The modified integral method and real electromagnetic properties of echelles

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ABSTRACT

The deep research of all types of echelle gratings, working from low (8) up to very high (1431) diffraction orders with use of the rigorous modified integral method of the analysis is presented. The modified integral approach allows one, with the help of the standard program (PCGrate™ 2000X) and a rather small PC, to simulate one of the most hard-to-converge diffraction efficiency problems, what the behaviour of echelle is. In comparison with detailed paper of E. Loewen *et al.* "Echelles: scalar, electromagnetic, and real-groove properties" the significant difference was found in calculation values for some examples in TM polarization. The difference between the compared theoretical data with the same refractive index for 316 gr/mm r-2 echelle at 632.8 nm in the 9 order and for TM polarization is up to 25% of absolute efficiency. The difference between calculated curve and measured data for the same grating and polarization at 441.6 nm in 12 and 13 orders is small (one-two percents) in opposite to the data of E. Loewen *et al.*, where the difference is many times more because of weak convergence of their method. The appreciable difference also exists for the medium and high orders. The presented results for the given refractive indices (basically, taken from the book E. Palik) have the best coincidence to experiment in all cases. Numerical research of two largest monolithic echelles, made on the project SOFIA also is included. The new record of rigorous calculations for r-10 EXES echelle, working in 1431 order was achieved at 10.6 μm. Because of the very small a wavelength-to-period ratios (~0.001) it is necessary to increase truncation parameter for such a case up to such value, that in result the matrices with the order about three thousands turn out.

Keywords: echelle, integral method, PCGrate software, echelle grating, diffraction grating, electromagnetic theory, efficiency modeling, relief gratings, reflecting gratings

1. INTRODUCTION

Diffraction of a grating echelle are well known and for a long time are used in various optical systems and especially in the cases when there are no alternative because of their special properties.[1] Even at application of advanced ruling engines and technology of copying, they are frequently produced on a limit of possible accuracy, and sometimes behind its limits. Also it is rather difficult and the process of measurement of the echelle characteristics limited for some reasons, including the measurements of form of the groove profile and diffraction efficiencies.[2] Thus, the high value of the efiiciency for echelles is one of the main reasons of their preferable use in devices.

The theoretical researches of behaviour of echelle efficiency long time were based only on the scalar theory of diffraction with its different adaptations for a case of echelle. The significant divergences between results obtained with the help of this simple and rather useful theory and experimental data, were explained by everything, only not by lacks of the scalar approach. But other theory for comparison until recently simply did not exist. Rigorous methods,[3] despite of their already long history, were developed away from problems of study of behaviour of echelle efficiency, both by virtue of significant complexity of this research, and because of lack of the measured data.

Rather recently, and only with the help of a well known integral method, two results,[4,5] speaking about convergence of algorithms, used by the authors for a really difficult case of the rigorous analysis of echelle efficiency were independently obtained. The further perfection of a method and programs has allowed rather easily to calculate reflecting ability of echelle, working in the very high orders and having multilayer coating and others.[6-9]

The purpose of the present work is the illumination, basically, such features of a used integral method (named earlier "modified"[10]) and programs, developed by the author,[11] including commercial,[9] which allow to calculate exact value of absolute echelle efficiency in a very wide range of parameters. For typical examples of behaviour of the energy characteristics of echelle

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the convergence of a method will be analyzed and some recommendations are given at the choice of optimum parameters of the calculation. The detailed comparison is made with the basic theoretical and experimental results given in paper,[5] in which rather compplete and regular study of echelle diffraction properties will be carried out, but in which, however, there are inaccuracies. A rather interesting sample of account of efficiency in the high orders for the largest on a today monolithic aluminum grating,[12] made recently for AIRES[13] under the project SOFIA also is presented. At last, for an illustration of opportunities of our programs the record calculation of absolute efficiency of r-10 echelle made for EXES[14] under the project SOFIA,[12] working for TM polarization in 1431 order is carried out at 10.6 μm.

2. MODIFIED INTEGRAL METHOD FOR ANALYSIS OF ECHELLE

The rigorous solution of diffraction problems for echelle at any numerical approach is characterized by the whole bouquet of difficulties: the small a wavelength-to-period ratios, blaze in the high order, high depth of a profile, steep working cut, grazing incidence, possible high conductivity of metal (for IR range), possible additional dielectric layer(s) on surface which has, generally speaking, variable thickness etc. Except for these heavy for numerical realization of "ideal" parameters of a task, there are still large difficulties connected with calculation of real gratings: definition (measurement or modeling) exact form of a groove profile or exact value of blaze angle, selection from the literature (or calculation) of refractive indices of used materials appropriating to actually used technology of manufacturing of echelle, account of periodic and aperiodic terms of roughness layers etc. That is why such task, despite of development of rigorous methods and computer facilities, has appeared under force only for the most powerful and flexible approach, known today, which are integral one, and, in the best its realizations.[8,11] As to used by the author in some publications of the term the "modified" integral method,[10,11] it concerns, first of all, to set of having basic meaning of techniques used at numerical implementation of the theory, about what in brief there will be discussed below. In detail theory of an integral method together with updatings allowing to calculate rigorously efficiency of any gratings, including echelles, is stated in.[11]

Perhaps, a choice of points of integration has the most basic value for a considered case. As it is offered in[4,5] and shown in[8,11] it should be curvilinear integration along a surface of a profile , that allows to increase amount of points coming on an steep cut (as against a choice of points in regular intervals along the period) and, thus, it allows much more precisely to integrate quickly oscillating integrands . Our experience shows, that at such curvilinear integration (rather simple in practice[11]) the number of used points of collocation in difficult cases, as with echelle, decreases approximately on the order. Hence,[11] necessary for calculation RAM decreases approximately in 100 times, and time - approximately in 1000 times!

It is not less important, that the groove profile was not represented as expansion into Fourier series, as it was used in,[3,15] but was specified point-by-point.[10] Expansion into Fourier series , besides basically inexact representation of function of a profile , gives at the large number of the used members of expansion quickly oscillating harmonics at edges of a profile, that very strongly deforms representation of its form having paramount value for calculations of echelle efficiency. Thus, the refusal of expansion into Fourier series, at which ribbed forms of profiles smooth out, on calculations near to these edges, has no effect. In case of modeling echelles with a real complex groove profile, Fourier representation of a profile, apparently,[2] in general is unacceptable.

At last, we shall note necessity of optimization of term numbers of expansion of Green's functions and their normal derivatives. For usual (sometimes rather complex) calculations the selection of this parameter practically is not required,[11] or is used some universal rule for the certain type of gratings.[3,4,10,16,17] For echelles, by virtue of complexity of computations, in each concrete case it is desirable to carry out optimization on this parameter. It frequently allows to reduce total time of calculations typical curve to the order and more, especially for TM polarization (see Section 3).

