



Crossed Grating

**Diffraction gratings design and analysis
by Modal and Chandezon methods**

2015

User Manual

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Introduction

The Crossed Grating package was designed by Nikolay Lyndin, PhD, the senior physicist of General Physics Institute of Russian Academy of Science, lyndin@ran.gpi.ru

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The Crossed Grating package is designed to run on any Windows® OS. The codes interface is written in Delphi. The most critical matrix routines (LAPACK) are taken from Intel® MKL 11.1 version. The routines in MKL are hand optimized by exploiting today's multicore and many core processors, wider vector units and other processor architectural features.

The two methods are implemented in this package.

- The C-method¹⁻⁵ based code is intended to calculate gratings with a smooth profile and includes two *Classic* and *Extended* options. The *Classic* option implies identical corrugation at all interfaces while the *Extended* method implies independent corrugation of all interfaces under the restriction that the period is the same and interfaces do not intersect.
- In the Modal code the Fourier Modes Method⁶⁻¹² (FMM) also known as RCWA is implemented. This code is intended to calculate gratings with a binary profile and the "Normal Vector Field" idea⁹⁻¹¹ with automatic generation of NV-Field is implemented. This provides the fastest known convergence for dielectric gratings of a binary profile.

The codes calculate the interaction of a plane electromagnetic wave with the multilayer corrugated structure providing the efficiencies (complex amplitude and power) of all reflected and transmitted diffraction waves and also calculate the complex field distribution and power flow in the multilayer structure and ambient media. Codes are based on a complex permittivity of layers for the electromagnetic wave. Incident wave has a unity amplitude of vector \mathbf{E} and zero phase at position $x = 0$, $y = 0$ and $z = 0$. Incident wave power flow always equals to unity.

Both codes have almost the same interface adapted for particular code possibilities. The main form is a container for independent project editor windows. The project editor window may display a text with a structure parameters or a text table with results of calculation. The graphic tools take data from the results text table. This seems to be reasonable because the user has an opportunity to edit the data before displaying and to display in a graphic form a saved data files. The user can change the results precision and diffraction orders of interest to display in the text table without repeating calculation because a complete result data is kept in a PC memory. The user is provided with the possibility of insertion any comment before the structure parameters text. The comment should not contain the structure first line text specification. The structure parameters can be edited as from the text window or from the *Settings Dialog* window. Lines of more than 2500 characters length are displayed by editor in truncated form and it is safely to edit them only as a whole (delete, copy, paste). The software will use full length lines. Dialog windows are also used to access any other tool options.

The codes also include:

1. An optimization possibility in multidimensional space¹³ for sophisticated criterion function.
2. General and 3D graphics for results presentation of one or two parameters scanning.
3. A refractive index materials catalog.
4. Automatic generation of Normal vector field⁹⁻¹¹ in Modal code.

C-method restrictions

Chandezon method domain of applicability is mainly defined by the ratio of grating depth to its period.

C method for crossed grating gives reliable results when the full grating depth is less than maximum of X or Y periods. If the grating depth is close to the critical value there are an optimal number of field decomposition orders providing the best result. In practice it was found that the optimal number of decomposition orders for calculating deep gratings does not exceed 30 for both X and Y axes. Most likely this restriction is similar to the Rayleigh method convergence problem¹, and finally because of insufficient calculation accuracy of high order harmonics.

The implemented method has a peculiarity under incident angles close to the normal (see Ref. 5). Around the incident angles less than 0.01 degrees a special processing is implemented. Nevertheless this domain of incident angles needs a special care. The increasing number of decomposition orders usually improves the convergence in this situation.

Calculation of grating structures with long periods needs large number of decomposition orders and has the restriction mentioned above.

The balance (sum of all diffraction orders power) is a good criterion of results reliability. In case of lossless structures this value should be close to unity and less than unity for dissipative structures.

Fourier modal method restrictions

The Fourier Modes Method, also known as RCWA, has not any restriction on grating depth. The method problem is an electromagnetic field discontinuity at interfaces of different permittivity. Theoretically for infinite number of modes the fields at interfaces are matched correctly. For dielectric structures always there is a smooth convergence with the truncated number of modes increasing but the convergence rate depends on permittivity discontinuity contrast - the less contrast the larger convergence rate. The implementation of NV-field approach increases the convergence rate dramatically.

The largest convergence problems arise for highly conductive metal gratings. In this case the permittivity changes sign at discontinuity interfaces and as a result there are two consequences. First, so called plasmon modes may exist. As usual, these modes field has very sharp coordinate dependence leading to the convergence rate decreasing. And second, the modes propagation constants spectrum became irregular – the effect analogous to the spurious modes generation by truncation the number of modes in the case of one dimensional gratings¹². In some cases the suggested in this paper modes filtering (also implemented in present code) may help.

Despite the problems described above this method gives practically acceptable results (accuracy is not less than fraction of percent) for moderate number of modes taken for calculation.

In the designing of the codes the following publications were used:

1. J. Chandezon, D. Maystre, G. Raoult, “A new theoretical method for diffraction gratings and its numerical application”, J. Optics (Paris), Vol. **11**, No. 4, p.235 (1980)
2. J. Chandezon, M. T. Dupuis, and G. Cornet, “Multicoated gratings: a differential formalism applicable in the entire optical region”, J. Opt. Soc. Am. **72**, 839-846 (1982)

