



## Unigit Version V1.02.04

Version V1.02.04 is a consequent development continuation based on the former version V1.02.02. The main focus was on 2D gratings with regard to both speed and ease of use. There are the following essential new achievements in this new version:

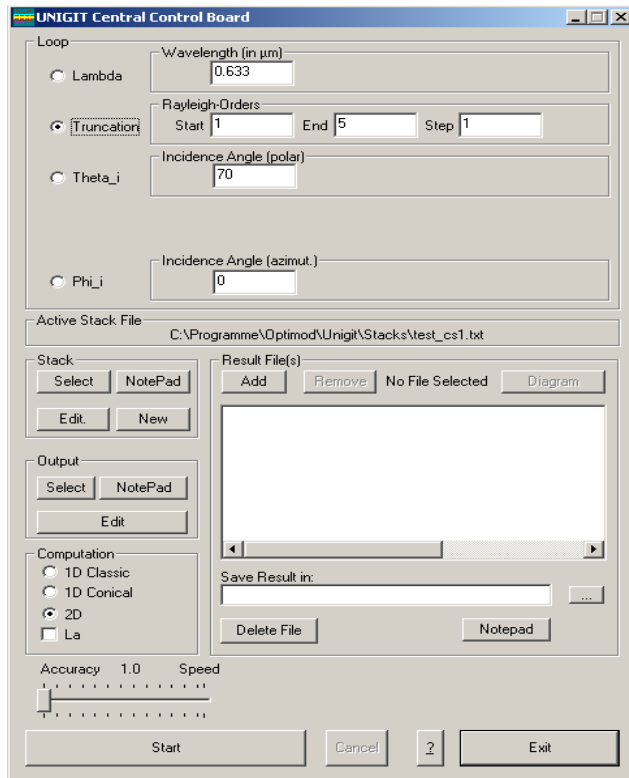
- Speed Accelerator for 2D-gratings (crossed gratings),
- New Layer Types for 2D-layers
  - Nested generalized ellipses
  - Generalized 3D cone
- Hot Keys for the most essential control buttons
- Log File for Unigit Runs

A detailed description of these new features is given in the following.

### 1. Speed Accelerator

Diffraction computations of 2D gratings are usually very time consuming. The main reason for this is the inherent Eigen solver which is required to solve the Differential Equation System (DES) resulting from Maxwell's Equations. While for 1D-gratings  $M = 2m+1$  orders are required (when truncated symmetrically with  $m$  being the order to be input in Unigit), 2D gratings have orders in  $x$ - and  $y$ -direction. Thus, the total number of orders is  $O = M*N$  with  $N = 2n+1$  ( $n$  = orders in  $y$ -direction). The costs for the Eigen solve scale as  $C = O^3$ . To give an example, assume you need  $m = 5$  orders in  $x$ - and  $y$ - direction. This will result in  $O = 11$  for 1D and  $O = 121$  for 2D. Then, the costs are  $C_{1D} = 11^3 = 1331$  and  $C_{2D} = 121^3 = 1771561$  meaning that the 2D computation for the same order is about  $((11*11)/11)^3 = 11^3 = 1331$  slower.

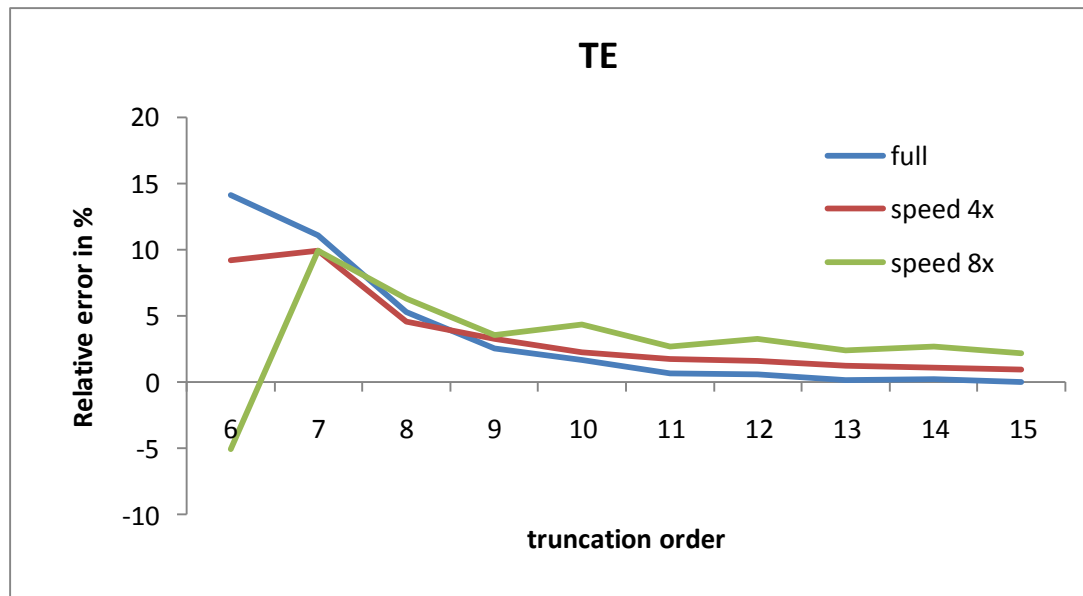
However, the energy distribution in the spatial frequency domain of a 2D grating is not uniform. Therefore, advantage can be taken by a smart order management to speed up the computation. The algorithm does not depend on any symmetries and can be applied to all types of grating and incidence settings (in terms of incidence and orthogonality). It was implemented in Unigit V1.02.04 in a way not to bother the user with the details. All, she or he has to do is to decide between speed and accuracy. To this end, the slider on the bottom of the central control board (see figure 1) has to be moved to the right. When doing this, the predicted speed gain factor is updated (see figure 2). The default is the standard case with no speed gain (factor = 1).