Except for above named basic features, there are also others, also rather important for reception of exact and quickly converging results in this most difficult case of efficiency calculations. To them it is possible to attribute: generalization of the law of preservation of energy on a case of absorbing gratings,[11] forms of representation of Green's functions,[3,11] account of singularity of kernels of the integral equations,[3,11] accounts of Rayleigh wavelengths,[3] definition of the minimal number of points of collocation[4,5,7,8,10,11,16,17] and some others.

3. CONVERGENCE OF CALCULATIONS

For demonstration of convergence of the modified integral method and opportunities of the programs, made on its basis, including commercial ones,[9] with reference to modeling of echelle efficiency, pair of enough difficult examples was picked up from:[5] one for the low orders, another - for high orders . They are interesting because for these examples there are significant discrepancies for TM efficiency (especially for the low orders) with results from very useful and ample work in comparison of electromagnetic properties of echelle with scalar representations and experimental data which have been carried out by E. Loewen with colleagues.[5] At it, for chosen wavelength at 632.8 nm a refractive index ($n = 1.09 + i5.31$) known from[5] was used. Here will be investigated dependences both on optimizing parameter P (term numbers taken into account in expansion of Green's functions and their normal derivatives), and for truncation parameter N (number of collocation points).[11]

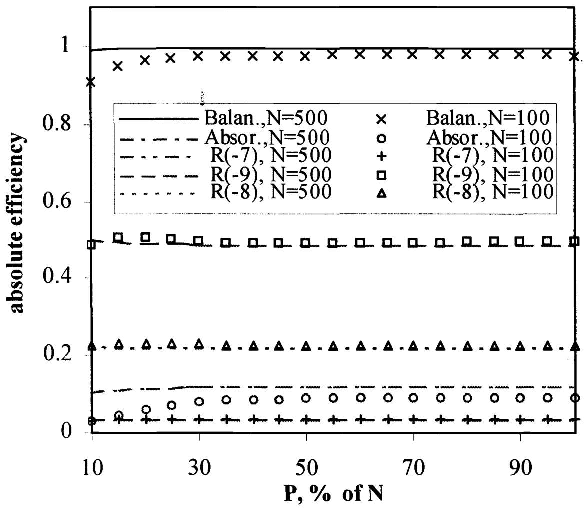

Fig.1. Balance, absorption, and efficiency in –7, –8, and –9 orders of r-2 316 gr/mm echelle at 632.8 nm & TE plane with 64° angle of incidence, as a function of P for N = 100, 500.

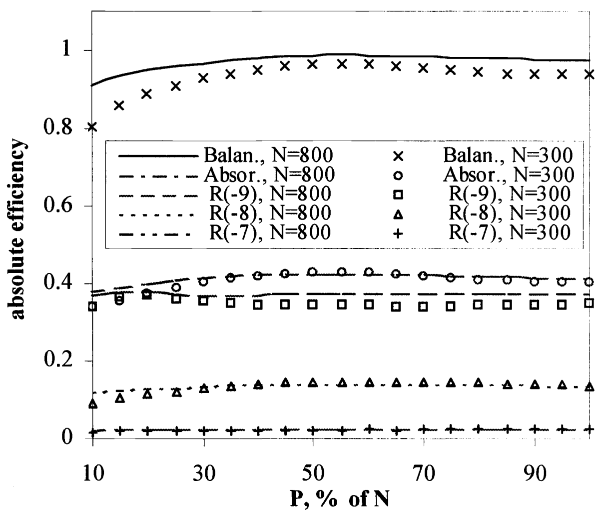

Fig.2. Balance, absorption, and efficiency in –7, –8, and –9 orders of r-2 316 gr/mm echelle at 632.8 nm & TM plane with 64° angle of incidence, as a function of P for N = 300, 800.

In Fig.1-2 the efficiencies for –7, –8, –9 orders, absorption and total balance of energy are presented accordingly for TE & TM polarizations of 316 gr/mm r-2 echelle (angle of an inclination of a facet is 63.4°) at wavelength 632.8 nm & incidence angle 64° dependent on optimizing parameter P. For TE polarization one can consider, that results in all orders and absorption are converged already at P = 30 of % from N for various N. It is especially pleasant, as dependence of computing time on term numbers in expansion of Green's functions and their derivatives has cubed form.[11] However, as it is visible from the Fig.1, truncation parameter N should be large enough, that the results converged to exact enough value. During the calculations it is easily supervised on value of total energy balance: for N = 500 it is close for converged (on parameter P) values to 100%, while for similar values at N = 100 it is insufficiently good and makes 97-98 %%. A little bit other pictures are observed for TM polarization. Convergence on parameter P is not so fast, as for TE plane: it reaches the saturation, when P is approximately equal to half of N. This value of P corresponds to so-called "a gold rule,"[11] recommended by the author as universal (starting) value of this parameter for accounts of any gratings[8,10,11,17] About such value P we also notice a maximum of approach of energy balance to 100%. At the further increase of P efficiencies, absorption and balance vary slightly. The curves for various N are similar, as well as in a case of TE polarization. And also, as for TE polarization, for insufficiently large N = 300 curves converge to not so exact value, in comparison with N = 800. However, as against the Fig.1 the –9 order is most sensitive to change of value N but not the absorption.

For research of convergence of obtained results of calculations on truncation parameter N we shall consider other interesting example. In Fig.3-4 efficiencies are presented in –89, –90, –91 orders, absorption and balance, accordingly, for TE & TM polarizations of 31.6 gr/mm r-2 echelle (assumed in[5] facet angle is 64.48°) at same wavelength and incidence angle, that in Fig.1-2, as function from N for P = 30, 50%% from N. For TE polarization the results begin to converge for various values P at

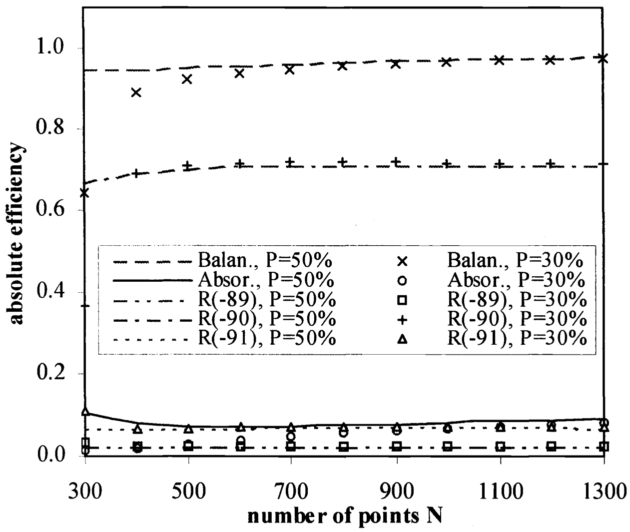

Fig.3. Balance, absorption, and efficiency in –89, –90, and –91 orders of r-2 31.6 gr/mm echelle at 632.8 nm & TE plane with 64° angle of incidence, as a function of N for P = 30, 50 %%.