3. Lifeng Li, "Multilayer-coated diffraction gratings: differential method of Chandezon et al. revisited", J. Opt. Soc. Am. **11**, 2816-2828 (1994)
4. Lifeng Li, G. Granet, J. P. Plumey, and J. Chandezon, "Some topics in extending the C method to multilayer gratings of different profiles", Pure Appl. Opt. **5**, 141-156 (1996)
5. G. Granet, "Analysis of diffraction by surface-relief crossed gratings with use of the Chandezon method: application to multilayer crossed gratings", J. Opt. Soc. Am. A **15**, 1121-1131 (1998).
6. Lifeng Li, "A modal analysis of lamella diffraction gratings in conical mountings", Journal of Modern Optics, **40**, 553-573 (1993);
7. P. Lalanne and G. M. Morris, "Highly improved convergence of the coupled-wave method for TM polarization", J. Opt. Soc. Am. A **13**, No. 4, p. 779 (1996).
8. L. Li, "Use of Fourier series in the analysis of discontinuous periodic structures", J. Opt. Soc. Am. A **13**, No. 9, p. 1870 (1996).
9. Evgeni Popov, Michel Nevie`re, "Grating theory: new equations in Fourier space leading to fast converging results for TM polarization", J. Opt. Soc. Am. A **17**, No. 10, p. 1773 (2000).
10. Evgeni Popov, Michel Nevie`re, "Maxwell equations in Fourier space: fast-converging formulation for diffraction by arbitrary shaped, periodic, anisotropic media", J. Opt. Soc. Am. A **18**, No. 11, p. 2886 (2001).
11. Thomas Schuster, Johannes Ruoff, Norbert Kerwien, Stephan Rafler, and Wolfgang Osten¹, "Normal vector method for convergence improvement using the RCWA for crossed gratings", J. Opt. Soc. Am. A **24**, No. 9, p. 2880 (2007).
12. N. Lyndin, O. Parriaux and A.V. Tishchenko, "Modal analysis and suppression of the FMM instabilities in highly conductive gratings", J. Opt. Soc. Am. A, Vol. **24**, No. 12, p. 3781 (2007).
13. R. Fletcher, M.J.D. Powell, "A rapidly convergent descent method for minimization", The Computer Journal, 6 163-168 (1963).

Project window and menus

The user is provided with several ways to open a project. Click the frame file menu **File** to choose one of three options:

- **Samples** provides the possibility to start a new project with several options:
C-method code – the example of a grating profile as a sum of two sinusoidal functions versus x and y ; the example of a grating profile as a sum of two triangular functions versus x and y (functions points presentation followed by its sinus decomposition); the example of a smooth hills (rectangular geometry); the example of a two smooth hills (hexagonal geometry).;
Modal method code - the example of chessboard grating layer; the example of a single cylinder pillar grating layer and the example of two cylinder pillars grating layer (hexagonal geometry).
- **Open** is a standard menu to open previously saved projects.
- **Reopen** contains the list of recently saved files.

The project window has an editor type and starts with the text representation of the structure (project) parameters. At the bottom of this window there are some controls with obvious functions. Four functions **Graph**, **Run**, **Settings** and **Optimize** are repeated in the main frame menu. The button **Result/Structure** switches the edit window between text representation of the structure parameters or of the results of calculations. If the *Structure* editor is activated the user can save the structure parameters and settings in a file with the extension CHA (*C-method code*) or MDL (*Modal method code*). If the *Result* editor is activated the user can save the calculated result in a file with the extension DAT. The Editor provides the possibility to edit results table and structure parameters but it is recommended to use the **Settings** dialog window for the last purpose.

After opening the project window the additional items appear in the main menu:

- **Edit** is a standard item and its items are not fully functional while the editor is read only. The user can switch this attribute by **Read only** control.
- **Font...** is a standard menu item for editing.
- **Settings** opens dialog window for editing the structure parameters, settings and calculation options.
- **Run** starts the process (calculation).
- **Optimize** opens dialog window for defining the structure optimization parameters, user defined criterion function and for optimization process control.
- **Graph** represents the results of the calculations in a graphical form. If the results are not applicable to this option, or there are no results at all, the **Graph** is inactive.
- **Slider** provides the possibility for an express analysis of the result graph behavior versus the input polarization state.
- **Duplicate** duplicates the active project into a new project window. This procedure is safe at any stage.
- **Service Window** permanently contains the **Structure Geometry** submenu for viewing the coordinate system, grating orientation and incident and diffracted plane wave definitions.

Depending on the project state, additional submenu references on the grating profile or activated graphs can appear.

- **Window** is a standard item.
- **Help** is a standard item. The *Version* in *Help* -> *About* has YYYY-MM-DD format of the code compilation date.

Settings Dialog

This dialog contains several pages:

- **Genera**
- **Layers**
- ^C **Grating** (from here the prefix ^C means that corresponding item is present only for C-method code)
- **Scanning**
- **Fields** and power flows.
- **Options**
- ^M **NV Field** visualization (from here the prefix ^M means that corresponding item is present only for modal method code)

Under the pagers there are three buttons:

- **Ok** applies all changes in this dialog and hides it.
- **Run** applies all changes in this dialog, hides it and starts the calculations.
If changes concern only the representation of the results data (number of digits, format of output: power or amplitude, number of displayed diffraction orders and also selected field or power flow component), the data already saved in memory will be used to recalculate the new representation. The real calculation of the structure will start only if the essential structure or scanning parameters are changed.
- **Cancel** abolishes all changes in this dialog and closes it.

General

- ^C **Maximum Order of Field Decomposition** defines $2*Order+1$ of Fourier components along *X* and *Y* directions (the total number of components is the product of these values). The order values should be adequate to the number of appropriate diffraction orders in every layer. There is a possibility of automatic fixing of this problem (see page **Options**).
- ^M **Number of Orders** allow to define the number of orders along *X* and *Y* directions (the total number of modes is the product of these values). The order values should be adequate to the number of appropriate diffraction orders in every layer. There is a possibility of automatic fixing of this problem (see page **Options**).
- **Wavelength**, measurement unit is nm.
- Grating **Period** field has two editor controls for periods along *X* and *Y* directions, measurement unit is *nm*. The selected Check box between these editor controls imposes constrain on period values preserving their ratio.

