RIGOROUS COUPLED WAVE ANALYSIS pdf

1: mrcwa - Multilayer Rigorous Coupled Wave Analysis

Rigorous coupled-wave analysis (RCWA) is a semi-analytical method in computational electromagnetics that is most typically applied to solve scattering from periodic dielectric structures. It is a Fourier-space method so devices and fields are represented as a sum of spatial harmonics.

Gaylord School of Electrical Engineering, Georgia Institute of Technology, Atlanta, Georgia Received July 7,; revised manuscript received February 18, A rigorous coupled-wave approach is used to analyze diffraction by general planar gratings bounded by two differ- ent media. The grating fringes may have any orientation slanted or unslanted with respect to the grating sur- faces. The analysis is based on a state-variables representation and results in a unifying, easily computer-imple- mentable matrix formulation of the general planar-grating diffraction problem. This present rigorous formulation is compared with rigorous modal theory, approximate two-wave modal theory, approximate multiwave coupled-wave theory, and approximate two-wave coupled-wavetheory. Typical errors in the diffraction character- istics introduced by these various approximate theories are evaluated for transmission, slanted, and reflection grat- ings. Inclusion of higher-order waves in a theory is important for obtaining accurate predictions when forward-dif- fracted orders are dominant transmission-grating behavior. Conversely, when backward-diffracted orders domi- nate reflection-grating behavior , second derivatives of the field amplitudes and boundary diffraction need to be included to produce accurate results. Bergstein and Kermisch12 applied the The diffraction of electromagnetic waves by planar gratings modal approach to slanted gratings, but they assumed a has been extensively studied in recent years. These periodic two-wave regime to obtain solutions. Chu and Kong17 have structures have applications in several diverse areas, such as also presented a generalized modal approach formulation for acousto-optics, integrated optics, holography, and spectros- the general slanted-gratings case. However, they did not copy. Several different techniques have been used to analyze present any calculated results for general slanted gratings the diffraction of electromagnetic waves by spatially modu- because the formulation for slanted gratings in the modal lated media. As such they have fraction results for slanted gratings. This paper presents a straightforward precise effect of using the various approximations mentioned rigorous coupled-wave analysis that is easily implemented on above. The effect of neglecting boundary diffraction and a computer. The method of solution is based on a state-space second derivatives of field amplitudes is studied by comparing representation of the governing set of differential equa- the present theory with multiwave coupled-wave theory. The effect of neglecting higher-order waves retaining only The coupled-wave approach has long been known to offer one diffracted wave is analyzed by comparing the present superior physical insight into wave-diffraction phenomena, theory and the two-wave modal theory. In this approach several assumptions typically are present theory with the two-wave coupled-wave theory. The first two of these approximations are lyzes the diffraction of an electromagnetic plane wave incident interconnected and cannot be separated for the case of a obliquely at a planar grating bounded by two different media. The full modal approach is a rigorous exact In general, these gratings simultaneously exhibit both trans- analysis, but solutions have been published only for the un- mission and reflection behavior, as indicated by the for- slanted pure transmission case in which the grating vector is ward-diffracted and backward-diffracted waves shown in Fig. Several authors have at- 1. This analysis is applicable 1 to holographic gratings in tempted to analyze general slanted gratings. For a given value of i, the wave field inside the grating is not a simple plane wave. It may be expressed as a superposition of an infinite number of plane waves inherent K in the coupled-wave formulation. Geometry for planar-grating diffraction. It is consideration is the diffraction of an obliquelyincident plane important to point out that the above analysis is valid for all wave on a lossless pure phase sinusoidal grating with the slant angles p except when the slant angle is identically zero incident wave polarized perpendicular to the plane of inci- pure reflection grating. In this case, the modulation is no dence H mode. Therefore the electric field will have only longer periodic since it has only a finite number of cycles. The di- modulation along its boundaries. It is assumed that each of the calculated. As p approaches zero, all the reflected wave three regions has the permeability of free space. For a more detailed termine the unknown constants resulting from solving the discussion of planar reflection gratings, see Ref. In region 1, backward-diffracted waves exist. These diffraction processes produce To obtain the diffracted amplitudes 9i z , Eqs. Therefore the present analysis is as rigorous and as exact as 16 the modal approach. The In regions 1 and 3, tIi is either positive real propagating wave composite parameters used in Eq. The system of terms of these parameters. Other equivalent sets of param- linear equations given by Eqs. The regime parameter Cm, and then Ri and Ti can be calculated from Eqs. Note that the number of equations available is exactly intermediate diffraction regime. For example, if n waves sents the Bragg condition, i. The parameter K iS the widely used coupling This is because the coefficient matrix [b] in Eq. Alternatively, this