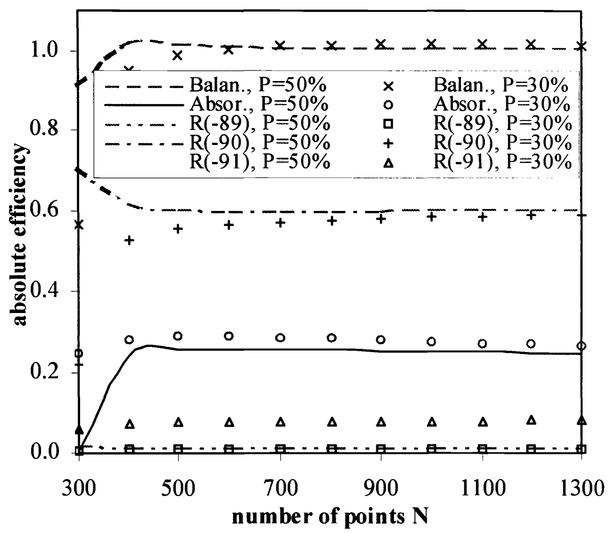

Fig.4. Balance, absorption, and efficiency in –89, –90, and –91 orders of r-2 31.6 gr/mm echelle at 632.8 nm & TM plane with 64° angle of incidence, as a function of N for P = 30, 50 %%.

N~400. With increase N the efficiencies slightly vary, and the energetic balance and absorption monotonously but, unfortunately, slowly comes nearer to exact values for different P. For P = 30 of % convergence is the slower, than for P = 50%. The difference in values of efficiencies for various P is small. In the Fig.4 for TM polarization the convergence begins to saturate for various P, as well as in a case for TE at N~400. However as against the Fig.3, absorption slowly and poorly oscillates and, together with it, oscillates about value 100% of energetic balance. For this example convergence is faster at P = 50%, and values of efficiencies and the absorption for various P differ slightly and tend to the same values.

In the considered examples the choice of optimum parameter P is not a complex task in both polarizations and the universal rule P = N/2 is suitable, for example.[11] The definition of suitable truncation parameter N is more essential in reception of exact results, that it is easy to make the analysis of convergence of results of the calculation (by energetic balance or main order). Unfortunately, the convenient rule P = N/2 for echelles works not always, especially in TM polarization. Then, it is more favorable at first to optimize parameter P at small N, and then with found optimum P to compute efficiencies with required accuracy on N. Let's note, that by virtue of disagreements with,[5] convergence was checked in addition up at the large values of N, but without allocation of logarithmic singularity of Green's functions.[3,11] All thus obtained results refer with given in Fig.1-4 to within the graphic image. The typical calculation of one point on specified in subsection 5.2 PC takes time from several seconds up to several tens minutes.

4. COMPARISON WITH RESULTS OF PAPER[5]

Behaviour of echelle efficiency in the low, medium and high orders we shall show by means of comparison of results obtained for some examples in[5] (section 3) and in this paper. In connection with the appreciable difference, found out by the author, with several theoretical examples from[5] for TM polarization, this aspect will be in detail investigated in this part. The comparison is carried out not only between calculated values for identical refractive indecies, but also with the measured data and computations executed with other refractive indecies. Unfortunately, at comparison the author used the data taken from the diagrams of papers[1,5] with an error of extraction approximately 0.5-1%% for absolute efficiency for the highly effective orders. About the same error corresponds to calculations carried out by the author. The similar total error does not influence comparison for strongly discrepancy cases of TM efficiency, where the difference makes up to 25 % of absolute efficiency.

4.1. Example of Comparison of Efficiencies in Low Orders

Let us investigate angular dependences of reflection of 316 gr/mm r-2 echelle (facet angle is 63.4°), working from –8 up to –13 orders at both types of polarization and two laser wavelengths: 441.6 nm and 632.8 nm. As from[5] the exact refractive index at wavelength 632.8 nm is known, the comparison for this wavelength represents the special interest.

In Fig.5-6 the results of comparison of angular dependences of efficiencies of chosen echelle in –8, –9 orders, computed in[5] and by the author at the given study are presented, accordingly, in TE and TM polarizations. For TE polarization the maximal spread of the compared data makes 1-2%% of absolute efficiency for –8 order and 3-4%% for –9 order, that approximately corresponds to a total error of similar calculations and extraction of the graphic data. Completely other picture is observed for TM polarization. The difference in the low effective –8 order almost for all values of a curve makes approximately 5% of absolute efficiency. For –9 order it makes almost for all values of a curve value about 25% of absolute efficiency! It is clear, that the so large difference can not be caused by a usual error by numerical realization of the used integral methods, but it is connected with an inaccuracy of prediction of one of them.

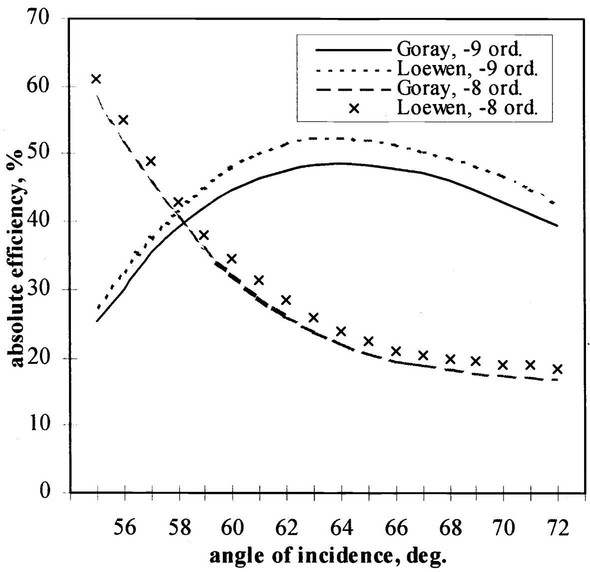

Fig.5. Absolute efficiency in –8 and –9 orders of r-2 316 gr/mm echelle at 632.8 nm & TE plane, as a function of incidence.

