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FAR-INFRARED OPTICS DESIGN & VERIFICATION

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Abstract: Compact quasi-optics are difficult to design with any confidence using techniques developed for visible wavelengths. In this paper we investigate the performance of existing software design tools (ASAP, CODE V, GLAD) as well as a Gaussian beam mode analysis technique not yet available as commercial software. We have devised a set of test cases and used these to study the underlying methodologies and physics of these packages and we probe their suitability for the analysis of submillimetre-wave systems and components. We have used the physical optics package GRASP as our benchmark software.

1. Introduction

In this paper we investigate the performance of a range of commercial optical design software packages (GLAD, ASAP, CODE V) in analysing the behaviour of far-IR optical systems. Although these packages are not specifically intended for use at submillimetre wavelengths, nevertheless they represent the only classes of commercial optical design tools available with some diffraction capability. In reality, long wavelength, far-infrared and terahertz optical systems are unique, requiring a different approach to those commonly used at visible wavelengths. In this paper therefore we identify those theoretical techniques that can be used to analyse long wavelength systems in which diffraction effects inevitably become important. Some of these techniques have been used in typical computer-aided design packages and we particularly assess their applicability to long-wavelength optical design. We do not intend to discuss the limitations of the packages as such, but rather probe the fundamental approximations that are inherent in the theoretical method on which the software analysis is based.

Several test examples have been chosen that highlight some of the discrepancies that can arise between field predictions from a selection of different software packages when applied to the far infra-red. We present the results of our investigations, which illustrate for the reader the level of confidence that can be placed in the predictions of commercially available software. We have taken the physical optics package, GRASP, an extremely powerful software tool for reflector antenna design and analysis, as our benchmark software against which the results of the other packages can be compared. It should be noted that GRASP because of its complexity and computational intensity is more suited to the concept verification phase rather than the instrument design phase. Future work will involve an experimental verification of some GRASP results.

2. Theoretical Analysis Techniques

Optical design is essentially concerned with the problem of calculating an electromagnetic field over a surface in an optical system when the field, or currents, over some other surface is known. The full solution to Maxwell's equations is usually extremely difficult to find and in practice approximations have to be made. Figure 1 shows the relationship between some of those approximate methods that can be used to analyse far infra-red systems. Many theoretical techniques listed in figure 1 have not however been used in commercial software at all.

In optical design a source field must be determined and then propagated from one optical component to the next. It is often difficult to rigorously calculate the source field in the first place. When a field is scattered by a metallic surface, such as a mirror, two analytical procedures are possible: either Maxwell's equations can be solved rigorously in the vicinity of the mirror, or the locally scattered field can be estimated. There is a major difference between those methods that attempt to calculate the scattered field in a rigorous manner and those that make approximations (termed 'Approximate Source Field' methods in figure 1). When a field is incident upon an aperture, for example, it is often assumed that the field, or its normal derivative, over the opaque region is zero, whereas over the transparent region they are the same as they were in the absence of the aperture. Techniques such as the Method of Moments attempt to calculate the current distribution over a surface precisely [1].

In general terms the field over the input surface is a vector field, and it is necessary to calculate the full vector field that results. In some cases, considering only one component of the field leads to relatively simple scalar solutions. These tend to emerge when a co-ordinate system is chosen so that the components of the vector field separate. For sequences of co-linear components it is best to separate out the direction of propagation. If the field is assumed to propagate in a paraxial manner, scalar solutions emerge. For THz systems the question of whether a vector or a scalar solution is sought is intrinsically related to whether the field is of a paraxial or wide-angle nature.

Propagating the field onto the next optical component (solving the wave equation) requires diffraction integrals to be calculated for each field point calculated. The Rayleigh-Sommerfield techniques (see *e.g.* [2]) are formal, rigorous solutions of the wave equation when either the scalar quantity under consideration (Dirichlet solution) or its normal derivative (Neumann solution) is known over a closed surface bounding the region of interest. Vector components of a field are considered to propagate independently of each other. These techniques require a source field to be assumed, and a two dimensional integral must be evaluated for every field-point calculated. Kirchhoff's approximation is essentially the arithmetic average of the two Rayleigh-Sommerfield equations when there is ambiguity over which vector quantity (**E** or **H**) is being analysed. The averaging process appears in the form of the well-known $(1+\cos\theta)/2$ obliquity term.