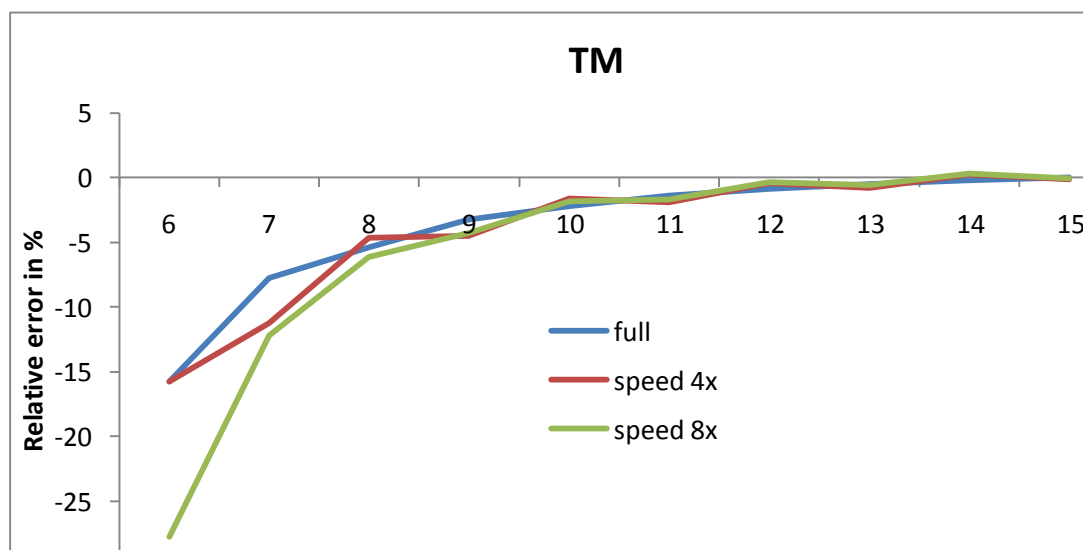
**Fig. 1:** Central Control Board with speed slider for 2D acceleration

However, this does not at all mean that accuracy is seriously jeopardized when handled with care. In order to make sure that the speed level does not risk the accuracy, the best recommendation is to run a convergence test with a certain speed factor and then relate this computation to the value which is obtained by speed factor = 1 and maximum order.

In the following, two examples are given for the use of the accelerator. The first example is a quarter micron, quadratic Silicon post etched from Si substrate with a grating period of half a micron. Figures 2a and 2b exhibit the relative errors for speed factors of 1x, 4x and 8x versus  $\pm$ truncation order for the zeroth reflection order in TE- and TM-polarization. The reference value is the  $\pm 15$  orders value for no acceleration (speed factor = 1x).