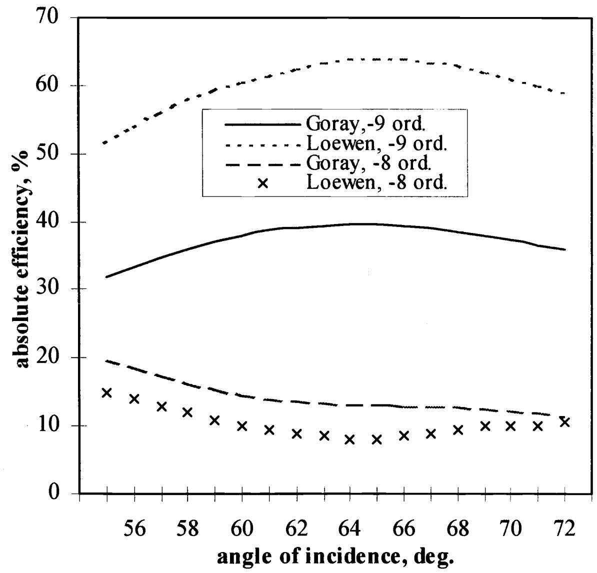

Fig.6. Absolute efficiency in –8 and –9 orders of r-2 316 gr/mm echelle at 632.8 nm & TM plane, as a function of incidence.

For finding out of a situation we will address to experimental data from same paper.[5] In Fig.7-8 the angular dependences of efficiencies of the same grating for, accordingly, two cases of polarization are presented: measured and calculated from[5] and computed by the author for refractive index n = 0.93 + i6.33.[18] The refractive index, chosen by the author, is not necessarily optimum, most appropriate to used technology of evaporation of aluminum films. However, its imaginary part is represented to more realistic for wavelength 632.8 nm, in comparison with an imaginary part of one used in[5] (1.09+i5.31). It proves to be true also by data (1.37+i7.62) from the book E. Palik[19] preferred by the author in many cases.

From comparison of Fig.5, 7 it follows, that the influence change of refractive index on reflection in –8 and –9 orders in TE polarization is insignificant. On the contrary, from Fig.6, 8 it is visible, that rather small (approximately on unit) increase of an imaginary part of refractive index strongly influences value diffraction of efficiency in –9 order for TM polarization. Efficiency in this order found with refractive index from[18] (Fig. 8) is increased approximately by 20% of absolute units in comparison with the data computed by the author for n from[5] (Fig. 6). If one assumes, that approximately on as much the values of TM efficiencies in –9 order at use of refractive index from[18] for an integral method from,[5] will increase (and that they will increase - undoubtedly) that the difference with experiment would make for this method huge value about 35-40%%. That is such calculated values would be more measured one almost in 2 times. Thus the difference from the Fig.8 between the measured results and results obtained with the help of our program for refractive index from,[18] makes on the average about 5%, and it makes about 20% for a method from[5] at use of an improper refractive index.[5] It becomes clear, that rigorous integral method[5] with such value of a error of a prediction, obviously has weak convergence for a case of TM polarization.

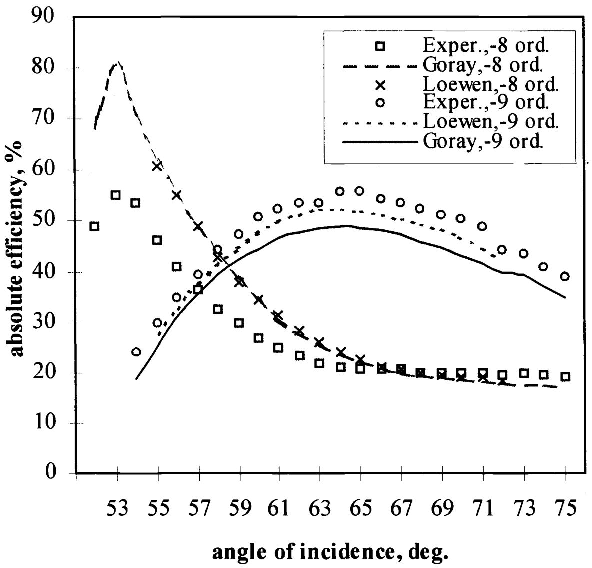

Fig.7. Same as Fig.5, except for Goray's data n=0.93+i6.33.

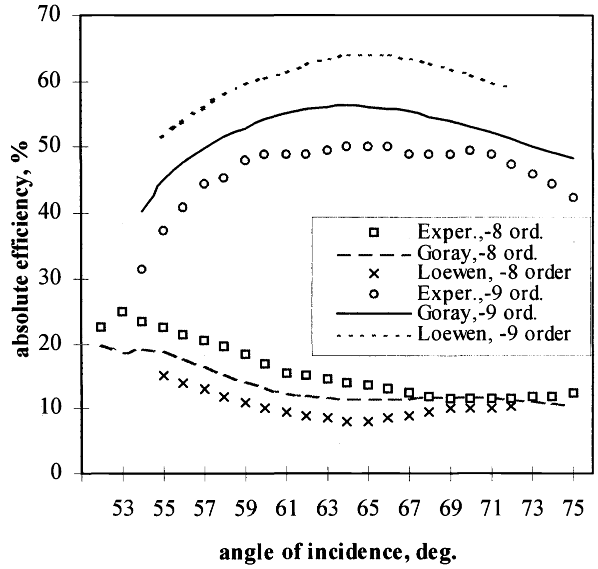

Fig.8. Same as Fig.6, except for Goray's data n=0.93+i6.33.

Not less indicative situation and for the low effective –8 order. For it the increase of an imaginary part of refractive index results in some decrease of values of efficiencies in TM polarization. Thus, as well as in a case with –9 order, difference between experimental data and calculated data in[5] is some times worse, in comparison with the computed here results at any combinations of refractive indecies chosen for comparison. In the conclusion of the analysis of this example we shall note, that the large difference between the measured and computed by both methods data for –8 order in TE polarization in the left part of curves in the Fig.7 is explained, most likely, by difference of a real groove profile from ideal one. Besides the error of measurement (as, however, and calculation) is increased at approach to a mode of disappearance of one of the orders that takes place near to an incidence angle 53° for –9 and +1 orders.

In Fig.9, 10 the results of comparison of efficiency angular dependences in –12 and –13 orders for same echelle are presented at 441.6 nm, obtained in[5] and by the author of the given study, accordingly, in TE and TM polarizations. The refractive index for this wavelength is not given in,[5] therefore the author used an refractive index from[19] (0.59+i5.37). Let's remind,[5] that for dark blue wavelength the influence of refractive index on TM efficiency is weaker, than for red one. For TE polarization the maximal spread of the compared calculated data makes less than 1% of absolute efficiency that speaks about perfect coincidence of results obtained by different methods for this plane of polarization. Excellent coincidence of the theory with experiment for –13 order also is observed in TE polarization. For –12 order in the left part of the diagram in the Fig.9 for TE polarization the excess of theoretical efficiency above experimental values approximately on 10% is observed, that, as well as in the previous example, is explained by difference of a real groove profile from ideal one. For TM polarization in the Fig.10 we again notice the large difference for both orders between numerical results. The difference for all values of a curve in –13 order makes value about 10% of absolute efficiency. For –12 order this difference also is equal 10% of absolute efficiency the left part of a curve and decreases approximately down to 5% in its right part. The comparison of the calculated data obtained by the author with experimental data for TM polarization, speaks about accuracy of this approach. For –13 order the average difference between experimental and numerical values obtained here makes value all in 1%, while this difference in[5] makes about 10%, i.e. it is worse on the order. For –12 order the difference between the measured values and data of the author makes on the average 2%, and by results of paper[5] it makes about 7%, i.e. it is worse in 3.5 times. Let's notice, that the author did not carry out for this work the detailed statistical analysis of comparison of different data in view of obvious discrepancy of approach[5] for TM polarization.

