beams, then the figure of merit is the maximum flux into a small spot. For a demagnifying KB mirror system, as the mirror becomes longer, the fraction of the source divergence that is collected increases, but the geometrical demagnification becomes less extreme and the object size must be decreased to maintain a small spot at the sample. The geometrical demagnification is simply $F_D(1+n/2)/(F_{10}-nF_D/2)=F_2/F_1$, and the beam collected by the mirror is θ_O. Again, the performance is nearly a universal function for small angles and large demagnifications (Fig. 5b).

Again a benefit of the significantly larger numerical aperture of Montel KB mirrors compared to sequential KB mirrors, is their ability to increase the flux on the sample. This is particularly important for neutron optics, where flux rather than diffraction limited spot size is the dominant concern. With neutron supermirrors nested in a Montel geometry, the total flux on the sample can be increased by about a factor of 2.6 compared with sequential KB mirrors. For example, a 0.5 m long Montel mirror system with 0.25 m of clearance has an n of 2. A similarly sized sequential mirror system has an n of 0.73. The difference in total flux collected into a small spot is ~2.5.

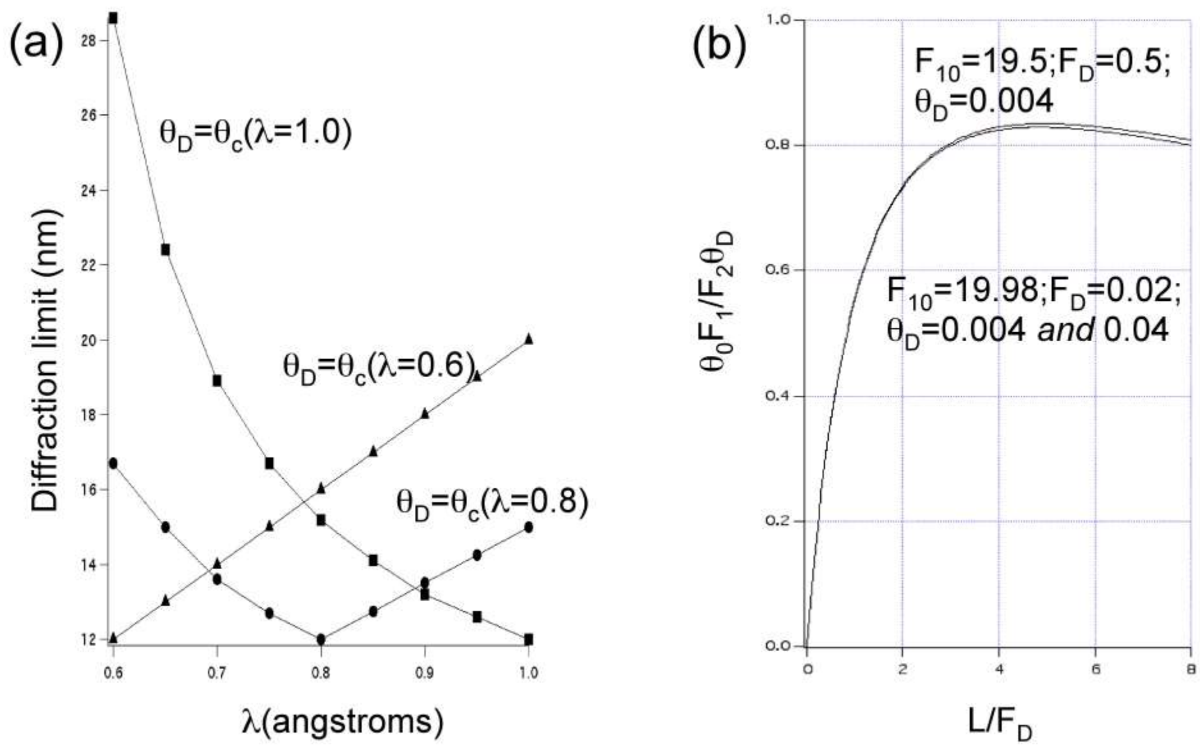

Fig. 5 a. Diffraction limit depending on whether the mirror is optimized for the shortest, longest or middle wavelength of a λ=0.6-1.0 Å bandpass. b. Relative flux as a function of L/F_D for an elliptical mirror.