Rather than evaluating diffraction integrals directly, it is possible to decompose the assumed source field into modes and then propagate the modes as required. Propagating modes through free space is usually straightforward and often simply consists of slipping the mode phases with respect to each other. One of the most attractive schemes is to break the field down into plane waves [3]. Plane waves are exact solutions of the Helmholtz equation, and therefore the only assumptions made relate to the field across the source plane. A plane wave analysis has the significant advantage that it is not limited to paraxial fields. Gaussian modes, on the other hand, are solutions of the paraxial wave equation [4]. They allow a field distribution to be traced using only the scale size of the beam, the large-scale radius of curvature of the phase front and the phase slippage between modes. An advantage of Gaussian modes is that, appropriately scaled, they allow an efficient representation of paraxial systems and only a relatively small number of modes is required for accurate representation of the system. In the Gabor approach [5], a field is decomposed into a discrete set of Gaussian beams shifted both laterally and in phase slope.

At optical wavelengths, away from boundary shadows and abrupt changes in intensity distribution, energy can be considered to be transported along certain curves, or light rays, obeying certain geometrical laws. For system design at visible wavelengths this technique is widely used and ray-tracing packages, such as Zemax, have proved to be very successful. In the far-infrared, however, the wavelength may be an appreciable fraction of component sizes and so cannot be neglected. In this regime diffraction effects become important and the approach of geometrical optics is inadequate.

The term physical optics, as we use it in this paper, refers to the calculation of the field radiated by a reflector using an approximate surface current distribution determined from the incident magnetic field. Central to the method is the assumption that the field on that part of the reflector not directly illuminated by the incoming field is zero. The method is appropriate where the radius of curvature of the reflector is many wavelengths, which of course is not valid at an edge. To correct for edge effects the Physical Theory of Diffraction (PTD) has been developed. Here an attempt is made to introduce currents associated with the edge into the assumed current distribution .

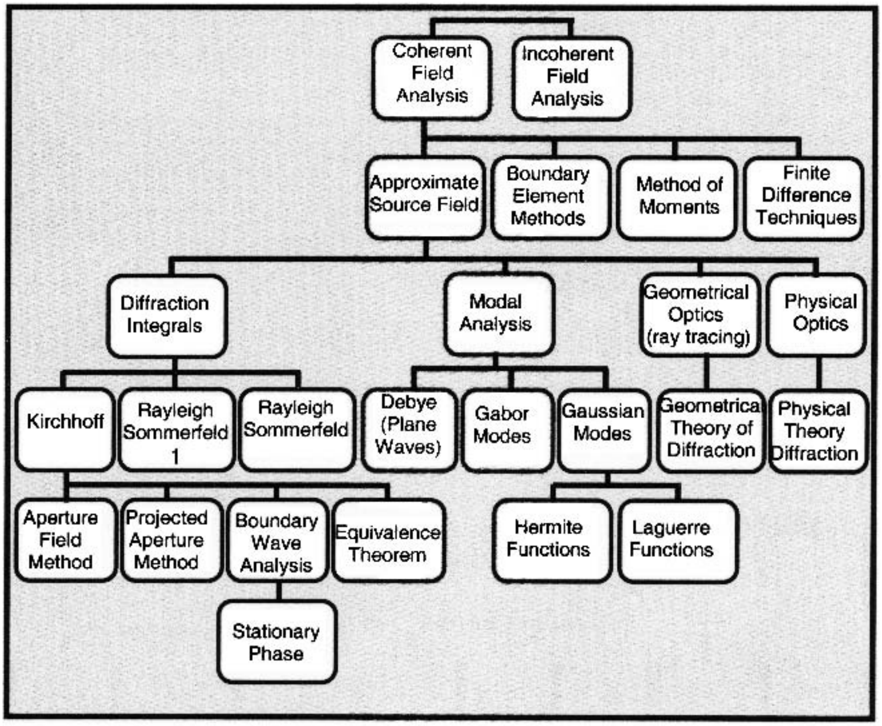

Figure 1 Schematic diagram showing the relationship between some methods used for diffraction analysis.