may be as viewed as being due to the n coupled-wave equations, each being a second-order differential equation, and thus there are [brs] [IS] 7 2n roots or eigenvalues and 2n unknown constants Cmto be determined from the boundary conditions. Therefore the total number of unknowns is 4n, and Eqs. The quantity [b]is the coefficient To summarize, the algorithm used to solve this problem matrix specified from Eq. Equation 7 corresponds to proceeds as follows: First the coefficient matrix [b] is con- an unforced state equation in the state-space description of structed, and then eigenvalues and eigenvectors are calculated linear systems. The system of differential equations given typically by using a computer library program. The system by Eq. It is Equations 9 and 11 are then used to calculate the diffracted amplitudes Ri and Ti. The coefficients Cm are unknown constants to be de- 1 and 3, respectively. Eliminating Ti and 4. The diffraction efficiencies of the transmitted waves for pure Fig. The diffraction ef- The diffraction efficiencies of all reflected and transmitted waves not ficiencies of all reflected and transmitted waves not shown in the shown in the figure are less than 0. Here and in Figs. The diffraction efficiencies of the transmitted waves for a Fig. These two waves are the only waves that 0. The eigenvalue problem, termine all the unknowns. The main difference between the although not simple, has been extensively studied, and nu- two approaches is in the technique used to find solutions of merous efficient and straightforward computer programs to the wave equation in the modulated region. In the present calculate the eigenvalues and the eigenvectors are available coupled-wave approach, the resulting system of coupled-wave in typical computer-program libraries. The modal approach, equations is formulated into a simple matrix form for which on the other hand, requires that a transcendental relationship M. These analyses are based on solving the half-space grating problem. They do not and cannot, because of the various C. Evaluation of Approximate Approaches 4 The rigorous coupled-wave theory presented in this paper is 0. As such, this analysis is a powerful tool for analyzing the precise effect of using the various assumptions employed in the above approximate methods. It is difficult to quantify 0. However, the trends shown here 0. Figures show, for some typical cases, the 0. These two waves are the only waves that general, these grating structures do not behave simply as propagate in the unmodulated regions. This is most obvious in slanted gratings such as that shown in Fig. A in the form of a continued fraction expansion be solved to find combination of transmission and reflection behaviors is typ- the wavenumbers and their corresponding coefficients that ically present, even though one or the other dominates in each are needed to solve the wave equation in the modulated region. For the slanted grating of Fig. Only for the unslanted, tirely to the inclusion of second derivatives in this rigorous physically symmetric case is the resulting matrix for the modal theory. The corresponding The gratings represented in Figs. The effect of neglecting negative square roots of the eigenvalues. The vector of boundary diffraction and second derivatives of field ampli- coefficients, which is the same for both the positive and neg- tudes is determined by the absolute error that results from ative wave numbers, is the corresponding eigenvector of the using multiwave coupled-wave theory. As is shown in Figs. For slanted gratings the resulting modal-approach 7 and 8, this error is relatively small when forward-diffracted n X n matrix is not in the form of a standard eigenvalue waves are dominant transmission-grating behavior. Therefore the wave numbers occurring in the ma- ever, when backward-diffracted waves are dominant reflec- trix cannot be systematically determined. The effect of neglecting higher-order waves B. Approximate Modal and Coupled-Wave Analyses and thus retaining only one diffracted wave is determined by With the exception of the rigorous modal theory, previous the absolute error that results in using two-wave modal theory. The present In a complementary way to the preceding results, Figs. For example, it reduces to ward-diffracted waves are dominant. This last approximation, which is common in almost portant in the reflection case. Further, these basic conclu- J. Gaylord equal to the larger of the two constituent errors. The errors shown in Figs. For a large 0 ar variety of cases analyzed, it was found in every case that if I 0. As 0 approaches zero, all the forward-diffracted and all the backward-diffracted waves outside the modulated region converge to a single forward and a single backward direction, respectively. The directions of 0. The error associatedwith the total backward-diffracted wave is shown in Fig. In this case, the errors that are due I- 0. For equal grating modulations, higher- 0 C- 0. The combined effect of neglecting both higher-order waves and second derivatives and boundary diffraction is determined by the absolute error 0. From the two-wave cou- pled-wave theory error, it is consistently found that the total Fig. Absolute error in the first-order diffraction efficiency as predicted by a two-wave coupled-wave theory, b multiwave cou- error that is due to neglecting both higher-order waves and pled-wave theory, and c two-wave modal theory for the grating second derivatives and boundary diffraction is approximately conditions shown in Fig. It was shown that in- 11 clusion of higher-order waves is more important than the in- I0 0. Conversely, it was shown that inclusion of second However, it is especially 11 valuable in applications in which slanted gratings and re- 0I 0 0.