3. EMERGING IMPLEMENTATIONS

3.1 Neutron mirrors for SNAP at the SNS

A Montel mirror system has been designed and tested on the Spallation Neutrons at Pressure (SNAP) beamline. The system is based on elliptical mirrors that are independently bent, and then brought together with a manual micrometer stage (Fig. 6). The prototype system utilizes mirrors with straight sides, which creates a gap between the mirrors when they are nested against each other. This gap can grows with mirror length and inversely with mirror radius. Because X rays and neutrons reflect near the intersection of Montel mirrors, the gap reduces the mirror system throughput and creates a double-peak in the divergence focused onto the image plane. Even so, the mirror focal spot size of the prototype was very close [6] to the size predicted from the figure errors measured with a special long-trace profiler (LTP) [7]. A detailed description of the mirror calibration and metrology of the mirror edge is provided in reference 6. Beams as small as ~70 microns were measured. Additional efforts are now underway to more precisely bend the mirrors to the optimum figure, to improve the quality of the mirror surface at the edge of the mirror and to shape the mirror edge to allow the two mirrors to nest against each other with a minimum gap. The required figure errors are < 10 microradians, which should be achievable with careful bending. By figuring the edges of one of the mirrors to < 50 microns of the ideal elliptical shape, it should be possible to achieve better than 97% of the theoretical throughput. A recent announcement by Swiss Neutronics of advanced metal neutron supermirrors [8] provides a possible path forward to figure the edge of the nested mirrors with electro-discharge machining.

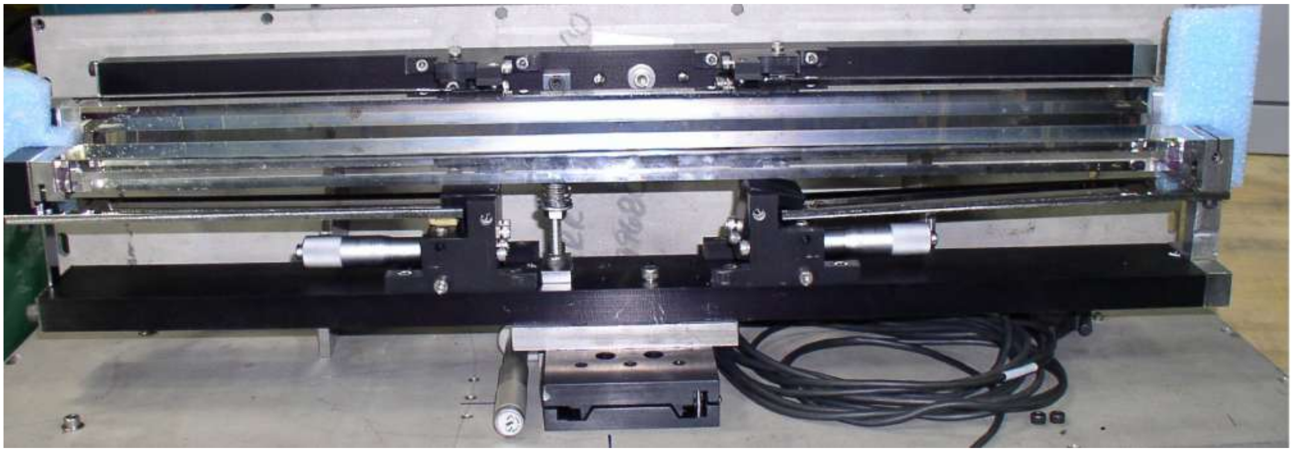

Fig. 6. Nested mirror pair for SNAP.

3.2 Polychromatic X-ray Nanofocusing for Beamline 33-ID at the APS

Another emerging application of nesting is to achieve ultra-small and ultra-stable polychromatic x-ray nanobeams. Here it is important to improve the stability, geometrical demagnification and diffraction limit of the optics. Montel optics are ideal because the are more compact, have better geometrical demagnification and have a better ultimate diffraction limit than with sequential KB optics. They are also easier to pre-align which simplifies alignment in the field. The main challenge is to maintain state-of-the-art surface quality near the edge of one of the mirrors, and to shape the mirror edge so it nests against the elliptical surface of the partner mirror.

One of our present approaches involves dividing a pre-figured elliptical mirror into two parts that can be used as the of Montel mirror pair. This approach is primarily driven by the fact that in a conventionally polished mirror, the clear aperture area (the central part of a polished surface) has the best figure and finish. As such, using two halves of a pre-figured mirror cut in the middle has several advantages- including consistency and economy. There are major challenges however. First, the mirror surface must be protected against damage and deformation during cutting and subsequent figuring operations. After cutting into two, the cut sites must be treated (e.g., etched) to remove any subsurface damages that could alter a mirror's figure. Then the mating side of one of the mirrors must be contoured and polished such that when it is placed against the partner mirror, it makes a nearly perfect fit with good surface quality all the way to the contact edge.