In a multi-moded infrared optical system the radiation field will be partially spatially coherent. Each true component mode of propagation, although having no fixed phase relationship with other modes, will of course propagate according to the laws of diffraction and the total field intensity at any point will be given by the sum of the intensities of the component modes (fields add in quadrature). Ray tracing can be employed in highly over-moded systems as an efficient accurate approach. However, in the long wavelength limit systems tend to be at most few moded and an approach incorporating diffraction techniques discussed above is necessary. When this is applied to a modal approach, for example, propagation can be very elegantly described in terms of coherence matrices. These track the evolution of the mutual coherence function [6].

In this paper we compare some results obtained using the commercial packages ASAP, GLAD, and CODE V (beam propagation algorithm). These are scalar diffraction packages based on a modal analysis of fields. GLAD and CODE V decompose the fields into plane waves, ASAP uses Gabor modes. In addition we have used results from the 'in-house' software package, PROFILE, which is based on Gaussian Beam Mode Analysis (GBM) techniques specifically applied to submillimetre-wave optical systems (*e.g.* [4], [7]). We use GRASP, a commercial software package combining Physical Optics and PTD, as our benchmark. GRASP has been developed as an effective tool for modelling reflector systems, when the full 4π radiation pattern is required and is ideal for accurate reflector antenna design purposes. It can therefore be computationally slow and inefficient in the design and analysis process of multi-element systems. In practice more approximate methods are therefore desirable for quasi-optical beam guides commonly used at submillimetre wavelengths.

4. Test Cases

A number of criteria were used when setting up the example test systems to analyse in detail. Our aim is to elucidate the essential differences between packages using a relatively small number of components with a combination of source fields typical of submillimetre-wave systems (e.g. horn antennas, Gaussian beams). As well as examples chosen from regimes where the approximations made by all packages are valid and good agreement would be expected, we have also probed more extreme examples, though still typical of quasi-optical systems in the far infra-red. The cases we describe in this paper, aperture stops and off-axis reflectors, are the basic fundamental components of many quasi-optical systems. They illustrate many of the essential features of modelling techniques and the results we present allow the estimation of the accuracy with which more complex multi-element systems can be analysed. In addition, for benchmark comparison purposes, apertures and off-axis mirrors are readily modelled by GRASP. In the case of ideal lenses the re-focussing effect on the beam can be represented as a pure phase transformation. We do not present any examples as all the optical packages have the ability to model such an ideal component and are in good agreement. Furthermore for GRASP the lens has to be described in terms of its physical parameters.

We have investigated components with diameters down to a few wavelengths and quasi-collimated beams with F-numbers between 3 and 30, as well as including uniform illumination by an infinite plane wave in certain examples. An F3 beam is typical of a horn antenna, whereas an F10 beam is quite often encountered at the focal plane of a Cassegrain telescope. An F30 beam is quasi-collimated and having a large depth of field could be used in interferometric diplexers and single-sidelobe filters. These range of F numbers, as well as the quasi-optical component diameters and separations in terms of wavelength are not necessarily those for which the software packages were initially intended. The off-axis mirrors we investigate have a large angle-of-throw typical of many current designs (*e.g.* HIFI [8]). Large angles of throw are necessary to avoid vignetting effects in compact optical systems. In the following sections we describe in detail the example test cases chosen and summarise the conclusions drawn from comparisons between the simulations

4.1. Apertures

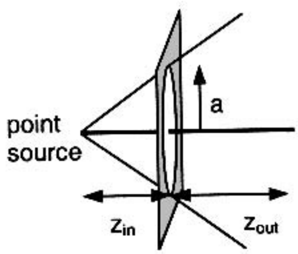

Figure 2 Aperture test cases. An aperture of radius a is illuminated by a point source located a distance z_{in} away. The beam pattern at z_{out} is calculated.