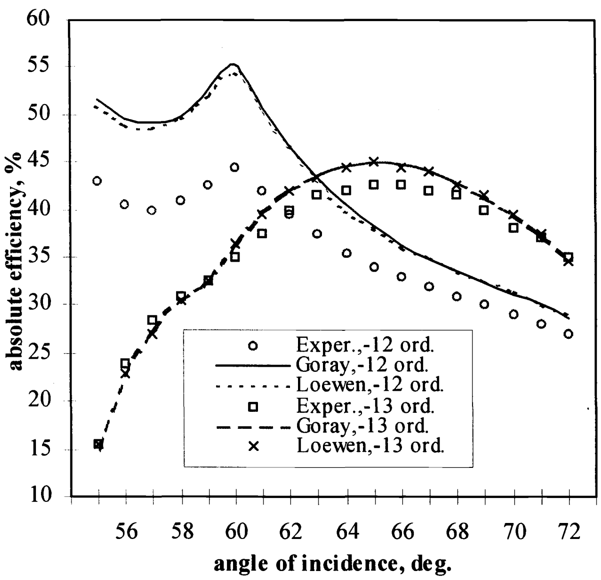

Fig.9. Same as Fig.5, except –12 and –13 orders at 441.6 nm.

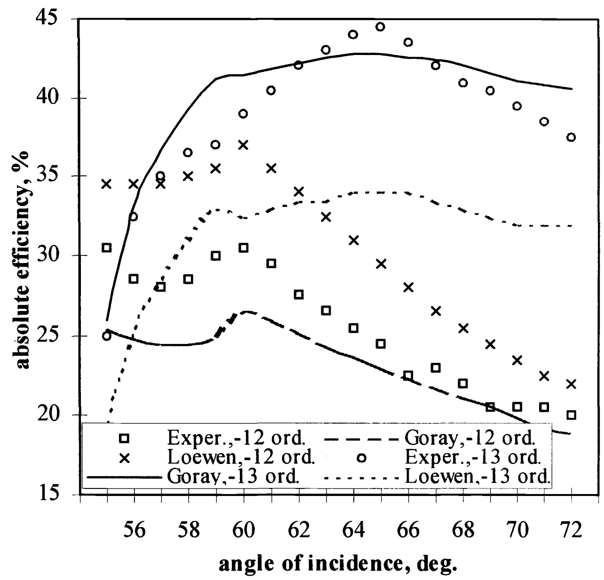

Fig.10. Same as Fig.6, except –12 and –13 orders at 441.6 nm.

4.2. Example of Comparison of Efficiencies in Medium Orders

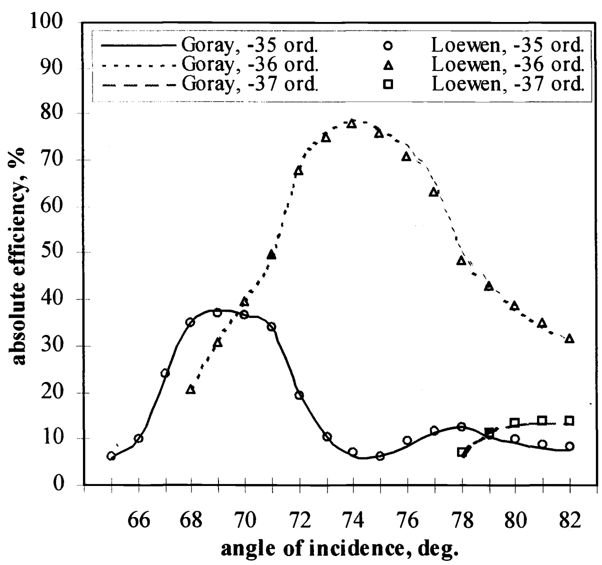

Fig.11. Absolute efficiency in –35, –36, and –37 orders of r-4 79 gr/mm echelle at 676.4 nm & TE plane, as a function of incidence.

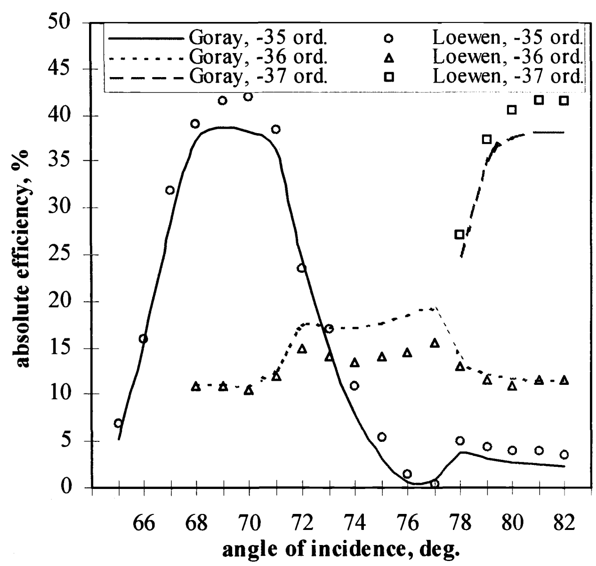

Fig.12. Absolute efficiency in –35, –36, and –37 orders of r-4 79 gr/mm echelle at 676.4 nm & TM plane, as a function of incidence.

As an example of calculations in the medium orders with results a little bit distinguished from[5] we shall study angular dependences of reflection of 79 gr/mm r-4 echelle (facet angle 76°), working in –35, –36, –37 orders at wavelength 676.4 nm. Refractive index n = 1.3 + i7.11 for this wavelength also was taken from.[5]

For TE polarization the values for all orders coincide to within graphic extraction and construction. On the contrary, in TM polarization in the Fig.12 some discrepancy with results of paper[5] is observed for all orders. Efficiencies in a maximum differ approximately on four absolute percents. Let's note also, that the results obtained by the author in the Fig.12, also, as well as in the previous examples, correspond better to experimental dependence from.[5] However, as it is noted in[5] refractive indecies used for calculations for this grating are improper for good coincidence with experiment.