2: Rigorous coupled-wave analysis - Wikipedia

A rigorous coupled-wave approach is used to analyze diffraction by general planar gratings bounded by two different media. The grating fringes may have any orientation (slanted or unslanted) with respect to the grating surfaces.

 Abstract We numerically evaluate the optical response of a Kretschmann surface plasmon resonance SPR biosensor featuring metallic nanogratings and patterned immobilization of surface receptors. Parameters are chosen such that the biosensor is operated near the generated bandgap of the surface plasmon dispersion. In this paper, we demonstrate that the sensitivity can be increased by concentrating the surface receptors and adsorbed analytes on regions where the field intensity is the greatest. Specifically, a surface presenting receptors on the grating mesas is shown to be twice as sensitive as that of a uniformly functionalized corrugated surface. The grating geometries are also studied; it is found that higher aspect ratio features show increased SPR response. The analysis differs from existing studies of enhanced SPR as the sensitivity improvement originating from the concentration and mapping of surface receptors to the plasmon field distribution is studied rather than the absorption or scattering enhancement effect of the nanostructures. Introduction Current and future demands for biosensors for use in point-of-care clinical diagnosis require increasingly compact and sensitive devices. Metallic nanogratings are studied owing to their capacity to perturb a propagating surface plasmon wave; it has been shown that these perturbations create strong field gradients and modify the surface plasmon dispersion relation. The development of novel surface functionalization techniques including polymer matrices, self-assembled monolayers, and nanocolloidal particles adds further potential for sensitivity improvements [1 â€” 5]. In a traditional surface plasmon resonance SPR biosensor configuration, known as the Kretschmann or Attenuated Total Reflection ATR configuration, surface plasmon waves are excited on a metallic-dielectric interface via a high refractive index prism [6]. Incident photons, propagating with increased momentum through the prism, are coupled to a surface electron density wave surface plasmon at a specific energy and momentum, collectively referred to as the resonance condition. The coupling of energy is observed as a dip in the reflectance spectrum when measured as a function of incident angle or wavelength of the excitation light. It has been shown that sensitivity of the SPR biosensor can be increased by the modification of the metallic surface with a periodic grating for both propagating and localized surface plasmon. Numerous studies have been presented in which nanoposts, nanowires, and gratings are used for enhancement [7 â€” 14]. Unlike grating-coupled SPR [6] and localized SPR spectroscopy [15 , 16], in the presented configuration, the coupling to the plasmon mode is achieved via a dielectric prism in a traditional setup. As a result of the surface corrugations, the electric field intensity of the propagating surface plasmon is redistributed between the grating mesa and trough. In this article, the focus is not on the surface plasmon enhancement due to the presence of the nanostructures, as previously explored elsewhere. Rather, we seek to determine whether there is a significant increase in sensitivity if the surface receptors are immobilized specifically where the field intensities are at their strongest, thus allowing the detection of lower concentrations of biomolecules than for a uniform distribution. In this context, we assume that the biosensor interface is not saturated with the adsorbed biomolecules, and thus we hypothesize that concentrating the adsorption to regions of field enhancement is advantageous. Furthermore, we will examine the effect of the grating duty factor, the grating height, and the underlying gold thickness on the SPR response for the concentration of adsorbed surface receptors and analytes. Model and Simulation Methods The SPR interface consists of thin layer of gold of thickness on top of which a binary grating of depth and period is introduced Figure 1 a. Surface receptors are immobilized on the gold surface. The biomolecules or analytes of interest are captured by the receptors as the sample solution flows over them. A background refractive index of 1. Four different receptor immobilization patterns are considered. First, the adsorption of a single receptor-analyte complex is modeled. In this case, it is represented by a active element per period Figure 