- **Polarization.** The **TE** (*s*) polarization when the electric field is in the *X-Y* plane and the **TM** (*p*) polarization when the magnetic field is in the *X-Y* plane. Generally the polarization state is defined by two amplitudes of the electric field in the plane normal to the ***k*** – vector of the incident wave i.e. ***E_s*** (in the *X-Y* plane) and ***E_p*** (perpendicular to ***E_s***). Amplitudes of these components are defined by the **State** polarization angle and phase shift of the ***E_p*** component with respect to the ***E_s*** component is defined by the **Phase** angle. Angles measurement unit is *degrees*.
- **Incidence Angles,** the angles definition is explained in the **Structure Geometry** picture (definition depends on **Coordinate System**). Theirs meaning are obvious from the pictures presented at the same page. Measurement unit is *degrees*.
- ^C **Method** defines the calculation method Classic or Extended. If classic method is selected then on this control exit a zero interface will be applied to all interfaces.

Layers

- The incidence always takes place from the cover medium and the layers are enumerated from the cover to substrate medium. If the user wants to illuminate the structure from the substrate medium, the role of cover and substrate must be swapped. Button **C-S** swaps the role of cover and substrate and reverses the order of the layers inclusive of the grating.
- For the Modal and Chandezon classic method by clicking the right mouse button at **Layer** control the user activates the **Pop-up Menu** for editing the whole layer (copy, paste, etc).
- ^M The elementary grating cell of each layer of given **Layer** index and given **Thickness** may contain more than one cylindrical pillars of identical height. The user can edit the pillars parameters individually. The **N Pillars** and **Index** controls define the number of pillars and the pillar index for edit controls in the panel at the right. If the user wants to increase **N Pillars**, the software duplicates the pillar with the higher index, so at this stage the user will not see any difference in the layer plot. For the insertion of the different pillar the user has to edit the parameters (X- and Y-coordinates and/or refractive index) of the last (duplicated) or previous pillar. Note that the pillar with the higher index overrides all pillars of lower index in case of pillars intersection.
- ^M There are two possible pillar shapes. For **P Points** equals to two the pillar is a cylinder with an ellipse cross-section inscribed into appropriate rectangle. In the case of **P Points** greater than two the pillar has a polygon cross-section. The user may set the diagonal coordinates of the ellipse rectangle or polygon point coordinates by using **Index** and **X** and **Y** controls. The coordinates measurement units are defined by **Pillar Units** control. If the **Fraction of Period** of **Pillar Units** control is selected the user can edit pillar coordinates under following constrains:

$$-1 \leq x_i \leq 2; \quad \text{Max}(x_i) - \text{Min}(x_i) \leq 1;$$

$$-1 \leq y_i \leq 2; \quad \text{Max}(y_i) - \text{Min}(y_i) \leq 1;$$

If the another of **Pillar Units** control is selected the constrains are multiplied by an appropriate factor. The pillar will be automatically inscribed in a single *X-Y* periods cell.

- ^M If the **Pillar Plot** control is checked the layer pillars structure is illustrated in separate graphic window.
- This page contains the **“Material”** control. If any of corresponding to the medium edit field is focused, by clicking this control the user can access to the Material Catalog through the **Material** dialog window. If a medium is assigned with a Material the **“Material”** control caption indicates the *Material name* and the software will always take a refractive index of this Material for a current value of wavelength otherwise the **“Material”** control caption is *Select Material* and medium refractive index will be fixed for all wavelengths.
- By clicking the right mouse button at the **“Material”** control the user activates the *Popup Menu* which helps to manipulate with the already set materials bypassing the **Material** dialog window.
- Other fields are obvious. It is necessary to emphasize the useful property of the *Permittivity* and *Refractive index* fields: after exiting from any field or after pressing the Enter key, all other fields in a line will be automatically recalculated.

Note 1 Every layer grating cell is defined in FFT grid. Pillars coordinates take values corresponding to the FFT grid nodes. FFT grid size depends on maximum *Number of Orders* (**General** page) and indicated in **Pillar Units** control.

Note 2 The imagine part positive sign of the *Permittivity* and *Refractive index* corresponds to the dissipative media while the negative sign corresponds to the media with amplification.

^C Grating

- The field **Period** has two editor controls for periods along *X* and *Y* directions, measurement unit is *nm*. The selected Check box between these editor controls imposes constrain on period values preserving their ratio.
- The field **Depth** has two controls: **Grating** and $f(x)$ or $g(y)$ functions. **Grating** represents the minimum thickness of the imaginary layer which contains the grating profile. After exiting from these controls or after pressing the Enter key, all sinusoidal harmonics and points values in the representation of the grating profile or the function will be automatically recalculated preserving the functional shape.
- The **Profile type** control has three options: first two represent the grating profile as the sum or the product of functions $f(x)$ and $g(y)$ and third - as an arbitrary 2D harmonics presentation.
 - First two options allow editing functions $f(x)$ and $g(y)$ individually. The state of corresponding fields for selected function depends on the state of button **Conversion to** i.e. on the text under this button. If this text is *“X Points Presentation”* or *“Y Points Presentation”*, the user can edit any sinusoidal harmonic (defined by **Harmonic Order**) individually. The user can also change the total number of harmonics in the field **Number of Sinus Harmonics**. After pressing the button **Conversion to** and after the appearance of the text *“X Harmonics Presentation”* or *“Y Harmonics Presentation”*, the user can insert the data of the function profile point by point (the original function profile will be deleted) and should choose the **Number of Approximating Harmonics** to decompose the inserted function as a harmonic set. In this regime by right mouse click of the **Point Index** control the user activates a *Popup Menu* which helps to edit points of a grating profile. After finishing the data insertion, the user can convert these data to the pure harmonics presentation or leave it as it is. This operation does not affect the result of the calculation but it is irreversible in

the representation of the function profile.

- Third option activates the button **Load profile**. If there is not 2D harmonics data the button **Profile plot** is inactive.