4.3. Example of Comparison of Efficiencies in High Orders

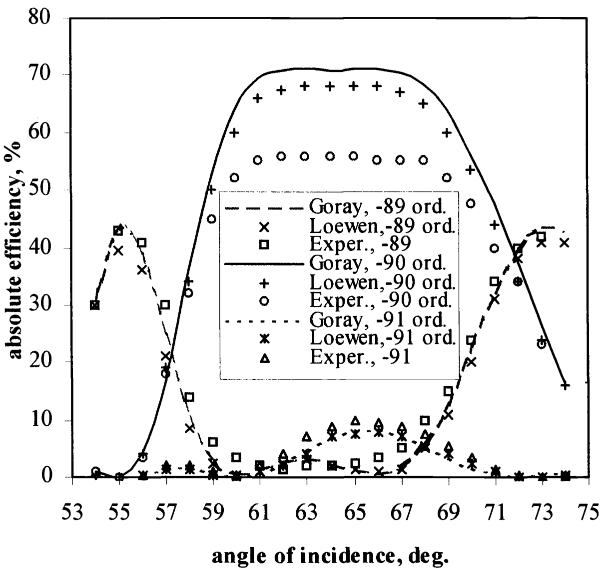

Fig.13. Same as Fig.5, except 31.6 gr/mm and –89, –90, –91 orders.

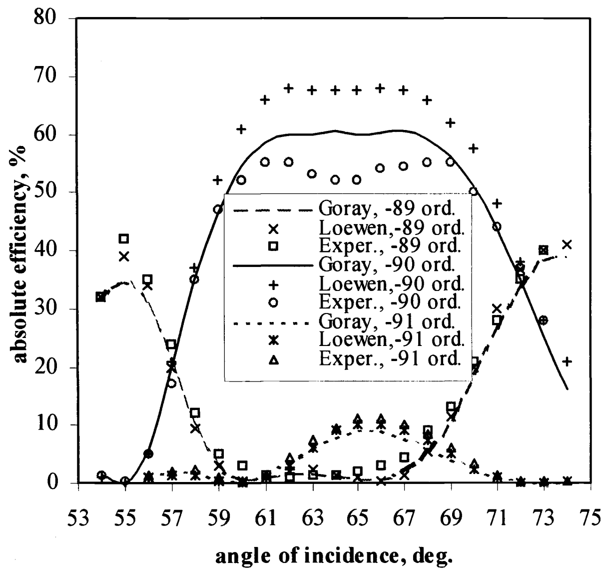

Fig.14. Same as Fig.6, except 31.6 gr/mm and –89, –90, –91 orders.

As an example of calculations of efficiencies in the high orders we shall consider angular dependences of reflection of 31.6 gr/mm r-2 echelle (supposed in[5] facet angle 64.48°), working in –89, –90, –91 orders at wavelength 632.8 nm. The refractive index (n =1.09 + i5.31) for this wavelength was taken from.[5] As well as in the previous examples, the difference in efficiencies for TE polarization does not exceed several percents for theoretical predictions of the author and calculations from.[5] Difference more, than on 10% for –90 order between the measured and calculated data is explained, as before, by non-ideal geometry of a groove of a real grating. For TM polarization, still, there is an appreciable quantitative difference (about 8%) in a maximum of basic –90 order between two rigorous calculations. And difference between experiment and computations of the author for flat top of this order is less in several times than difference with calculations from.[5] Let us note, that executed by the author for this example of calculation with rather small of wavelength-to-period ratios (~0.02) speak about greater difference between TE and TM efficiencies, in comparison with data from.[5]

In the conclusion of this part we shall note, that the compared results, given in it, differ quantitatively for TM polarization from similar one from,[5] especially for the low orders, where the polarizing effects are strong. On the contrary, all compared accounts practically do not differ in a case TE of polarization. Thus, very good qualitative coincidences are achieved for all data for TM of polarization, including fine electromagnetic effects. Carried out by the author detailed comparison with experimental data and deep research of convergence of the method, developed by him, allow to approve, that the method from[5] has insufficiently good convergence in a case of TM polarization. Let's notice also, that the strong dependence of results of account on values of refractive index for TM polarization, is especial in red area, requires an accurate choice of this parameter.

5. EXAMPLES OF CALCULATION OF ECHELLE IN VERY HIGH ORDERS

For examples of calculations in the very high orders there were chosen two largest on today in the world monolithic echelle gratings,[11] which were made under the project NASA Stratospheric Observatory For Infrared Astronomy (SOFIA). One of them was made for NASA-AMES Airborne Infrared Echelle Spectrometer (ARIES),[12] another - for Echelon-cross-echelle Spectrograph (EXES)[13] on the order University of Texas at Austin. These gratings are characterized by the very large periods and blaze angles and are intended for work in the medium and far IR ranges in the orders from 9 up to 2500!

The modeling of efficiencies of various gratings for SOFIA with the help of the programs PCGrate already was successfully carried out by different scientists.[4,12,13,20,21] As these two unique gratings are cut rather recently and the investigations of their characteristics still proceeds, it is rather interesting to study behaviour of diffraction efficiency of so unusual echelle, for example, near to laser wavelength 10.6 μm. The spectral and angular dependences, obtained in this work, further, can be compared with the measured data. In connection with non-standard technology of manufacturing of these gratings and very large periods, there are bases to consider, that for them a blaze angle and form of a profile, in particular apex angle, are executed with good accuracy, that facilitates a theoretical prediction of efficiency. The traditional technology of manufacturing of echelle[1,5] frequently deforms strongly a real groove profile. For an integral method, used in this work, and the algorithms, created on its basis, practically there are no difference what profile is used for an input in the program: ideal or real one. However, till now measurement of a real groove profile of the majority of echelles is difficult scientific and technical task.[1,2,9]

For EXES echelle the record rigorous calculation of efficiency in –1431 order was carried out, namely for TM polarization. Previous record[5] of numerical calculations was established for 660 order for TE polarization, and one managed to exceed it more, than in 2 times.

5.1. Calculation of Efficiency of ARIES Echelle

The largest of monolithic gratings, which was ever cut, is considered to be a 1254 x 1066.8 mm light-weighted aluminum cryogenic-cooled r-4 (with blaze angle 76°) echelle with the period 980.2 μm, made for ARIES.[12] The spectral dependence of efficiency, for example, in autocollimation for the –182 order in the 9.5-10.6 μm range and for the angular range from 61.88° to 79.76° is rather interesting from the point of view of use of this echelle. In Fig.15-16 such dependences to gether with the adjacent orders are presented for TE and TM polarization, accordingly.