The first set of test cases modelled the diffraction effects of beam truncation at an aperture stop in a screen. The near and far field intensity patterns were calculated for uniform plane wave illumination ($z_{in} = \infty$ in figure 2) of apertures of radius between 3λ and 30λ. Results are shown in figures 3 and 4. Figure 3 shows an example of the near-field results for the paraxial packages (GBM analysis results closely matched those of GLAD). In fact, for the paraxial packages the results simply scale with aperture diameter as expected. Although this would be an unusual example for a typical far-infrared system in the sense that the aperture is uniformly illuminated, it is one of the standard classic examples of Fresnel diffraction and so is instructive in terms of probing the limitation of paraxially based packages. These examples were chosen so that an on-axis minimum is predicted using a simple Fresnel diffraction calculation (a sort of inverse Poisson spot, as predicted using Babinet's principle). The packages do produce the on-axis minimum indicating that they are correct within the limits of Fresnel Diffraction.

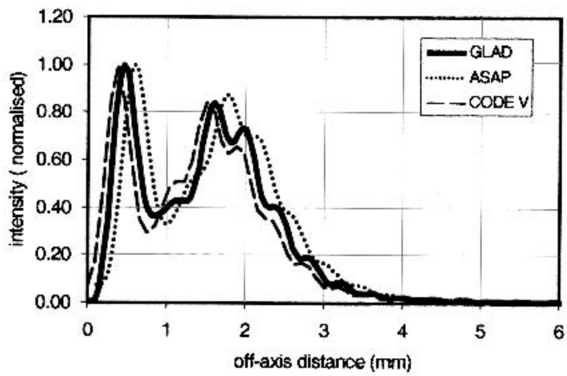

Figure 3 Intensity distribution in the near field (z_{out} = *25*mm) of an aperture of radius 10mm calculated using GLAD ASAP and CODE V. λ = 1mm.

However, when compared with GRASP (figure 4), some interesting differences become apparent. There is a significant discrepancy between predicted patterns, particularly in the case of the smallest aperture (3λ). In the GRASP data there is no on-axis minimum for the case of a = 3λ and the overall pattern is smoother and subject to less high-frequency ringing.

Clearly, the lack of agreement between GRASP and the other packages must be associated with the approximations made in the paraxial packages. In terms of paraxial Fresnel diffraction, the on-axis minimum