- The state of other fields depends on the state of button **Conversion to** i.e. on the text under this button. If this text is “*Two points Line*”, the user can edit any sinusoidal harmonic (defined by **Harmonic Order**) individually. The user can also change the total number of harmonics in the field **Number of Sinus Harmonics**. After pressing the button **Conversion to** and after the appearance of the text “*Harmonics Presentation*”, the user can insert the data of the grating profile point by point (the original grating profile will be deleted) and should choose the **Number of Approximating Harmonics** to decompose the inserted function as a harmonic set. In this regime by right mouse click of the **Point Index** control the user activates a *Popup Menu* which helps to edit points of a grating profile. After finishing the data insertion, the user can convert these data to the pure harmonics presentation or leave it as it is. The last operation does not affect the result of the calculation but it is irreversible in the representation of the grating profile.
- Pressing the **Load profile** button opens the intermediate *Profile 1D to Harmonics* or *Profile 2D to Harmonics* window depending on the state of Profile Type control.
In case of 1D Profile window the user may load the data text file (extensions .dat or .txt) followed by selection of profile depth and number of harmonics approximation of loaded profile. Profile must be single-valued function on a unit cell of the grating. File should contain two columns X or Y (arbitrary) and Z (nanometer) coordinates respectively. The length of the profile table must be greater than or equal to 2. The first line of the columns names is allowed. Columns should be separated by tab or double space. Values in the X or Y column will be normalized by software to a corresponding single period.
In case of 2D Profile window the user may load user defined or one of the predefined profiles followed by selection of profile depth and number of X and Y Fourier harmonics in profile presentation.
The user 2D Profile must be defined on a unit cell of the grating and must be single-valued function. Two text file formats are accepted by software. First format is a simple N_x (number of lines) by N_y (number of entries in each row) *FFT* grid table of profile height values in *nm* separated by tab or double space character. The numbers N_x and N_y must be power of 2 and belong to a range of 8-512. Second format is a general table of profile height values in *nm* with first column and first line representing X and Y coordinates respectively. The number of lines and the number of entries in each row must be greater than or equal to 3. Coordinates (X and Y) can be of any scale but in ascending order. These coordinates will be normalized by software to corresponding single periods. Common element of first line and column should be a simple string, for example “x-y”.
- The extended method implies the additional **Interface** field which provides possibility to choose the interface for editing. The interface indexes start from “0” and finish with the index of the last layer.
- For the extended method by clicking the right mouse button at **Interface** field the user activates the *Popup Menu* for manipulating the interfaces grating profiles (copy, paste, etc).
- The extended method implies additional button **Remove Interface**. This button is active if the layers adjacent to the interface have identical permittivity.

Scanning

A one dimensional scan can be represented in an appropriate graphics window. See the **Graph Dialog**.

A two dimensional scan can be represented in the **3D Graph** window.

- The panel **Scanning Range** defines the initial and final values of the scanning parameter and the number of intervals (number of points minus one).
- The panel **Scanning of** has an obvious meaning. The first option **Fixed Parameters** corresponds to the **General**, **Layers**, ^c **Grating** page parameters. The checked box **X-p/Y-p=const** imposes constrain on periods ratio defined by corresponding **General** page values. This constrain is valid only for scanning.
- If the check box in the **2D scan of** panel is checked then the user can get diffraction efficiency versus two different parameters from the **Scanning of** panel list. The diffraction efficiency order and component can be selected in the **Diffraction Orders Output** panel and in the **2D scan of** panel Combo Box. Scanning parameters, range and number of scanning points can be selected individually for rows and columns under appropriate **2D scan of** option.
- The other controls: **Output Format**, **Output Decimal Digits** and **Diffraction Orders Output** define the representation of result data in the edit window.
In the panel **Diffraction Orders Output** the user can choose any diffraction order to be displayed restricted by minus plus of a half **Number of Orders** in appropriate direction. Near by the appropriate fields there are tips about the extreme indexes of diffraction orders in the whole range of scanning which are updating with the changes of scanning range parameters.
- The **Output Polarizer** control has an effect only on the result data representation and not on the actual calculations. For more details see **Slider**.

Resonance

- The resonance search is aimed at searching for the true guided modes of the dielectric structure under modeling. It searches for the incidence angle and resonance width of waveguide excitation by selected polarization in the incidence plane normal to the grating plane and with an orientation defined by Plane Angle. At the page opening the software automatically calculates the mode effective indexes of the multilayer structure under the assumption of a structure with real refractive indexes, the grating regions being considered as suitably averaged uniform layers. The resonance search can be performed for a defined initial incidence angle and resonance width with the button **Find** and iteratively improved with the same button changed to **Repeat**. The main resonance parameters are calculated on the basis of the phenomenological resonance response approximation by *poles* functions using five (single resonance) or seven (double resonance) equidistant angular positions located within an angular range covering four **Half Resonance Width** symmetrically with respect to the resonance **Angle** position. If the **Double Resonance** check box is checked two consecutive poles will be calculated. This double resonance search is obligatory in two cases: first under normal incidence, secondly in the case of two neighboring resonances (poles).
- The full set of *poles* parameters can be found after the resonance searching in an appropriate page of **Analysis** dialog.

- It is the user responsibility to choose the grating period value (see *Analysis* dialog) and a corresponding mode effective index used for waveguide excitation.
- The all fields and controls of this page are rather obvious.

Fields

The purpose of this page is analogous to the purpose of the *Scanning* page and the meaning of most fields is obvious. The coordinate system is illustrated in *Service Window* then *Structure Geometry*.

- If Check Box **2D (x, z) Scan of** is not selected then depending on the *Scanning Direction* and *Cross-section* options the user will get all field or power flow components distribution along any axis at selected coordinates along other two axes.
- If Check Box **2D (x, z) Scan of** is selected then the user will get a distribution (along any two axes at selected third axis coordinate) of field or power flow component selected in the Combo Box at the right of Check Box **2D (x, z) Scan of**. Scanning range and number of points can be selected individually for both directions under appropriate *Scanning Direction* option. The final state of this control defines rows in data table. A change of selected component does not impose a field components recalculation.