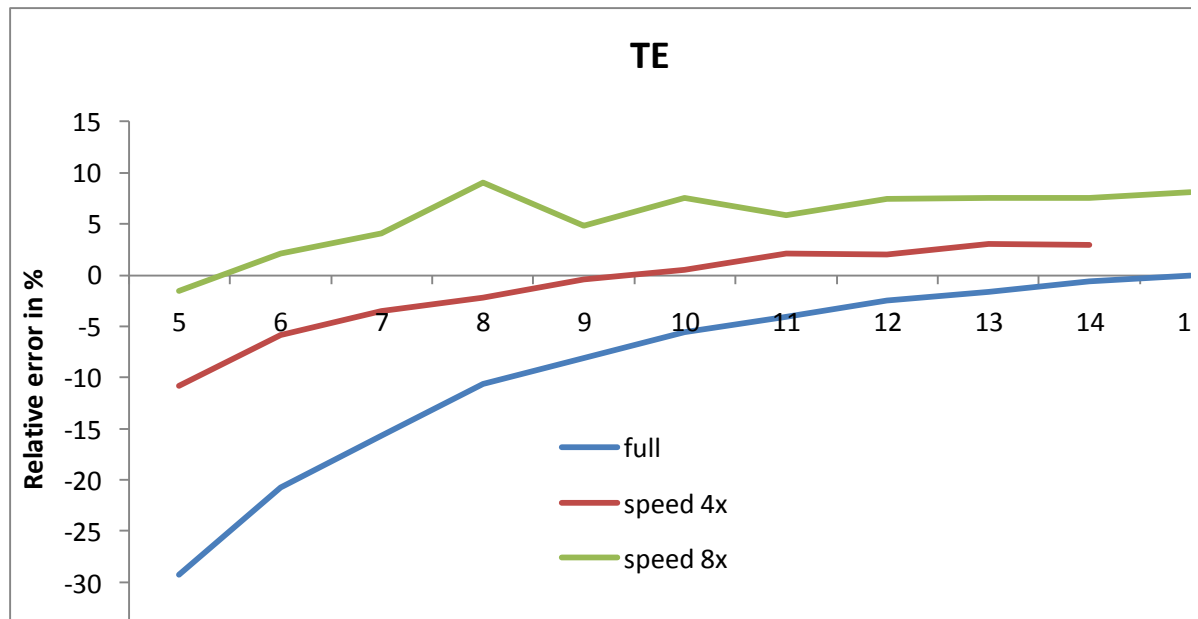
**Fig. 2a:** Relative error of the zeroth reflection order in TE polarisation vs. truncation order for speed factors of 1x (full order), 4x and 8x.



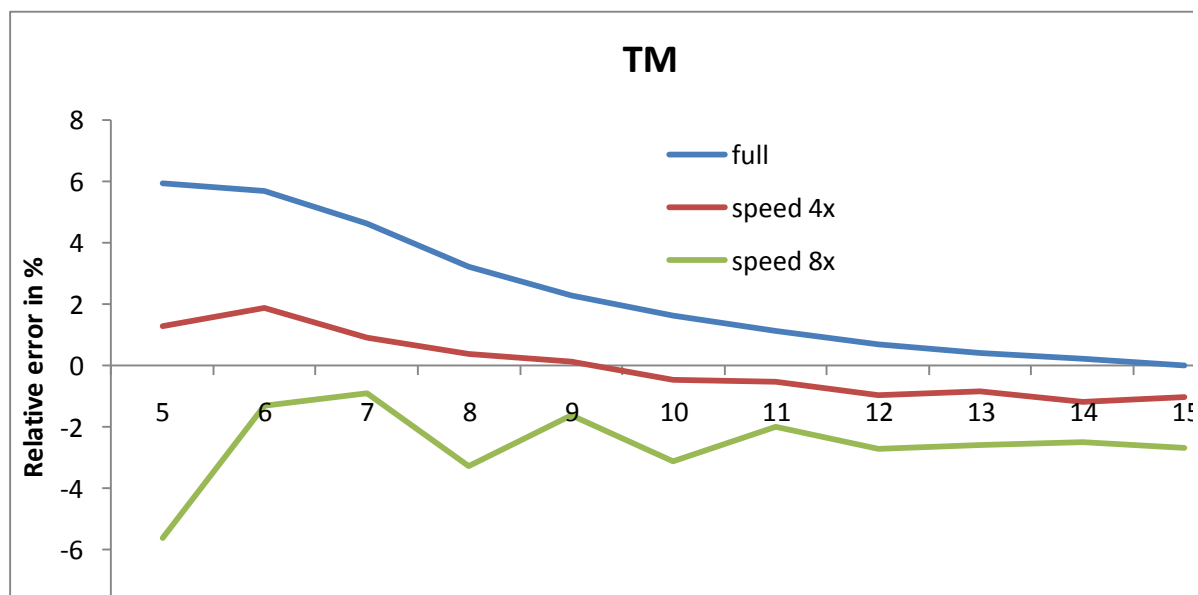
**Fig. 2b:** Relative error of the zeroth reflection order in TM polarisation vs. truncation order for speed factors of 1x (full order), 4x and 8x.