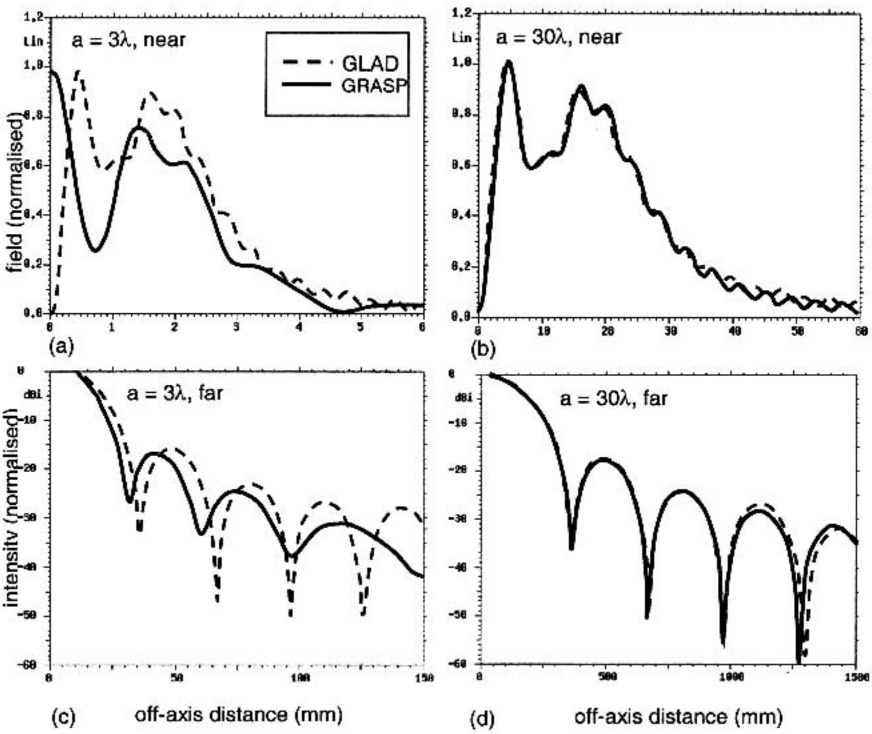

Figure 4 Beam amplitude in the near ($z_{out} = a^2/4\lambda$) and far ($z_{out} = 20a^2/\lambda$) field of an aperture of radius $a = 3\lambda$ and $a = 30\lambda$, calculated using GLAD and GRASP. GLAD is taken to be representative of the paraxial packages. λ = 1mm in all cases.

in these examples can be predicted by summing the the contribution to the overall fields of neighbouring Fresnel zones. The examples were chosen so that an even number of zones (four in our case) are seen to fill the aperture, and when viewed from the ouput plane their contributions will approximately cancel. However, the non-constant obliquity factor from zone to zone is not included in such calculations. As is clearly suggested by the GRASP plots such an omission has a significant effect on the beam patterns calculated for the smallest aperture, where the angle associated with the obliquity factor ($\theta_{obliq} = \tan^{-1}(a/z_{out})$) is largest, destroying the perfect cancellations of neighbouring Fresnel zones. At the centre of the focal plane the angle subtended by the edge of the 3λ aperture (θ_{obliq}) is 37°. For the largest (30λ) aperture, where the on-axis minimum is present in the GRASP data, the obliquity angle of the outermost zone is relatively small (7.6°). In that case the off-axis structure predicted by the paraxial packages is very good agreement with those predicted GRASP. The similarity of the GRASP near-field results when calculated with and without PTD show that it is the obliquity factor rather than edge effects that is the dominant source error in these cases. This indicates as a rule of thumb that propagation over short distances of $z < 2.5a$ can result in errors in the fine structure of the beam pattern for collimated beams.

In the far field, by contrast, the angles associated with the obliquity factor are always relatively small and one would expect much closer agreement in the form of the beam between GRASP and the paraxial packages. This is clearly seen in plots (c) and (d) of figure 4 which show the far field ($z_{out} = 20a^2/\lambda$) patterns of two of the apertures examined. Our data show that the paraxial packages are in broad agreement with each other, predicting the familiar Fraunhofer radiation pattern.

The discrepancy that appears in the small aperture far-field result (figure 4(c)) is not due to an obliquity term, but rather due to the fact that the beam spreads out into a large angle. The first point to note in the case of the far-field of a narrow aperture is that the high spatial frequencies are associated with non-paraxial far-field angles. This implies for the modal approach used in some packages, for example, that the highest order modes may not be propagating paraxially, resulting in the edge of the mode spreading out into too large an angle. However, in all cases examined here the discrepancies were not very significant for aperture diameters greater than 6λ. Thus, the main lobes are well matched in all examples. This indicates as a rule of thumb that the paraxial packages will be accurate for beam truncation at diameters greater than 6 λ.

There is also the issue that, in far field calculations involving the paraxial approximation, it is assumed that $\theta \approx \sin\theta \approx \tan\theta$. Far-field Fresnel diffraction calculations are more accurate if applied in k space. In other words, the off-axis radial distance r should be replaced with a term proportional to $ka\sin\theta$ for greater accuracy at high off-axis angles. Since r depends on $\tan\theta$, an increasing lateral discrepancy between GRASP and the other paraxial programs in terms of the positions of the sidelobe peaks and nulls will occur at off-axis distances corresponding to large angles as viewed from the beam waist (or phase centre).