All changes in this page do not impose a recalculation of the structure. By default this page is disabled. To enable it select an appropriate option in the *Options* page.

Options

- If the *Save Settings* box is checked then all *Scanning*, *Fields* and *Options* parameters will be saved in the structure file in addition to the parameters from the *General* and *Layers* pages. The part of the structure text file with settings is hidden for the user but accessible with any external text redactor.
- The check box *Background calculation* disables the output to the result editor window during the calculation process.
- ^C If the *Decomposition Order Correction* box is checked, then if necessary the software will automatically increase the values of *Minimal Order of Field Decomposition* to the adequate number of Cover and Substrate X and Y diffraction orders.
- ^M If the *Number of Modes Correction* box is checked, then if necessary the software will automatically increase the *Number of Orders* values to the adequate number of Cover and Substrate X and Y diffraction orders..
- *Calculation Direction* option is useful for calculation of structures with a uniform layers stack. Calculation is faster if it starts from this stack section.
- For the Field calculation and to activate the page *Fields* the box *Field Calculation* should be checked at that the page *Scanning* becomes inactive. The *Autoselect* check box allows enabling/disabling of a conformation dialog appearance while the user enters the *Fields* or *Scanning* disabled pages. The fields are calculated in two steps: calculation of the structure for the fixed parameters followed by the field distribution calculation in accordance to the page *Field* settings.
- If the *Automatically Start Second Stage* box is not checked, then the calculation will be stopped after the first step and the user should press *Run* to proceed with the second step.

This option is useful to check the intermediate results in the editor window. Changes in page *Fields* do not activate the first step.

- If the ***Favor Memory Consumption*** box is checked the software needs minimum possible memory to complete calculation. This option is incompatible with the field calculation.
- For a reasonable response of the other windows applications it is not recommended to increase the ***Calculation Priority*** greater than Idle.
- ^C If ***Profile Plot Real Position*** box is checked the *Profile Plot* displays real Z coordinates of interface otherwise coordinates correspond to the profile defined in ***Grating*** page.
- ^M In the case of the *TM* polarization and a binary highly conductive metal grating the truncation of Fourier representation of Maxwell's equations generates spurious plasmon-like modes. These modes have anomalously high effective refractive indexes and are responsible for the so called numerical instabilities. They do not present in the real lamellar structure (TMM) modes spectrum. If the ***Neff Filter Level*** box is checked the software considers the modes with effective refractive index above the specified level as no propagating in the layers. These modes are still used at the interfaces field matching. This option may be used to suppress so called numerical instabilities. For more details see Ref.7 in the ***Introduction***.
- ^M If ***Using NV Field*** box is checked the *NV Field Method* is applied (Ref. 4-6 in the ***Introduction***) and the ***Smoothing NV Field*** option can be applied with the corresponding smoothing parameters. The resulting *Normal Vector Field* can be checked with the tools of *NV Field* panel.

^M NV Field

This page is intended for *Normal Vector Field* visualization.

The structure calculation is completely independent from this page controls.

- ***Layer Index*** defines the grating layer index.
Above this control the FFT grid size is indicated.
- ***Graph Type*** control has two options:
 - ***Interface*** displays in the FFT grid the *NV Field* at interfaces only.
 - ***Full Field*** displays full *NV Field* in the FFT grid.
 - ***NV Field component*** selects *NV Field* component to display.
- The user may display in the FFT grid the original *NV Field* with smoothing or not (see page ***Options***) or the *NV Field* image used in real calculation. The last depends on number of orders (***General*** page) repeated in the *Root-mean-square error at Interface* panel. This panel presents average difference between the original and the image of three *NV Field* components. These values are calculated during the *NV Field* displaying. The *NV Field* values are significant only at interfaces. So, minimizing these errors by playing with smoothing parameters page (***Options*** page) will increase the reliability of *NV Field* using.

Analysis Dialog

This dialog allows calculating reflection and transmission of a finite Gaussian beam of two incident polarizations the TE (s) or the TM (p) in the incident plane normal to the grating plane and with orientation defined by a Plane Angle (**Resonance** page). In the case of the TE polarization the software uses E_s electrical field component. In the case of the TM polarization the software uses $E_p = H_p/n$ (n is the propagation medium refractive index) electromagnetic field component. The FFT (Fast Fourier Transform) and Pole functions of a resonance search are implemented.

The reflected and transmitted Gaussian beam is calculated as a sum of corresponding plane waves. The **Analysis** button is active only if a result data is in the form of scanning versus angle or **Resonance** was found or external data file is a scanning versus angle of complex reflected and/or transmitted amplitude calculated with switched on the **Output Polarizer** (Settings dialog -> Scanning page).

The **Analysis** dialog contains several pages:

- **General** page informs about the geometry, pole functions definition and input parameters. The user can switch the pictures with information by the **Picture** control. If the data was loaded from the external file, the edit fields can become active and it is necessary to fill them with appropriate values and press the button **Ok General**. The user can add appropriate data at the end of the input data file after the blank line and in individual lines. The format is: value, double space or tab followed by specifications (Wl, Per, Nc, Ns, Pol).
- **Gauss (FFT)** page appears only if the result data is in a form of scanning versus the incidence angle.
- **Gauss (Pole)** page appears every time when **Resonance** was found.

Under the pagers area there are three buttons:

- **Calculate** with obvious meaning. If the process takes long time the user can terminate calculations with the same button which changed its caption and functionality to **Terminate**.
- **OK** saves the state of dialog and hides it.
- **Cancel** closes the dialog.

The controls of data format output to the **Graph** and to the **Result window** also are placed here. By default the output data always contains the Power option.

Depending on resonance type (single or double) the **Single Resonance** and **Pole** or the **Double Resonance** and **Poles** pagers appear. These pagers represent the appropriate resonance and poles parameters. Under these pagers the button **Calculate** is replaced with the button **Data Window** which provides ability to save the page information in data file.