In conclusion of example 1, a deviation from full order of about 1% can be obtained for almost all orders with the 4x speed option in TE-polarization. Moreover, the error is almost negligible for both the 4x as well as 8x speed in the TM-case.

The second example relates to round Si posts on Si substrate being 500 nm in height. The results are plotted in figures 3a and 3b. Obviously, one has to take a bigger deviation into account when using the acceleration.



**Fig. 3a:** Relative error of the zeroth reflection order in TE polarisation vs. truncation order for speed factors of 1x (full order), 4x and 8x for circular Si posts.



**Fig. 3b:** Relative error of the zeroth reflection order in TM polarisation vs. truncation order for speed factors of 1x (full order), 4x and 8x for circular Si posts.

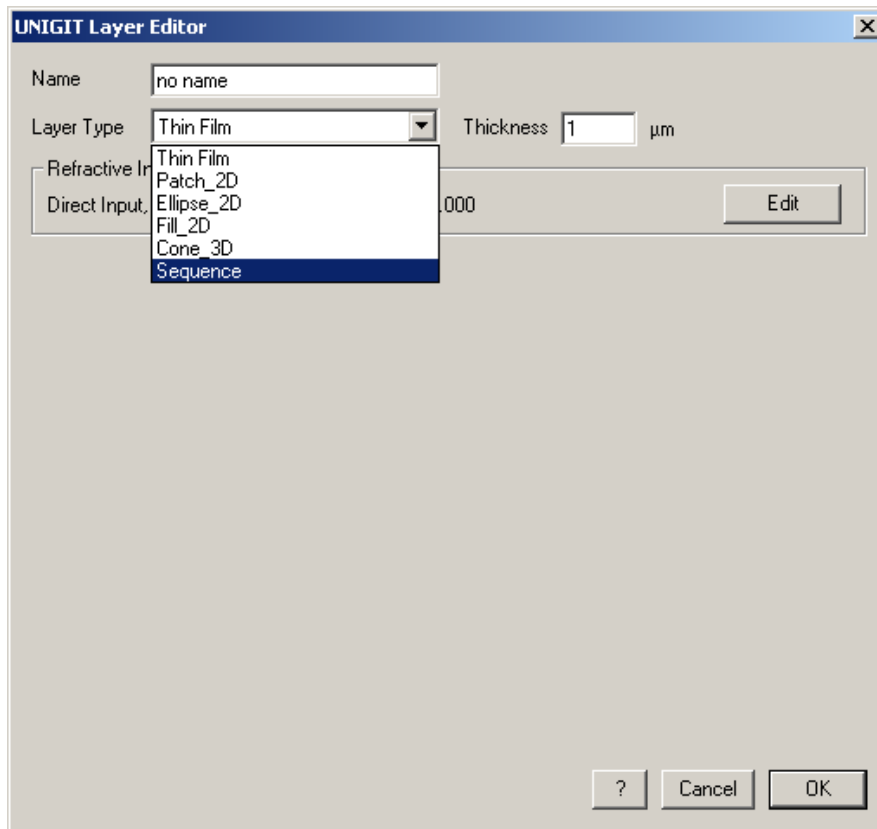
## 2. New 2D- and 3D- Layer Types

In order to facilitate the use of Unigit, new types of layers have been implemented. Beside the “Fill\_2D”, which was introduced with version 1.02.02 and enables the free user defined description of a 2D slice, two types of new layers for crossed gratings have been included in version 1.02.04 (as shown in figure 4):



- the generalized double ellipse (which is contained in the former “Ellipse\_2D”) and
- the Cone\_3D which is a true 3D-building block.