Of course a ray tracing analysis of the examples given above is completely inadequate as the rays will continue to propagate parallel to each other after the aperture since the original source is at $z_{in} = -\infty$. However, as the source approaches the aperture ray tracing becomes a good approximation in the regime where $z_{in} < \pi a^2/\lambda$ (effectively, where the aperture is in the far field of the source). Ray tracing in general, therefore, is not adequtae for quasi-optical long wavelength systems.

A more typical example in efficient quasi-optical systems would have a quasi-Gaussian beam illuminated aperture stop equivalent to an apodised plane wave. In that case of course although the Poisson spot affect is much deminished, there is still the same level of discrepancy between the GRASP results and those of other packages for small beam diameters of the order of 6λ when one is close to aperture. In general it also indicates that paraxial packages begin to become inaccurate for beam sizes of less than 6λ in diameter. In terms of a 6λ beam waist, this corresponds to an F number of approximately 4 (typical of many horn antennas).

4.2. Off-Axis Mirrors

This second set of test cases involved modelling diffraction effects associated with re-imaging a coherent beam at off-axis paraboloidal or ellipsoidal mirrors of finite size (see figure 5). Off axis mirrors are often used at submillimetre wavelengths for controlling free-space beams and have the advantage over lenses of not giving rise to partial reflections and absorption losses.

Curved mirrors in the form of paraboloids, hyperboloids and ellispoids of revolution are an excellent approximation to the true surface that is required in order to correctly transform the spherical phase front of the incident beam into an undistorted spherical phase front for the reflected beam. In the short wavelength limit ellipsoids and hyperboloids are perfect phase-transforming reflectors of wavefronts with a finite radius of curvature. In the submillimetre regime, however, projection effects give rise to cross-polar scattering and spatial aberrations even at the wavelength for which the mirror was designed. This is because the image

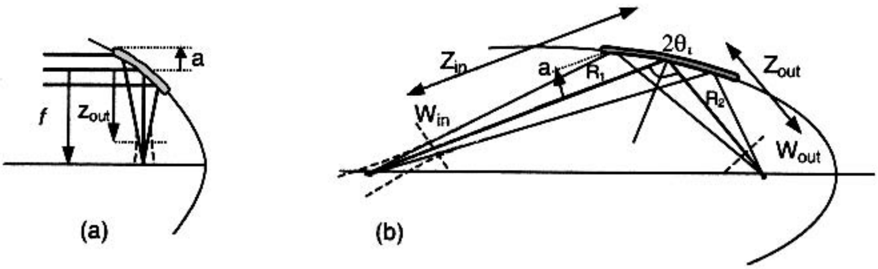

Figure 5 Off-axis mirror test cases. (a) Paraboloidal mirrors of focal length f and projected aperture a are used to reflect parallel beams forming a waist at z_{out}. (b) Ellipsoidal mirrors reflect wavefronts with a finite radius of curvature (R_1) producing an output beam waist at z_{out}.

is not a perfect point but rather a beam waist which must reproduce some of the asymmetries of the mirror geometry. Paraboloidal mirrors are similarly used as reflectors of parallel wavefronts.

We choose the test cases in this section to investigate the ability of the selected software packages to handle off-axis reflection and the resulting phase and amplitude distortions. The test cases were chosen to cover the range of typical parameters for the component in question, including some fairly extreme examples often found in modern quasi-optical systems. In all cases the mirror surface represents a perfect phase transformer (if one assumes no diffraction effects over the mirror volume defined by the tilt of the mirror). All our test cases involved a 90° angle of throw common in submillimetre-wave systems to prevent vignetting and for simplicity of design (especially in modular based systems). The sources investigated were Gaussian beams, with plane wave illumination chosen for one of the parabolic examples to mimic the operation of a telescope. Although idealised, these sources allow us to probe the fundamental limitations of the packages to deal with aberrations and truncation. An extension to the standard GRASP package can be used to model the more realistic sidelobe structure of, for example, a scalar horn.

Figure 6 shows poor agreement in general between the packages, especially in the plane of asymmetry. PROFILE, using a GBM analysis, predicts the same main-beam asymmetry as GRASP down to -25dB.