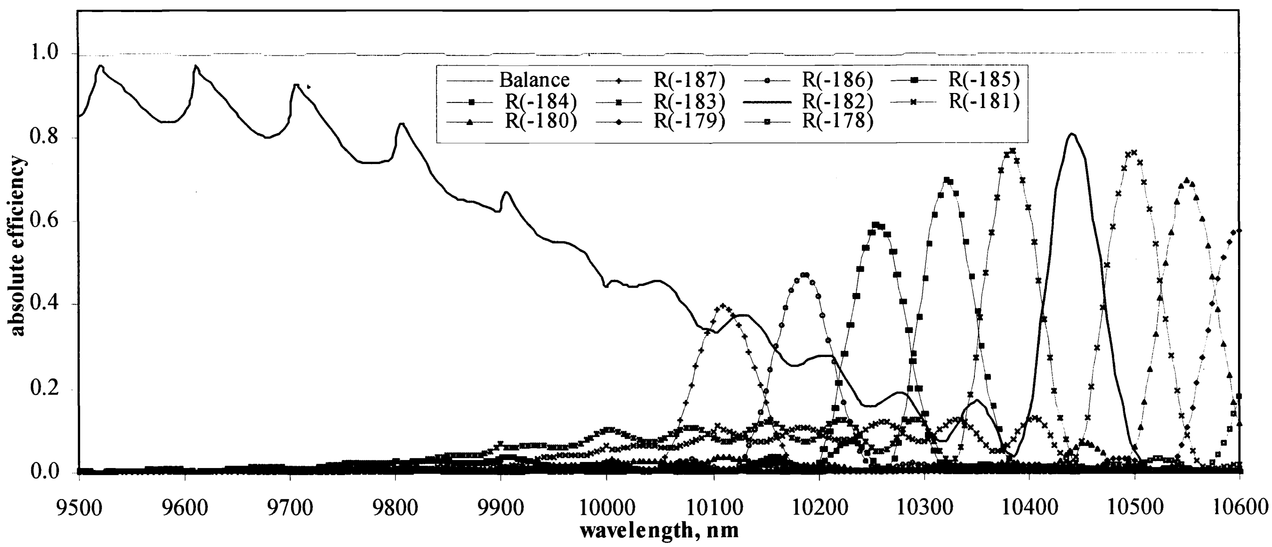

Fig.15. Theoretical TE efficiency of AIRES 1.02 gr/mm r-4 echelle for –182 Littrow and adjacent orders, as a function of wavelength.

In connection with conclusions made in,[11] despite of high conductivity for such wavelengths, previously test was made to compare approximations of ifinite and finite conductivities for several points in both polarizations. As the difference between two approaches in a prediction of efficiency has appeared to be for the working orders less than one relative percent for TM polarization and even less for TE polarization, all further calculations for this grating were carried out in approximation of perfect conductivity. In calculations only 500 points of a collocation were used, and the optimization on parameter P was carried out for TM plane of polarization. Thus the accuracy from total energy balance was in a range 99-101%%. The obtained reflectances for the orders in approximation of infinite conductivity then were multiplied on appropriate Fresnel reflectance. The behaviour of efficiency of this grating near to blaze for autocollimation order corresponds to classical representations about echelle.[1] Efficiency maximum for TE plane of –182 order is located near 10.44 μm and reaches 80% in absolute value approximately. The efficiency maximum for TM plane is located further, near 10.45 μm and reaches about 99%. The rigorous theory allows precisely to predict both positions of maxima, and their values. Besides of the basic mirror peak of efficiency for –182 order, there is one more maximum in both polarizations close 9.60 μm, appropriate to blaze for r-2 echelle (incident angle ~63°), when the grooves work as corner reflectors. Oscillations of efficiency in TE & TM polarizations for autocollimation order to the left of the basic maximum, to be characteristic only for the electromagnetic theory are explained by disappearance of the orders at the appropriate wavelengths and redistribution of energy between stayed orders.

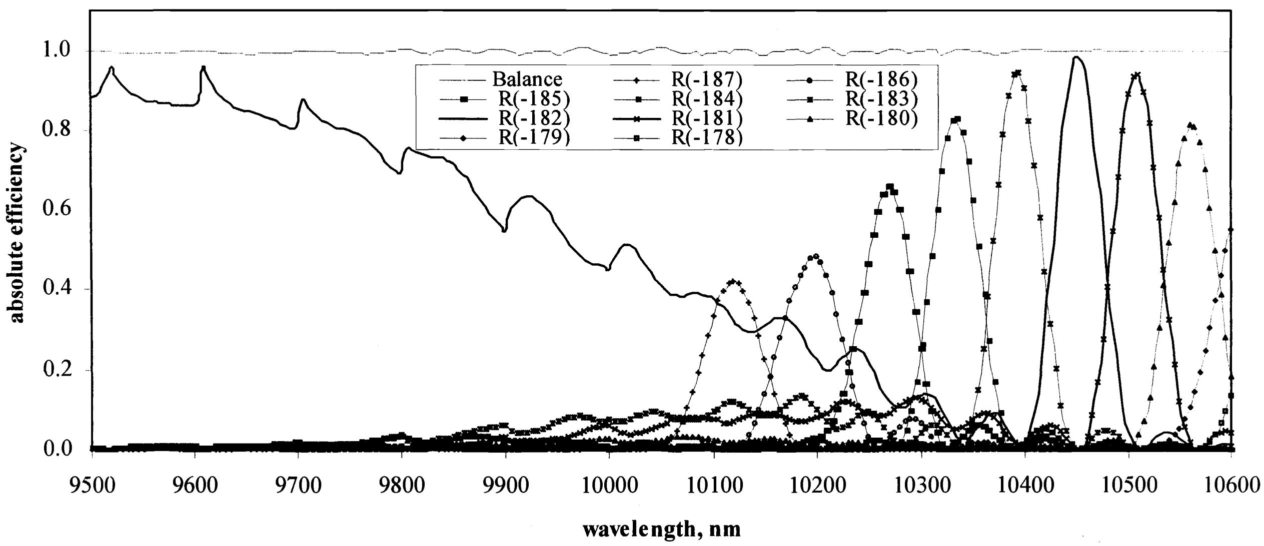

Fig.16. Theoretical TM efficiency of AIRES 1.02 gr/mm r-4 echelle for –182 Littrow and adjacent orders, as a function of wavelength.

5.2. Record Calculation of Efficiency of EXES Echelle

The other huge monolithic grating for SOFIA, which was cut with the period of 7.62 mm and record blaze angle 84.36 (r-10) on the same technology, as grating for ARIES,[11] is a cooled light-weighted aluminum 101.6 x 1016 mm EXES echelle.[13] The working range of this spectrograph is 5.5-28.5 μm and determines use of the very high orders: from 500 up to 2500.