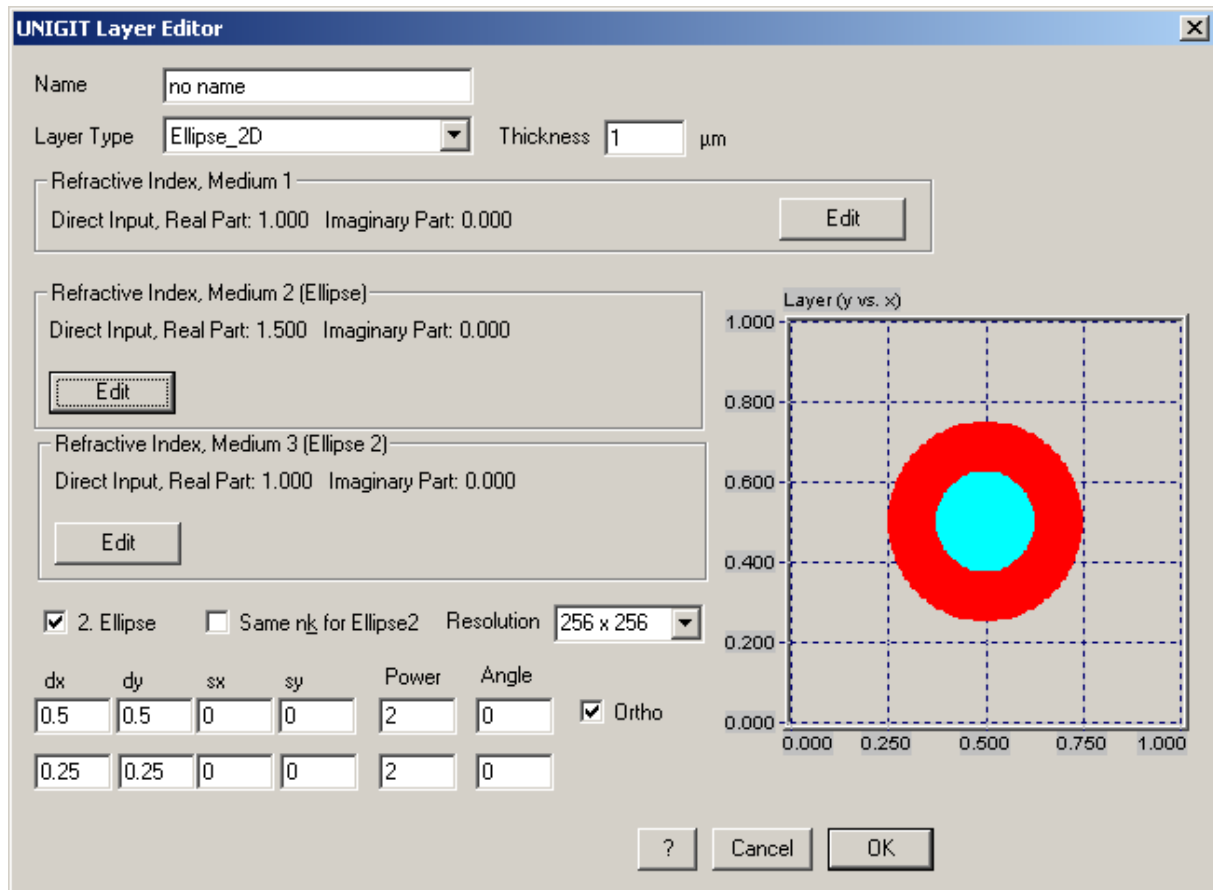
The functionality of these new “layer” types is detailed in the following subsections.