This last two-steps are crucial because if there is a significant gap or if the mirror surfaces in the vicinity of the interface are damaged, a significant part of the incident beam could be lost. As an example, we are developing a pair of Montel mirrors for polychromatic nanofocusing on Sector 33 at APS. This beam line will use 40 mm long elliptical mirrors for nano-focusing a 100 μm beam to a 50 nm spot at 2000x demagnification. This concave elliptical mirror has a maximum depression of about 6 μm at its center. If cut flat and placed against its mating mirror, a gap as large as 6 μm is created which loses about 10% of the 100 μm incident beam. Similarly, if the mirror surfaces near the intersection are damaged, then beam loss can be significant.

Another approach to making a pair of Montel mirrors from a single pre-figured substrate is to cut a pre-figured mirror into two parts and then grind the cut sites at a 45 degree angle as shown in the left pair of Fig. 7. Placing the two together makes a good fit with no gaps requiring no contouring of the mirror sides. This work is in progress and the results and we hope to have positive results shortly

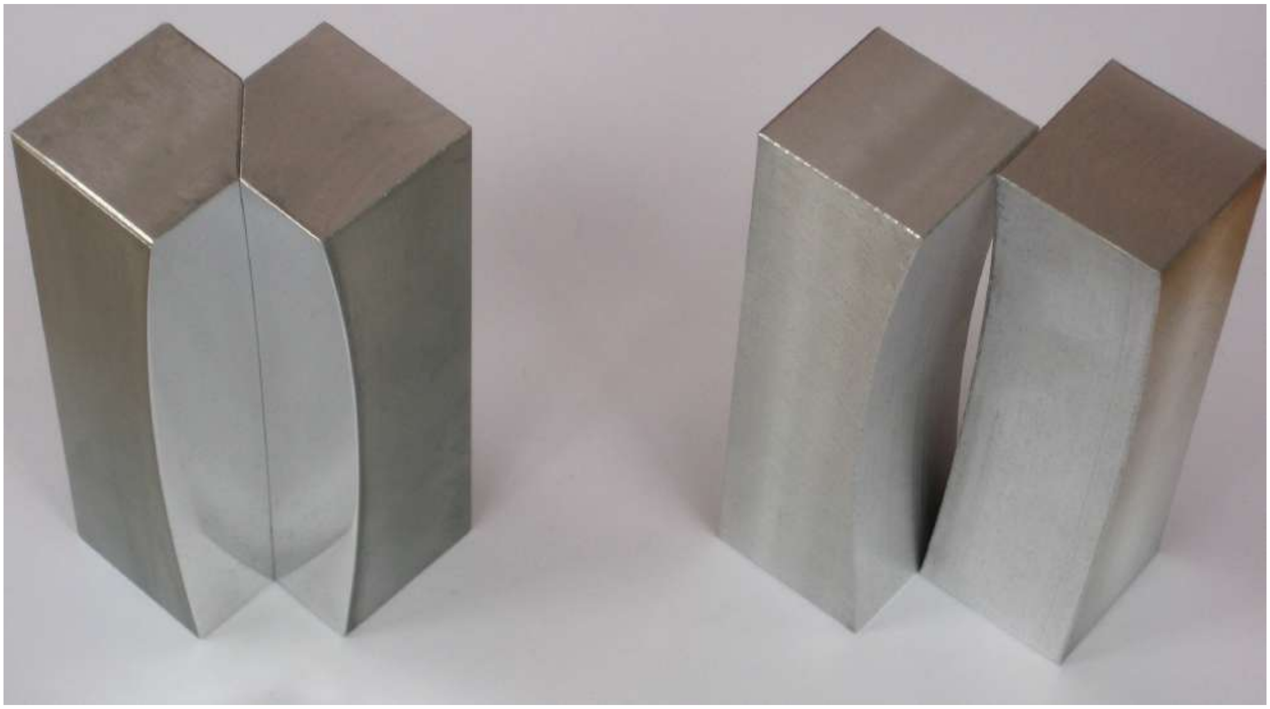

Fig. 7. If mirrors with elliptical surfaces are nested together their is a gap at the intersection (right pair) unless the edges are either cut at 45° to the surface (left pair) or one of the mirror edges is profiled to nest against the surface of its partner mirror. .

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