1 b. Then, configurations in which the surface receptors are placed uniformly over the entire grating Figure 1 c , exclusively in the trough Figure 1 d , and exclusively on the mesa Figure 1 e are modeled. The SPR angular resonance shifts are calculated for various index changes of the active medium from 1. A planar surface is also included in the comparison. While this study focuses on the enhancements from the mapped immobilization and not on the effect of the nanostructure, the conventional planar or flat surface serves as a control for the comparison. The simulations were carried out using a proprietary rigorous coupled wave analysis RCWA code. In the literature, RCWA has been extensively employed to study metallic corrugated surfaces, with significant pioneering work by Moharam and colleagues [7 , 10 , 17 â€” 20]. A period of nm and laser wavelength of nm and nm were chosen so that the biosensor operates near and above the bandgap in the dispersion map. It has been demonstrated that, for periodic structures, operating near the bandgap is more sensitive [8]. The optical properties of the metal and substrate were taken from Johnson and Christy [21] and the manufacturer, respectively. Calculations were carried out using harmonics in order to obtain an accuracy of , with 1 nm resolution in the grating depth axis and steps per grating period. Only TM polarization is considered. An initial grating thickness of 25 nm and grating height of 25 nm were chosen. Results and Discussion 3. Field Concentration and Patterned Reception Immobilization Figure 2 shows reflectance as a function of the incident angle for the two different wavelengths nm and nm. An evanescent field scattering off a grating receives a momentum change equal to an integral multiple of the grating vector. Consequently, multiple resonances are observed for nm illumination. The reflectance curve is shallow and broad. Generally, a narrower resonance is preferred for determining the resonance angle precisely, such as the response for nm illumination. Angular reflectance spectrum at nm and nm wavelength. The grating redistributes the field intensity of the propagating surface plasmon wave such that the highest field intensity is found near the grating edge, and with higher field strength on the grating mesa rather than in the trough as shown in Figure 3 a. The SPR response from the adsorption of a single biomolecule complex on the grating surface is simulated. Both the adsorption of the surface receptor active medium index change from 1. The sensitivities for both refractive index changes are similar, suggesting a linear response for the index range. The SPR response or sensitivity, defined as the angular shift of the resonance minimum per refractive index unit RIU change, is calculated at different points along the grating surface. A sensitivity of 0. It peaks at 0. The intensity distribution over the grating surface and consequently the selective sensitivity of the plasmon wave suggest that one can significantly enhance the SPR biosensor by guiding, selectively, the immobilization of surface receptors, such as antibodies for the detection of proteins, or oligonucleotide probes for the detection of DNA, onto the more sensitive area of the grating surface. The grating structure is simulated with the active medium uniformly distributed along the entire grating as in Figure 1 c , concentrated on the mesa Figure 1 d and in the trough Figure 1 e. For a fair comparison, an equal total concentration of biomolecules is assumed over a grating period. In the case of the uniformly distributed surface, this results in a lower surface density. In these simulations, the active medium refractive index is changed from 1. Numerically, the active medium represented as a grid of areas covering the entire mesa, trough, or both. The refractive indices of each area are increased accordingly. On the uniformly or evenly distributed active medium that is equally distributed on the mesas and in trough , only the refractive index of every second area is changed, such that in the three immobilization cases, the effective refractive index changes are the same over the entire grating. The resonance shift for the functionalized mesa is almost twice that of the uniformly covered grating and almost 3 times that of a conventional planar interface, while a small response is measured when the analyte is adsorbed in the trough Figure 4. This gives rise to another possibility for enhancement. By selecting a second excitation laser wavelength or angle for which the field intensities are localized in the trough, as exemplified by Figure 5 for measurement