**Fig. 4:** Layer editor showing the extended choice of layers in version 1.02.04

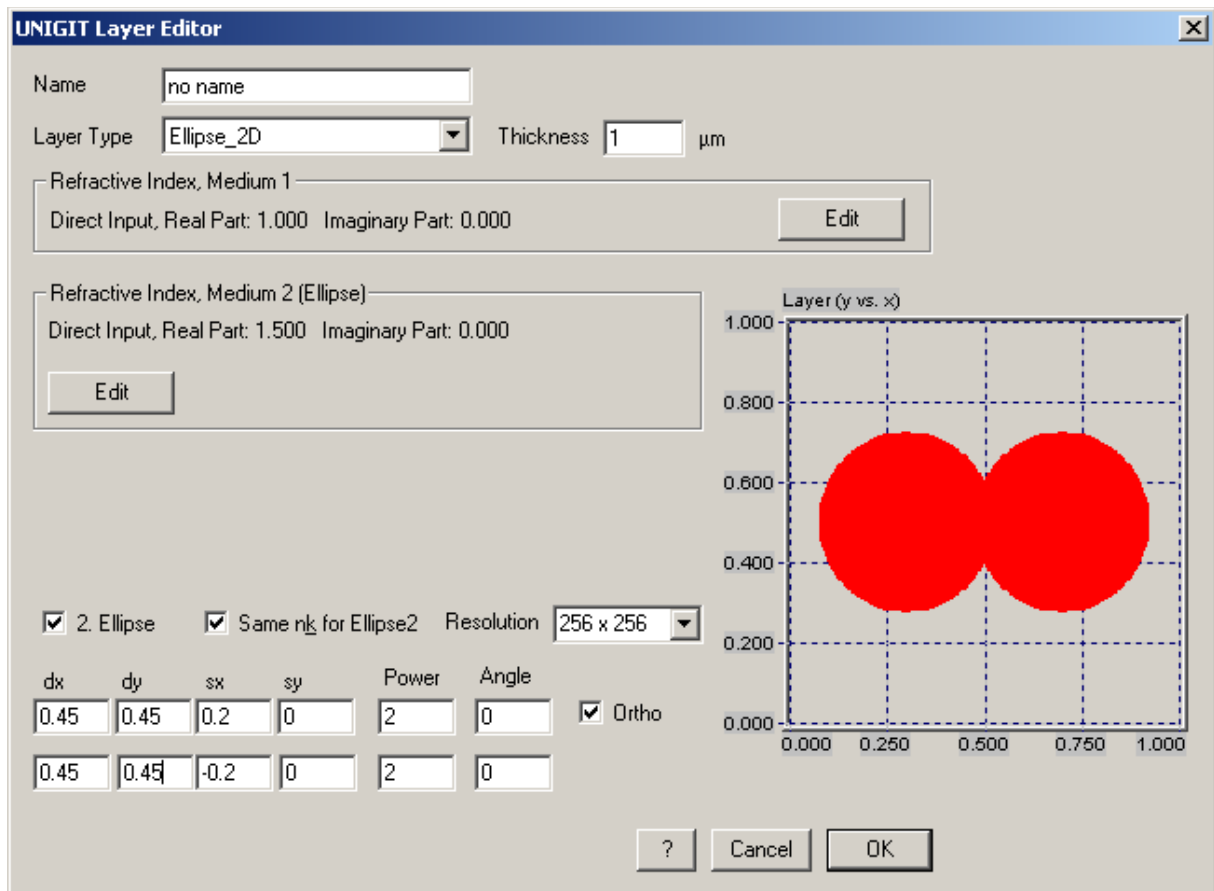
## 2.1. Generalized Double Ellipse

In order to activate the double ellipse layer, one has to select the Ellipse\_2D first. Then, the box “2. Ellipse” has to be checked as indicated in figure 5. Of course, the single ellipse is available when the box remains unchecked.



**Fig. 5:** Activation of the Double Ellipse

As you can see in figure 5, a block of edit fields becomes visible when deciding for the double ellipse. They have just the same functionality as those for the first ellipse arranged above, i.e. diameter in x and y (dx, dy), decentering in x and (sx, sy), ellipse power and rotation angle. The second ellipse allows all possibilities of two nested ellipses. It is important to say that the second ellipse always overwrites the first ellipse. There are several ways to make use of the second ellipse option. So, you can align both ellipses in order to describe an ellipse with a rim formed by different material. In this case, you have to make sure to select the material of your choice by means of the EDIT button in the panel “Refractive Index, Medium 3 (Ellipse 2)”. On the other hand, you can check the box “Same nk for Ellipse 2” (see figure 6) when you want to assign the same refraction index to ellipse 1 and 2. This makes sense when you want to input for instance a twin hole or post as shown in figure 6. By the way, the panel for the nk-selection of ellipse 3 disappears in this case.