Note Sometimes the **Graph** or **Result window** is not accessible with open **Analysis dialog**. In this case the user may press **OK** button to hide the dialog.

Gauss (FFT)

The input result data are recalculated by parabola fit procedure to correspond to **Number of FFT Points**. This value effects on the angular resolution. An incident Gaussian beam has two intrinsic parameters: **Waist Radius** and **Defocus** and the external parameter is the incidence angle (**Fixed Beam Angle**) calculated with respect to the beam axes. The minimum **Waist Radius** depends on the input data angular scanning range: the larger range - the smaller possible **Waist Radius**. The maximum **Waist Radius** depends pro rata on **Number of FFT Points**. The **Defocus** is the distance

along beam axes from the crossing point with the cover interface and the waist position. If waist is placed in the cover the sign of defocus is negative otherwise the sign is positive.

The user is able to get several structure responses from the incident Gaussian beam defined by the **Output Type** and **Output(Reflection/Transmission)** controls in the form of graph or table in editor window and in the format defined by the **Output Decimal Digits** and **Output(Real; Imagine/Module; Phase)** controls placed under the pagers area.

If the buttons **Graph** and **Result Window** are active this means that the result is already calculated otherwise it is necessary to press button **Calculate**.

This page contains the intrinsic checking of the page parameters on corresponding to the input data. This checking can be considered only as a guide and the user responsibility is to set reasonable parameters.

Gauss (Pole)

On this page the phenomenological approximation by pole functions of the plane wave reflection and transmission is used. For more details see the reference 9 of used sources in Introduction. The user is able to make a decision about what type of resonance is applicable to his situation: single or double. The other possibilities of this page are analogous to the **Gauss(FFT)** page with one exception: this page does not contain any intrinsic checking of the input parameters.

Optimization Dialog

The optimization method is based on the approach suggested by Davidon (1959), and further developed by Fletcher and Powell⁸. The Davidon - Fletcher - Powell method is a Quasi-Newton Method also known as a Variable Metrics Method.

The Optimization Dialog contains at the creating a copy of the initial structure of the parent project window. It comprises three pages:

- **Variable Parameters** page is destined for the assignment of the set of the structure variable parameters and their initial values. The user can change these initial values at will and in accordance of she's intuition.
- **Criterion Function** page which the user can use for defining the targeted output power of diffracted waves of the structure under established conditions (arguments).
- **Optimization** page contains the controls of an optimization process.

Under the pagers area there are three buttons:

- **Export** replaces the structure of the parent project window by the current structure of the Optimization Dialog and hides the Optimization Dialog. Only the current point **Criterion Function** Arguments of active fields will be exported as the parent project structure parameters. This action also exports the other content of the three Optimization Dialog pages which will be added to the structure text file in a form hidden for the user but accessible with any external text redactor.
- **Ok** hides the current Optimization Dialog.
- **Clear** abolishes all changes in the Optimization Dialog, removes the corresponding part in the structure text file and closes dialog.

Note If the Optimization Dialog already exists but hidden and the user opens it by pressing **Optimize** control a warning or conformation dialog may appear. The warning dialog corresponds to the parent project structure changes incompatible with the Optimization Dialog settings, for example number of layers was changed. The conformation dialog appears if the parent project structure changes influence the optimization result, for example invariable layer thickness was changed.

Variable parameters

A checked box means that the corresponding parameter (*Wavelength*, *Periods*, *Normal Angle* and *Plane Angle*) will be varied to optimize the **Criterion Function**. It also means that the user can edit the above variables as the starting optimization parameters. If a box is not checked these edit controls are inactive and display the current *criterion point arguments* values during the optimization. The above parameters can be set as variable only if the *Criterion function* has the same parameter value for all *Criterion points*.

The user can check the structure parameters under optimization by way of **Settings Dialog** after the **Export** procedure.

The structure media with identical refractive indexes can be combined in a group identified by its index number by selecting the check box in the **Material Group** control. If the **Add To Group** of the **Material Group** control is selected, the **Group** control indicates the index of group which corresponds to the selected Layer while the **Members** control indicates total number of elements in the current group. The maximum allowed **Group Index** always corresponds to an empty group; it automatically increases or decreases as soon as a first refractive index group member is introduced or the last refractive index group member is removed. If the **Set group Parameters** of the **Material Group** control is selected, the refractive index of the group and its variable status can be set while the **Member** control allows inspecting of current group member other parameters. After start the **Optimization** all material assignment for media in the group will be removed.

Note 1 The checked box $X\text{-}p/Y\text{-}p=\text{const}$ imposes constrain on periods ratio. This constrain is also valid for Criterion points.

Note 2 During the Optimization process the edit controls are disabled but they display every second the real time values. In addition, if the user changes the **Group Index** or **Layer Index** the related parameters will be updated immediately.

Criterion Function

The optimization procedure objective is the minimum mean-square deviation of the user defined values assigned in the *Criterion Function* from the calculated values. The user can construct this Function in the form of a number of (**Number of Points**) completely independent criterion points. The **Point** control provides the possibility to select the criterion point index. By clicking the mouse right button at this control the user activates the *Popup Menu* for editing the criterion points. Every criterion point targets the assigned power of the given diffraction order (edit control **Value**) with the **Weighting Factor** of this criterion point within the whole criterion function and its characteristics (**Diffraction Order** and **Cover/Substrate** propagation). The **Output Polarizer** and its orientation (edit control **Angle**) is an additional criterion point characteristic. All these characteristics are placed in the **Criterion Diffraction Order Power** panel. The right hand **Criterion Arguments** panel contains other parameters. These arguments are: the polarization type, the incident conditions **Normal Angle**, **Plane Angle**, **Wavelength** and the grating **X-Period** and **Y-Period**. The edit controls of the corresponding **Variable parameters** are inactive.