at nm, one could implement a two-analyte detection system or a differential measurement SPR approach. In the former approach, two types of receptors can be immobilized to the different parts of the gratings. The latter case requires that either the mesa or trough is passivated to repel any analyte adsorption. Resonance shift for nm operating wavelength for immobilization on the mesa, trough, or uniform across the grating and also for the flat conventional SPR surface. Field distribution for nm at top incident angle first resonance dip and bottom second resonance dip â€”See Figure 2. Grating Geometry and Duty Factor Effect with Mapped Immobilization The effects of the metallic grating height and the grating duty factor are also examined with the mapped immobilization of surface receptors. The plasmon field distributions are dependent on the features of the metallic gratings. For these simulations, the immobilization of surface receptors is assumed to be exclusively on the grating mesas, where field concentrations are the greatest, at nm wavelength. Furthermore, an equivalent effective refractive index change is assumed in all cases, as to model an equal adsorption of analytes. It assumes that in an actual system the surface and solution concentrations have reached equilibrium, with unsaturated surface receptors. Shown in Figure 6 a , the results point to an increased SPR response for gratings with smaller duty factors. As discussed, increased field concentrations are observed near the grating mesa edges Figure 1 a and thus point toward a greater response when analytes are increasingly concentrated on the mesas. However, in practice the smaller grating mesas are harder to implement given the small feature sizes; furthermore, the smaller effective coverage area reduces the accessibility of the solution analyte to the surface receptors, thus reducing the probability of binding. The optimum duty cycle is thus best determined experimentally. Similar to a planar SPR interface configuration, increasing the underlying metallic film narrows the angular resonance curve. A thin gold underlayer increases the loss of the propagating evanescent wave, reducing its propagation length, resulting in broad resonance responses Figure 6 b. The presence of the surface corrugations, while perturbing the electromagnetic field distribution and allowing for enhanced responses from the mapped immobilization, can be viewed as a change in the surface refractive index. By increasing the grating height, one can observe a shift toward a larger angular resonance response. The sensitivity with respect to an index change localized at the grating mesa increases with the higher aspect ratio features, suggesting a higher field gradient in these cases, as shown in Figure 6 c. A higher sensitivity is generally observed for gratings with deep troughs and a thinner underlying gold layer. For a very thin gold layer , the SPR resonance dips are generally broad, and the sensitivity is only weakly dependent on grating height. For shallow gratings and a thick gold layer, the resonance dips are narrow, much like planar interfaces. However, they show increased sensitivity with an increased grating height. The latter effect points to the advantage of corrugated surfaces in plasmonic biosensing. The effect of the nanograting on the SPR curves can also be measured by the figure of merit. It is defined as the ratio of the sensitivity and the full-width half maximum width of the SPR curves [22]. The figure of merit for the different grating geometries is shown in Figure 7. As one would expect, an increase in the underlying gold layer thickness results in an increased figure of merit due to the narrower SPR responses. As the grating height increases, both the angular sensitivity and width of the SPR curves increase, resulting in a generally constant figure of merit with a peak value at 15â€”30 nm in grating height depending on the gold thickness. Again, in practice, a compromise must be made between the degree of resonance shift and the width of the SPR curves for the measurement setup and fabrication process. Figure of merit for different grating geometries. The grating with 5 and 10 nm underlying gold layer is not included. A number of methods have been reported for the fabrication of nanometric metallic gratings or periodic structures, generally based on a metallic lift-off process of an electron-beam patterned polymeric resist or fast-replication techniques [23]. Features smaller than nm have been demonstrated [24]. Typically, molecules that are known to self-assemble on metallic surfaces alkanethiol are employed [31].