In the Fig.17 the record sample of calculation of absolute efficiency of r-10 EXES echelle for -1431 order is presented at 10.6 μm in TM polarization executed with the help of the commercial program PCGrate™ 2000X,[9] written on programming language C ++. To have an opportunity to carry out regularly similar heavy calculations, the code was essentially improved. The improvements have touched: structures of the program, optimization of compilation, acceleration of the program at the expense of use of its own cash memory for repeating expressions, more exact choice of points of integration, reduction of needed RAM using the subroutine of the solution of the linear equation system with the matrix inversion on a row, improvement of accuracy of the key equations, included in the program, and subroutines. It has allowed rather easily to carry out modeling efficiency of this grating on a PC with the processor Intel™ Pentium III 733 MHz, 256 KB Cash and 128 MB of RAM, working under MS™ Windows NT, v. 4.0. For this example one has to increase the truncation parameter up to 2500-3000 points and to optimize number of factors of expansion of Green's functions and their derivatives because of the very small wavelength-to-period ratio (~0.001) and huge numbers of the propagating orders at grazing incidence. Despite of the so small a wavelength-to-period ratio, the absolute efficiency in a maximum reaches value of about 84.5%. It speaks about impossibility of use of the scalar theory for calculations of efficiency even in such high orders, as it predicts value close to 100%.

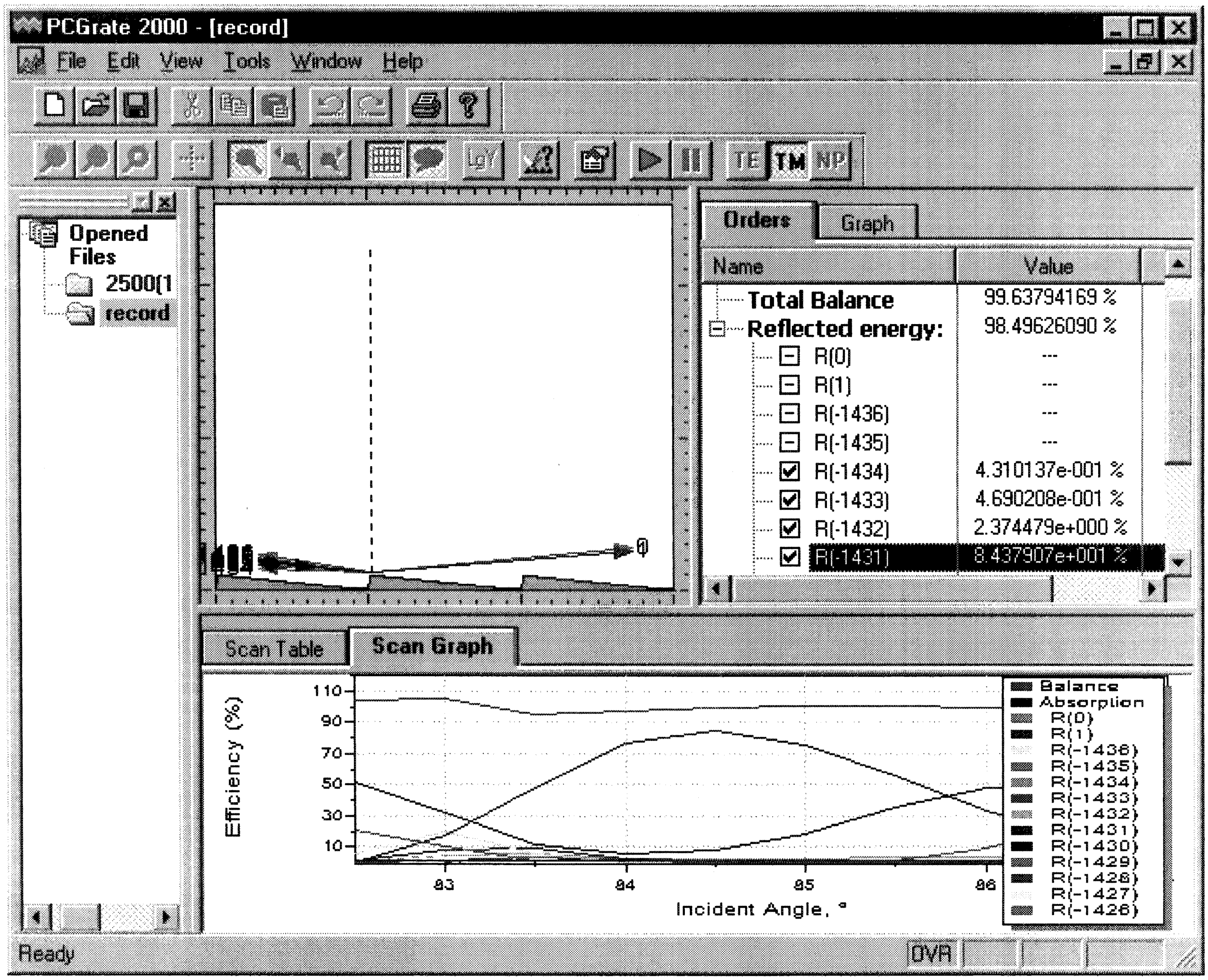

Fig.17. New record of numerical efficiency investigation of EXES 7.62 gr/mm r-10 (84.36° blaze angle) echelle for –1431 order, as a function of incident angle at 10.6 μm in TM polarization.

6. CONCLUSION

In the conclusion it would be desirable in brief to plan directions, on which it is necessary still to work for perfection of a technique of the echelle efficiency analysis, including a real groove profile. The rigorous modified integral method, presented in this work, allows to calculate efficiencies practically for any echelle, including for TM polarization and with a real groove profile, at rather small expenses of computer resources. However, as it was already marked, the rigorous research of echelles properties is one of the most difficult tasks of the electromagnetic theory of diffraction on gratings and still certain work for improvement of convergence of a method and acceleration of the existing programs is required. It is especially urgent for case of multilayer coating, and also for cases of conical diffraction and account of microroughnesses.

Speaking about opportunities of exact coincidence between the measured and calculated data for any echelle gratings, it is necessary to note two main problems: measurement of a real groove profile and correct choice of refractive indecies. First of them, apparently, can be solved with use of standard tools of the analysis, such as atomic-force microscope (AFM) or microinterferometer of high resolution.[2,9] Second can be solved rather easily, for example, by the analysis of the literary data or with the help of computer computations for definition of parameters appropriate to real technology of manufacturing grating.[9] The solution of both tasks on today is represented to be labour-consuming, but real work in view of opportunities of computer modeling. And it, in turn, allows to hope for improvement of existing technology of manufacturing echelle and, probably, even on development of another, more perfect technology. Such opportunities are necessary for taking into account at designing spectral instruments of next generation.

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