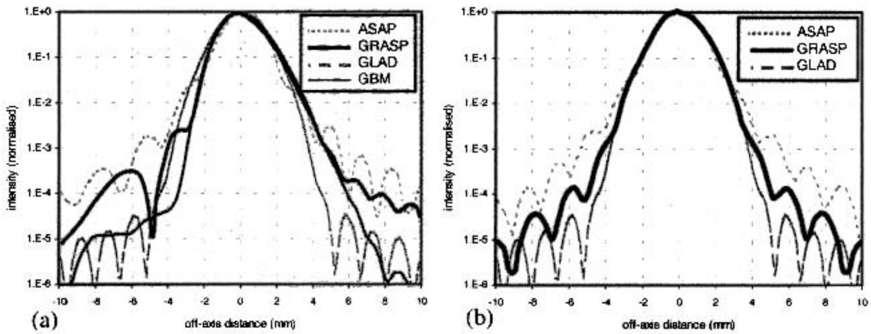

Figure 6 Intensity pattern at the output beam waist ($z_{in} = z_{out} = f$=12.57mm) for an ellipsoidal mirror of projected aperture a = 1.5×W. (a) shows a cut in the plane of asymmetry, (b) in the plane of symmetry. λ = 1mm and W_{in} = 2mm in both cases. The beams were calculated using ASAP, GLAD and GRASP.

Both ASAP and GLAD fail to predict the correct sidelobe structure and level. GLAD underestimates the sidelobe level by up to 10dB and predicts an almost symmetric beam. The sidelobe level and asymmetry calculated by ASAP are closer to those of GRASP, but the main beams differ by several dBs. There is better agreement in the other plane where the output beam is expected to be symmetric. GLAD and GRASP match down to -25dB, with GLAD's sidelobe level again lower, but in this case by about 5dB. ASAP, on the other hand overestimates the sidelobes by up to 10dB. The main beams show good agreement out to ~15°.

In order to understand the rather poor performance of the optical design packages we need to consider the approximations inherent in the packages. In the Gabor approach the electromagnetic field is decomposed into individual Gaussian beamlets, which can then be propagated through optical components using ray tracing methods and in that way take aberrations into account. While ASAP is based on such a Gaussian beam decomposition, however, the full Gabor representation is not implemented. One elementary Gaussian beam, rather than a fan of beams, is used to represent the field at each point on a spatial grid. This causes problems when attempting to model structure in beams on the scale of a few wavelengths. In any case the included beamlets propagate paraxially, although they follow rays travelling at non-paraxial angles to each other.

GLAD makes several simplifications which we might expect to affect the results of these test cases. The first is that it is restricted to apertures placed normal (or with small tilts) to the beam. Mirrors are assumed infinite and their edges are defined by placing a suitable aperture in front. In these test cases we would need a tilted aperture to correctly define the mirror edges but these are, as yet, not allowed in GLAD. The level of trucation by the mirror is therefore an approximation, and if the defining aperture is placed in front of the mirror the sidelobe levels will be underestimated. Placing an aperture after the mirror was often found to improve the predicted sidelobe level, but at the expense of the main-beam accuracy.

The second source of possible errors is the level of amplitude distortion caused by the mirror. If the mirror is designed correctly, it can act as an almost perfect phase transformer producing very little phase aberration, but projection effects will always introduce amplitude distortion. GLAD calculates aberrations by ray-tracing through the volume of conic sections before switching back to the usual diffraction propagation. When doing this it considers the optical path length difference introduced, and uses these to calculate the phase aberration imposed on the beam. Diffraction through the volume of the mirror is calculated for the centre of the beam. Other parts of the beam diffract either too much or two little, although introducing some phase error. More importantly, however, is that amplitude distortions, important at far-IR wavelengths, are not included in this analysis. After reflection by either a paraboloidal or ellipsoidal mirror, the fraction of power η in a reflected Gaussian beam (in the plane of the mirror) that is scattered out of the fundamental Gaussian beam mode is given by $\eta = w_m^2 \tan\theta_i^2 / 8f^2$, where f is the nominal focal length, w_m the beam waist at the mirror and θ_i is the angle of incidence [9]. Even though the power in the higher order modes may be small, there can be a significant effect on the sidelobe structure. We looked at another example (f = 125mm) where we would expect the amplitude aberration to be lower and the beam pattern at the output waist is shown in figure 8. In this case both the phase and amplitude aberrations are small and the paraxial packages agree with GRASP down to below -30dB.