3: CASA - A more Rigorous Coupled-Wave Analysis

1/8/ 1 Lecture 21 Slide 1 EE Computational Electromagnetics Lecture #21 Formulation of Rigorous Coupledâ€•Wave Analysis These notes may contain copyrighted material obtained under fair use rules.

Once this is done, the transmittance T is given by: Although the following description of some preferred embodiments of the invention will make reference to this example for clarity of description, the principles of the invention are broadly applicable to any kind of RCWA analysis. Step is to record a measured spectral reflectance from the sample of interest. Any reflected order can be selected, but it is typically preferred to measure the zero-order reflectance. Step is to define parameters Pl,j for each layer and region, where Ll is the lth layer or region, and j indexes the parameters. The parameters Pl,j are structural parameters of the diffraction grating, and can include any physical or geometrical properties of a grating layer or region that can affect an optical response of the grating. Such parameters include, but are not limited to: Step indicates that each parameter Pl,j can take on values selected from a corresponding set Sl,j. For example, if P3,1 is the thickness of layer 3, and P3,2 is the line width of layer 3, then S3,1 is the set of thicknesses to model for layer 3, and S3,2 is the set of linewidths to model for layer 3. It is helpful to define combined sets Sk, indexed by k, such that each Sk is a set of values for all relevant structural parameters of the grating, and every parameter combination of interest is included as one of the Sk. For example, if a single layer grating has three parameters of interest, thickness, line width, and refractive index, and each parameter can take on any of 10 values, then there would be different sets Sk, each corresponding to one of the possible combinations of parameter values. By calculating a modeled response for each of the Sk, a library of modeled responses can be constructed for use in characterization. As another example, Sk can include two sets differing only by a small change in value of a selected structural parameter. This situation can arise when it is necessary to provide an estimate of the derivative of the optical response with respect to the selected structural parameter. Since many curve fitting procedures require derivative estimates, or converge more rapidly when provided with derivative estimates, such numerical derivative capability is helpful in practice. Wavelength is a representative example of an incident radiation parameter. Other possible incident radiation parameters include frequency which is equivalent to wavelength and angle of incidence. As indicated above, a key aspect of the invention is to vary the incident radiation parameter in the outermost loop of the modeling calculations. In the example of FIG. The main reason it is helpful to vary the wavelength in the outermost loop is that everything in an RCWA calculation depends on the wavelength and other incident radiation parameters e. In contrast to wavelength, changing a structural parameter of the grating does not change everything in an RCWA calculation e. A sequential approach, as in Eqs. Let Ll be the lth layer in the grating structure. Condition indicates that calculations for all parameter value combinations relating to Ll and layers above Ll are performed while holding all parameters for layers below Ll at fixed values. Condition indicates that stored intermediate RCWA results relating to layers below Ll are employed, such that no recalculation relating to layers below Ll are needed when varying the parameters of Ll and layers above Ll. Step is to select a new wavelength and repeat the calculation of at the new wavelength. New wavelengths are selected until the wavelength range of interest is covered. Step is to provide estimates of grating structural parameters based on a best fit of modeled reflectance to measured reflectance. This method is similar to the method of FIG. Step is to record a measured spectral transmittance from the sample of interest. Any transmitted order can be selected, but it is typically preferred to measure the zero-order transmittance. Steps , and are as described in connection with FIG. Condition indicates that calculations for all parameter value combinations relating to Ll and layers below Ll are performed while holding all parameters for layers above Ll at fixed values. Condition indicates that stored intermediate RCWA results relating to layers above Ll are employed, such that no recalculation relating to layers above Ll are needed when varying the parameters of Ll and layers below Ll. Step is to provide estimates of grating structural parameters based on a best fit of modeled transmittance to measured transmittance. Optional step is to cache intermediate results that can be reused e. Whether the cached result is retained in computer memory or externally stored e. Since Q and W are obtained as a result of relatively time consuming eigenvalue decomposition calculations, it is significantly beneficial to cache these results. Note that caching as described here and organizing the calculations as described above are logically distinct. Thus embodiments of the invention can include or not include caching. Similarly, conventional RCWA approaches i. In some cases, the approach of optional steps and is possible, where calculations for all possible thicknesses of Ll are performed while holding all other parameters of Ll at fixed value. Stored intermediate results pertaining to all non-thickness parameters of Ll are employed such that no recalculations relating to parameters other than thickness are required while varying the thickness. In following this approach, it can be helpful to isolate the thickness dependence in the RCWA to the maximum extent. For example, if reflectance is of interest, it is helpful to make the following substitution in Eqs. The resulting equations corresponding to Eqs.