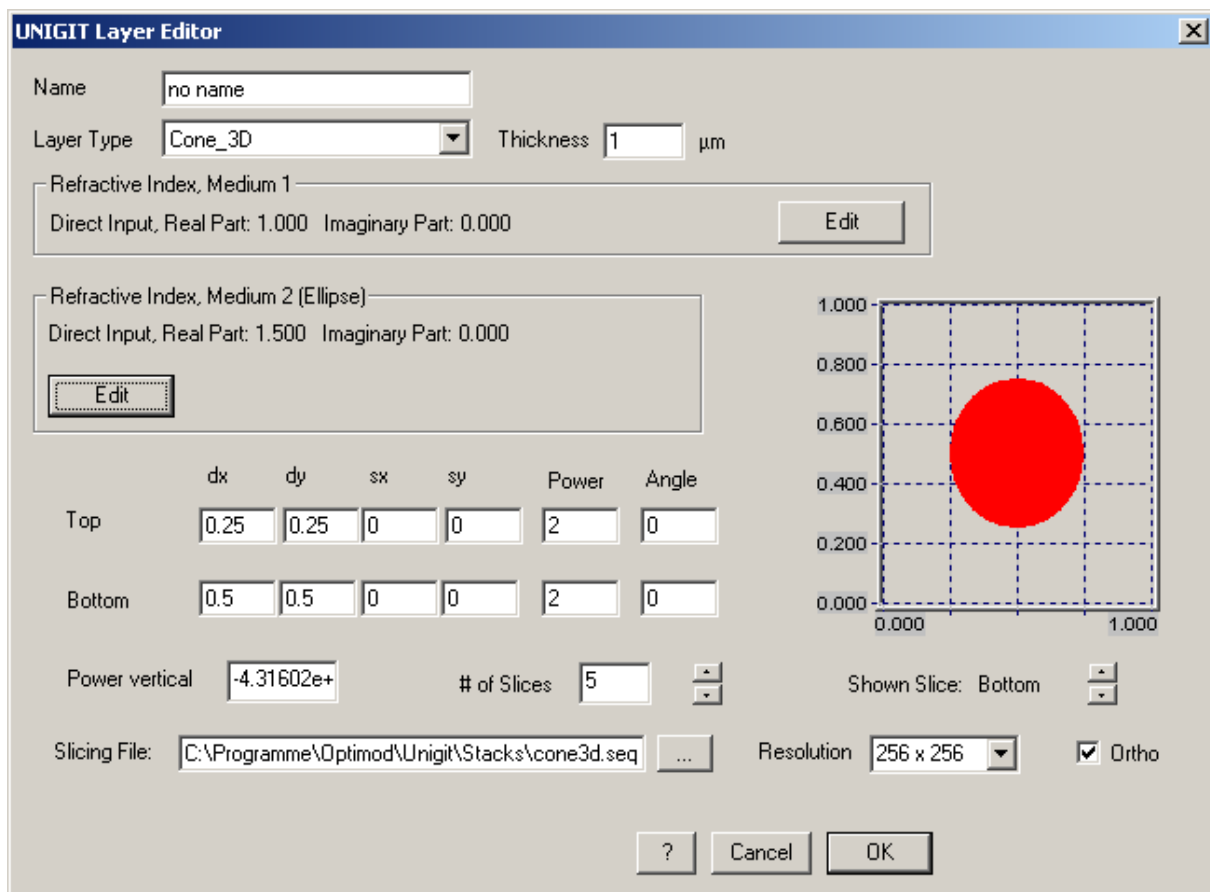


**Fig. 6:** Selecting the same index for both ellipses

Another interesting application of the double ellipse which is based on the enforced overwriting of the first by the second ellipse is to cut out shapes of the first ellipse. This can be done just by selecting the same refraction index for the second ellipse as for the surrounding medium 1 and overlap the parts to be cut out by selecting the appropriate shape and position of ellipse 2.

## 2.2. Generalized 3D Cone

The assembling of complex grating shapes is quite cumbersome when doing it only with slices. To this end, the stack editor for 1D gratings include the layer types “Slicing polygon” and “Slicing Fourier”. By means of this types, the user can describe the profile itself and does not need to bother with the slicing that is been done automatically in the background. In version 1.02.04, this successful concept is expanded to 2D gratings by means of the generalized 3D cone. Here, the user has to define the lateral cross section shape (i.e. the 2D slice) at the top and at the bottom of the 3D body to be input. To this end, the well known edit fields for the generalized ellipse are available (highlighted in figure 7). The outer shape of the cone is defined by the vertical power (input field below the top & bottom cross section input). And eventually, the number of slices can be entered in the “# of slices” input field (default is 5). Then, the 3D shape is computed by means of an interpolation between top and bottom cross section according to the position of the slice and depending on the vertical power. A vertical power (VP) = 1 will result in a regular straight cone (linear interpolation). A  $VP > 1$  yields a barrel-shaped body whereas  $VP < 1$  describes an hyperboloid.



**Fig. 7:** Layer Editor for the generalized 3D Cone (cross section of the bottom of the 3D body is shown)





The shape can be checked by sweeping through the slices by means of the up-& down-buttons below the graph (as indicated in figure 8). Then, the cross section of the active slice (numbered from top to bottom) is shown in the graphical window. When exiting the layer editor, the slicing information is written to a slicing file the same way as it is known from its 1D equivalent. To this end, the information where to locate this file has to be input in the corresponding field. A file requester button “...” is provided for your convenience.