During the *Optimization* process these two panels are inactive, but at the bottom of the left panel under the label **Current Power Value** the user can see the updated every second power of the appropriate diffracted wave. In addition this information will be updated every time the user changes the criterion **Point** index.

Optimization

This page contains several controls for the defining the optimization process parameters:

- **Iterations in Trial: N Variables plus** the number displayed in the related edit control. In accordance with the theory of the optimization method, in the ideal case of parabolic behavior of the *Criterion Function* versus *Variables*, the process converges after N iterations, where N is the number of variables. In many real cases it takes a much larger number of iterations and the efficiency of convergence is progressively decreasing. After defined number of iterations the optimization code continues the process from the achieved position and in the direction of the steepest descent.
- **Accuracy** defines the step for the numerical estimate of the derivative of the *Criterion Function* relative to each *Variable* and also defines the size of the multidimensional region of space around the targeted point in which the criterion function has an absolute minimum with respect to all variables. Once the above condition is satisfied, the process stops with the message “Optimized!”
- **Correction Coefficient** is simply the multiplier in the *Criterion Function*. This option is useful because the optimization procedure depends to some extent on the Criterion Function absolute value.
- **Factor** by default is the initial value of the determinant of the main Hessian matrix.
- **Automatic Scale**. By default the same **Accuracy** step is applied to every variable but the dependency of the *Criterion Function* on the variables can be very different. If the box **Automatic Scale** is checked the software analyses these dependencies after an iteration cycle and continues the process with the new individual step for every *Variable* to equalize the dependencies. This action also changes the **Correction Coefficient** in order to maintain the **Factor** value around unity.
- **Terminate** button terminates the optimization process but the current *Variables* values can be used for the start of the next optimization.

Under the *Mean-square Error* label there is an information about the mean square deviation (average taken with the *Weighting factors*) of the calculated values from the values assigned in the *Criterion Function*.

Note 1 The **Automatic Scale** regime does not always provide the best convergence and in addition after the completion of the optimization the accuracy of the result is unknown. In order to fix this accuracy problem, the user will uncheck the checked box **Automatic Scale** and restart the optimization process.

Note 2 Some times the optimization process finishes at the local extremum. The advice is to try the optimization with the new starting parameters or with other **Accuracy** value.

Note 3 If the variable parameter is going to a negative value and this is in contradiction with a physical sense then an error message appears and the optimization process will be terminated.

Graph

Graph Dialog

In case of a two parameters scan, after clicking the **Graph** control the **3D Graph** window will appear. In case of a one dimensional scan, after clicking **Graph** control the **Graph Dialog** window appears. This window provides possibility to relate columns of result data to the *X* and the *Y* axes as well as to choose the curve color and thickness.

This dialog also contains a **Smooth Phase** check box. This box is enabled for a phase column data, if it is checked all 2π phase jumps will be removed from the graph.

After clicking **OK** the Graph window will appear. There are several independent Graph windows for different options of **Scanning of** and **Scanning Direction** and for the external data. These windows are common for all projects.

The graph window has the **Edit** menu with submenus:

- **Clear All** clears all curves and closes the window.
- **Titles** is the option for editing titles of the *X* and *Y* axes.
- **Copy** copies the Image into Clipboard .
- **Save as** saves the graph in Bitmap, JPEG and Windows metafile formats.
- **Print**.

The second menu **Curves** contains the list of curves. By clicking the curve title the user can open dialog window for curve editing (color, thickness and curve title). The selected curve also can be deleted (**Delete** button) or saved in a data file (mouse click at the button with diskette icon opens the save dialog).

3D Graph

In case of a two parameters scan, after clicking the **Graph** control the 3D Graph window will appear. This window is common for all projects.

The **Edit** menu may provide the following options:

- **Titles** is the option for editing titles of the *Value*, *Row* and *Column* axes.
- **Copy** copies the Image into Clipboard .
- **Save as** saves the graph in Bitmap, JPEG and Windows metafile formats.
- **Print**.

The second menu **View** may contain the following options:

- **Front**
- **Back**
- **Top Color Image**

- *Node's Hint*
- *Color Scale*
- *Interfaces*
- *Aspect Ratio*

The **Front**, **Back** and **Top Color Image** items have an obvious meaning. If **Node's Hint** is checked then the user by pointing *Cursor* at a *Node* position can inspect its value and coordinates. The **Color Scale**, **Interfaces** and **Aspect Ratio** items are related to the **Top Color Image** option only. **Interfaces** item is not available for the external graph.

Additional view options (*Front* and *Back*):

- Horizontal View option. If the user presses the left mouse button and *Cursor* is at the 3D Graph area a vertical line crossing the front corner horizontal coordinate plane appears. Holding pressed the mouse button the user can lock *Cursor* to this line (*Cursor* changes shape and line disappears) and then change the horizontal position of this front corner that equivalent the Graph horizontal rotation in the range from -90 till 90 degrees.
- Vertical View option. With the right mouse button in the same manner the user can change the back corner horizontal coordinate plane vertical position that equivalent the Graph view changes in the range from horizontal till top view.

Additional view option (*Top Color Image*)

Right mouse click at image area opens Popup Menu for changing Color Scale Type (Blue-Green-Red; Black-Violet-Blue-Green-Red-White; Black-Grey-White).

Slider Dialog

The control which opens this dialog is active only if there is a result data of any type. For the any type of a scan result data this utility provides the possibility for an express analysis of the scan graph behavior versus the input polarization state of the incident beam and versus the orientation of the output polarizer. For the **Fixed Parameters** result data (including **Field Calculation** data) the slider graph is versus the output polarizer angle. The output polarizer is always placed in the plane perpendicular to the \mathbf{k} – vector of the wave impinging onto it. The polarizer angle corresponds to the angle between \mathbf{E}_s component of the incoming wave and the \mathbf{E} vector of the output wave.