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4: Rigorous coupled-wave analysis of planar-grating diffraction | Jerry Chang - www.enganchecubano.com

Gaylord, "Stable implementation of the rigorous coupled-wave analysis for surface-relief gratings: Enhanced transmittance matrix approach," J.

A device is divided into layers that are each uniform in the z direction. A staircase approximation is needed for curved devices with properties such as dielectric permittivity graded along the z-direction. The electromagnetic modes in each layer are calculated and analytically propagated through the layers. The overall problem is solved by matching boundary conditions at each of the interfaces between the layers using a technique like scattering matrices. With the cutting off of higher order Floquet functions, depending on the accuracy and convergence speed one needs, the infinitely large algebraic equations become finite and thus solvable by computers. Fourier factorization[edit] Being a Fourier-space method it suffers several drawbacks. Gibbs phenomenon is particularly severe for devices with high dielectric contrast. Truncating the number of spatial harmonics can also slow convergence and techniques like fast Fourier factorization FFF should be used. FFF is straightforward to implement for 1D gratings, but the community is still working on a straightforward approach for crossed grating devices. The difficulty with FFF in crossed grating devices is that the field must be decomposed into parallel and perpendicular components at all of the interfaces. This is not a straightforward calculation for arbitrarily shaped devices. Boundary conditions[edit] Boundary conditions must be enforced at the interfaces between all the layers. When many layers are used, this becomes too large to solve simultaneously. Instead, we borrow from network theory and calculate scattering matrices. This lets us solve the boundary conditions one layer at a time. Almost without exception, however, the scattering matrices implemented for RCWA are inefficient and do not follow long standing conventions in terms of how S11, S12, S21, and S22 are defined. ETM, for example, is considerably faster but less memory efficient. Applications[edit] RCWA analysis applied to a polarized broadband reflectometry measurement is used within the semiconductor power device industry as a measurement technique to obtain detailed profile information of periodic trench structures. This technique has been used to provide trench depth and critical dimension CD results comparable to cross-section SEM, while having the added benefit of being both high-throughput and non-destructive. In order to extract critical dimensions of a trench structure depth, CD, and sidewall angle , the measured polarized reflectance data must have a sufficiently large wavelength range and analyzed with a physically valid model for example:

5: S4 - Rigorous Coupled Wave Analysis â€" Solcore documentation

A MATLAB based rigorous coupled-wave analysis (RCWA) tool.. Built with the object-oriented programming of MATLAB, RicWaA provides a friendly user interface facilitating the implementation of RCWA to arbitrary 2D periodic photonic structures.