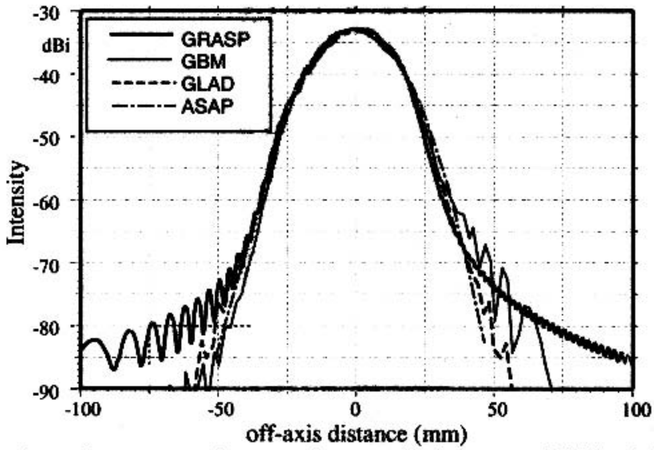

Figure 7 Intensity pattern at the output beam waist ($z_{in} = z_{out} = f$=125mm) for an ellipsoidal mirror of projected aperture a = 1.5×W. The cut was taken in the asymmetric plane. λ = 1mm and W_{in} = 2mm. The beams were calculated using ASAP, GLAD, PROFILE (GBM) and GRASP.

There is clear evidence that GLAD does therefore not include amplitude projection effects and will only show aberrational effects in mirrors whose surface is not a perfect phase transformer. This neglect of amplitude aberrations is not a consequence of the paraxial approximation however, and we have successfully modelled such aberrations using the GBM approach (figure 6(a)).

5. Summary

For all of the packages examined, with the exception of GRASP, one has to be aware that obliquity factors are not taken into account which may give rise to errors if fields are simulated for propagation distance that are too short. A good rule of thumb seems to be that the opening angle of the aperture as viewed from the on-axis point of the output plane should be less than about 10°. Far from apertures of modest radii (in terms of wavelength $a > 3\lambda$), and where obliquity effects are negligible, there is good agreement in terms of main beam widths and sidelobe levels out to relatively large off-axis angles (25°). For off-axis angle greater than about 25° a fundamental approximation used in paraxial packages, that for the off axis angle $\theta \approx \sin\theta \approx \tan\theta$, begins to break down with the consequence that the sidelobe structure is compressed and the positions of peaks and nulls becomes unreliable. The side-lobe structure roughly shift by an amount $(\tan\theta/\sin\theta)$.

The definition of off-axis mirror edges are a particular problem for some packages because it does not, as yet, allow tilted apertures. Phase aberrations introduced on reflection from a conic mirror are calculated correctly but amplitude aberrations, particularly important for large angles of throw and fast beams, appear to be ignored. The paraxial packages in general gave good agreement, down to -25dB in the plane of symmetry. Using ASAP it is difficult to model beam structure of less than several wavelengths. The particular Gaussian decomposition used is not suited to beams with sharp cut-offs, at the edge of a horn, for example.

In conclusion, it is clear that none of the commercially available software investigated is ideally suited to model submillimetre optical systems. Under certain conditions discussed they do give good results but it is important to bear their limitations in mind particularly when interested in sidelobe structure. All our results have been compared with those of GRASP, which we take to be correct, and our test cases have been restricted to those that can be easily modelled by it. Future work will look at an experimental verification of some GRASP models as well as development of PROFILE software, specifically aimed at the submillimetre regime.

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