Under the slider controls area there are additional controls with obvious meaning and two buttons:

- **Ok** hides the Slider Dialog and makes the slider graph window accessible.
- **Cancel** closes the Slider Dialog and the slider graph window.

Command line

- There is a possibility to run an executable file in command line with two obligatory parameters separated by space. First of them is a path to a structure file and second is a path to an output file.

- Software will start calculation with parameters stored in the structure file including settings parameters, for example *Background Calculation*. After finishing calculation the executable will be terminated.
- This option will be helpful for users familiar with external running of executable files and allow performing user defined type of scanning.

Material

This dialog window is accessible from the *Layers* page of *Settings Dialog*.

- The user is provided with two Materials catalogs: the Main catalog and the Custom catalog accessible through the material dialog.
- Materials from a current Material Catalog are listed in *List Box*. **Refractive index** edit controls represent the Material refractive index values of selected *Material name* for the wavelength specified in **General** page and indicated above refractive index values. The user also can check the refractive index wavelength dependence (the **Graph** button).
- The right mouse button click at *List Box* activates the *Popup Menu* with following options: **Add Material**, **Edit Material**, **Copy Material**, **Remove Material** and **Insert Material**.

The first two options open the **Material Edit** dialog window.

The other options allow reordering Materials in Catalogs or copying Material from one catalog to another for the user convenience.

To protect the Main catalog from an accidental changes the **Edit Material** option is available only for the Custom catalog. To edit the Main catalog record copy it to the Custom catalog and after editing copy it back to the Main catalog.

- **Clear Selection** button removes an assignment of Material for appropriate media from *Layers* page keeping the current refractive index value.
- **Sort** button allows sorting Materials names in alphabetical order.
- **Ok** applies all changes in this dialog as described below and hides it.
If Material name is selected this Material will be assigned to the specified medium which takes the Material refractive index for any given wavelength, otherwise the medium will not be related to any Material and current refractive index of this medium will be used for all wavelengths;
All Materials changes will be saved in both Material Catalogs.
- **Cancel** abolishes all current changes in this dialog and hides it.

Note In case the *Material name* is present in both catalogs the software will take a data from the Main catalog.

Material Editor

This dialog window is accessible from the **Material dialog**.

Three models of refraction index wavelength dependence are implemented: *Drude*, *Schott*, *Sellmeier*, *Herzberger*, and *Table*. The *Drude* and *Table* models are complex, the *Schott*, *Sellmeier*, and *Herzberger* models are real valued.

The *Drude* model requires two parameters. The index of refraction n is given as

$$n = \sqrt{1 + \frac{-C_2 + i\lambda C_1 C_2}{C_1^2 + \lambda^{-2}}}$$

The *Schott*, *Sellmeier*, and *Herzberger* formulas are defined by six parameters. These formulas assume that imaginary part of refractive index is identically 0, and gives n according to formulas.

The Schott formula

$$n(\lambda) = \sqrt{c_1 + c_2\lambda^2 + \frac{c_3}{\lambda^2} + \frac{c_4}{\lambda^4} + \frac{c_5}{\lambda^6} + \frac{c_6}{\lambda^8}}.$$

The Sellmeier formula

$$n(\lambda) = \sqrt{1 + \frac{c_1\lambda^2}{\lambda^2 - c_4} + \frac{c_2\lambda^2}{\lambda^2 - c_5} + \frac{c_3\lambda^2}{\lambda^2 - c_6}}.$$

The Sellmeier coefficients for many common optical materials can be found in the online database of RefractiveIndex.info.

The Herzberger formula

$$n(\lambda) = c_1 + c_2\lambda^2 + c_3\lambda^4 + c_4L + c_5L^2 + c_6L^3, \text{ where } L = \frac{1}{\lambda^2 + 0.028}.$$

The *Table* needs at least one data point. For two points in *Table* the linear approximation is used to calculate refractive indexes. If number of points exceeds two the parabolic approximation is used. By default the Material Catalog contains the data for calculation of Air refractive index by special formula:

$$n = C_1 + C_2 + \frac{C_3}{C_4 - \lambda^{-2}} + \frac{C_5}{C_6 - \lambda^{-2}}$$

Coefficients in Material Catalog for all formulas above assume that the wavelength is in micrometers.

The following dialog window items need explanation:

- **Minimum** and **Maximum** wavelength edit controls define the wavelength range where the *Table* and formulas are applicable. Outside this range the refractive index will be set to the value at the nearest wavelength limit. For the *Table* the *Minimum* and *Maximum* wavelength controls are disabled and display the minimum and maximum wavelengths in the *Table*.
- **Convert** button allows the user to convert a *Table* data into a new Material Catalog record of formula presentation.
For *Drude* formula the *Table* should contain at list one point and coefficients are calculated

for every *Table* point between *Minimum* and *Maximum* wavelengths followed by an averaging.

The *Schott* formula coefficients are calculated assuming minimum square deviation of formula and *Table* refractive index values between *Minimum* and *Maximum* wavelengths. In this case the *Table* should contain at list six points.

- **Ok** applies all changes in this dialog and closes it.
The *Table* data will be automatically sorted in wavelength ascending order.
- **Cancel** abolishes all changes in this dialog and closes it.

This dialog was used in composition of the main materials catalog and the following sources were used to retrieve some refractive index values:

1. From the reference book Physical values, ENERGOATOMIZDAT, Moscow (1991)
Reference in catalog: (Table Ru) and (Schott Ru).
2. From GratingSolver 4.20 Demo, <http://www.gsolver.com>
Reference in catalog: (Table GS) and (Drude GS).
3. From the website <http://www.luxpop.com/#index%20of%20refraction%A0>
Reference in catalog: (Table).
4. From the paper in Applied Optics Vol. 32 No. 28 p.5587 (1993)
Reference in catalog: Film (Table).
5. From the website RefractiveIndex.info
Reference in catalog: (Sellmeier).