**Fig. 8:** Layer Editor for the generalized 3D Cone – when sweeping through the 3D body (slice 5 is shown here)

### 3. Hot Keys

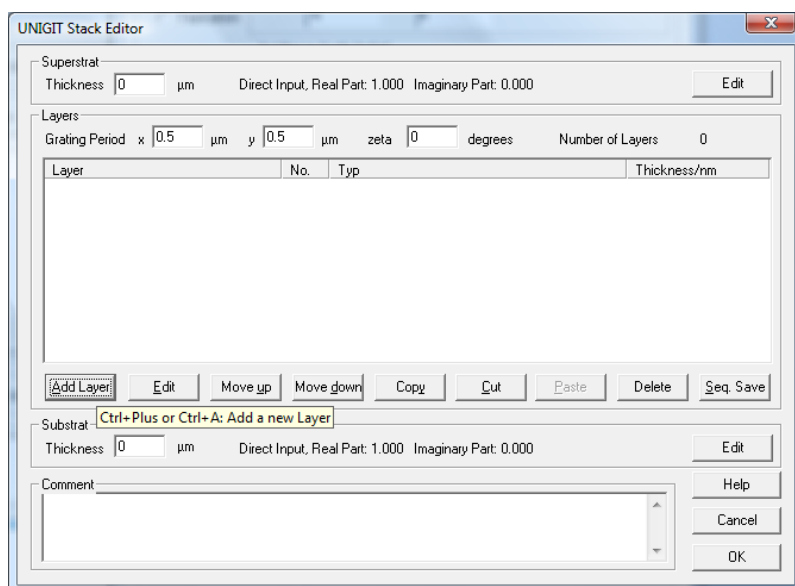
Hot keys are provided in the central control board, in the stack editor and in the layer editor.

#### 3.1. Hot Keys in the Stack Editor

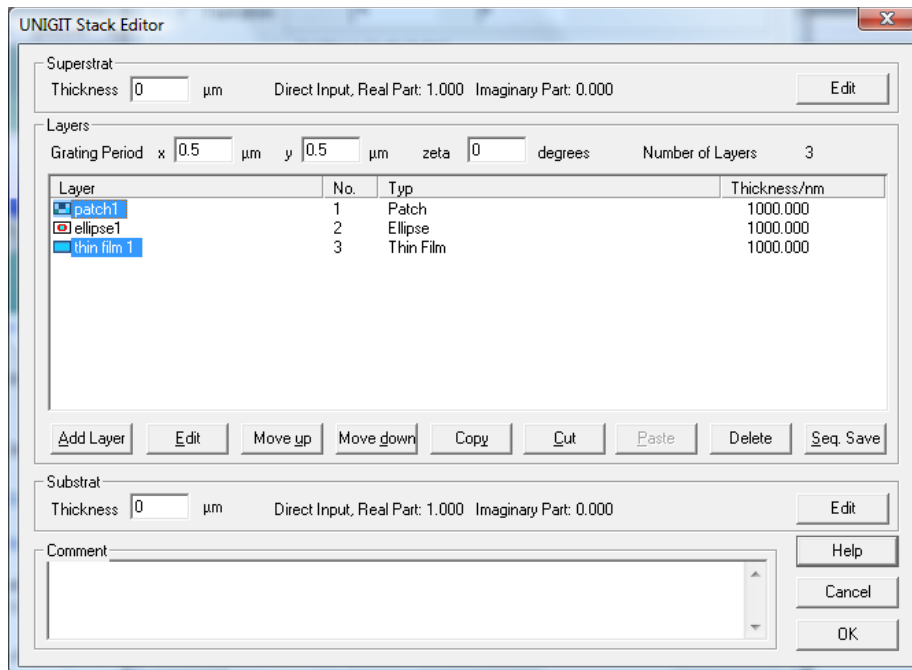
The hot keys which are available in the stack editor are summarized in the table below (table 1). However, the meaning can also be seen while moving the mouse over the corresponding buttons as shown in figure 9. Remember, some buttons and the associated hot keys and (e.g. copy) relate to the group of selected layers rather than only one layer (as shown in figure 10). As known from former versions, the selection can be done with the “Shift” or “Control” (CTR) keys while concurrently left mouse clicking the icon of the selected layer.

CTR C	Copy Layer or Group
CTR V	Paste
CTR D	Delete
CTR X	Cut out
CTR S	Save as Sequence
CTR E	Edit Layer
CTR A or CTR +	Add a Layer
CTR ↑	Move up
CTR ↓	Move down

**Table 1:** Hot keys in the layer editor



**Fig. 9:** Tool tip information for hot keys in the layer editor



**Fig. 10:** The operations triggered by the button or the corresponding hot key in the stack editor will impact all marked layers