How to Cite Abstract A variety of light management structures have been introduced in solar cells to improve light harvesting and further boost their conversion efficiency. Reliable and accurate simulation tools are required to design and optimize the individual structures and complete devices. In the first part of this paper, we analyze the performance of rigorous coupled-wave analysis RCWA for accurate three-dimensional optical simulation of solar cells, in particular heterojunction silicon HJ Si solar cells. The structure of HJ Si solar cells consists of thin and thick layers, and additionally, micro- and nano-textures are also introduced to further exploit the potential of light trapping. The RCWA was tested on the front substructure of the solar cell, including the texture, thin passivation and contact layers. Inverted pyramidal textures of different sizes were included in the simulations. The simulations rapidly converge as long as the textures are small in the sub micrometer range , while for larger microscale textures feature sizes of a few micrometers , this is not the case. Small textures were optimized to decrease the reflectance, and consequently, increase the absorption in the active layers of the solar cell. Decreasing the flat parts of the texture was shown to improve performance. For simulations of structures with microtextures, and for simulations of complete HJ Si cells, we propose a coupled modeling approach CMA , where the RCWA is coupled with raytracing and the transfer matrix method. By means of CMA and nanotexture optimization, we show the possible benefits of nanotextures at the front interface of HJ Si solar cells, demonstrating a We additionally demonstrate the ability to simulate a combination of nano- and microtextures at a single interface, although the considered structure did not show an improvement over the pyramidal textures. Such techniques aim to improve the coupling of light into the structure e. The latter is especially important in solar cells where indirect semiconductors such as silicon Si are used as an absorber layer, where the absorption coefficient at the photon energy approaching the value of energy bandgap is small. Nowadays different photonic structures and among them, mostly surface textures of different shapes and sizes are being tested in solar cells in order to exploit their potential to couple and trap light into solar cells []. The use of different techniques for the wet and dry etching of Si wafers [6] in combination with thermal or UV nanoimprint lithography [6,7] has opened new potential for design of nano textures with superior antireflection, light scattering and trapping properties. Besides the optical properties, proper passivation techniques of textured interfaces are crucial to keep surface recombination velocities as low as possible and thus to maintain the good electrical properties of the device [8,9]. The models that enable simulations of thick incoherent and thin coherent layers, including textures of nano-, micro- and several micro-macro meter size, are required. Different modeling techniques have been used in simulations of solar cells [] , and among them, rigorous coupled-wave analysis RCWA has been employed for the optical simulation of thin film or wafer-based solar cells with various textures [2,3,]. However, its applicability, limitations and accuracy in simulation of structures with textures of different types and sizes used in silicon solar cells have not been investigated systematically. In this paper, we report on three-dimensional optical modeling and simulations applied to a representative of Si-wafer-based technology aiming at low cost production and high conversion efficiency, namely, heterojunction silicon HJ Si solar cells [18]. First, we present our optical models and approaches: We proceed with the results of the analysis of the applicability and accuracy of the RCWA method for simulation of different textures in nano- and micrometer size, as applied to the front side of a solar cell structure. The analysis shows that RCWA is an efficient simulation tool for small textures, which is a further verification of the results obtained previously [20]. Additionally, RCWA may have convergence difficulties if systems of equations are large and the layers in the structure have low absorption. After the applicability and accuracy of RCWA have been successfully tested and analyzed, we apply the RCWA method to optimize inverted-pyramid nanotextures on the front side of the HJ Si solar cell to minimize the reflectivity losses. Modeling Rigorous coupled-wave analysis method RCWA, also called the Fourier modal method FMM , has been widely used in simulations of photovoltaic devices [2,3,] , including the structures similar to the ones explored in this paper [3]. It assumes lateral periodicity of the simulated structure. Inside a sublayer, materials with different complex refractive indices are involved in lateral directions x, y. No vertical dependence z of is assumed inside a sublayer, while lateral changes of are considered to be abrupt. This results in a staircase approximation of. While lateral periodicity of the simulated structure is assumed in RCWA, random textures can be simulated by including a sufficient segment of the structure to form a pseudo-periodic simulation domain, where the statistical parameters of the random roughness are still well represented [3]. Spatial 2D discrete Fourier transform of staircase distributions is applied to all N sublayers, obtaining a discrete power spectrum of distribution for each sublayer. These Fourier components are then combined with wavevectors in a matrix describing the propagation of light inside each sublayer separately. The matrix size depends on the number of modes considered. Based on this matrix, complex vectors of the electric and magnetic field, E and H, inside each sublayer can be defined at the end of the calculation. Eigenvectors of the matrix define lateral dependence of E and H, while eigenvalues describe their vertical dependence. Finally, boundary conditions at the interfaces of sublayers are defined considering that tangential components of E and H need to be conserved for conservation of momentum. When solving the system, an S-matrix algorithm is typically used in the RCWA method to couple equations between different sublayers []. Vertical cross-section of a sliced three-layer structure with texture applied to the bottom layer sine texture shown in this example. The different of the layers are indicated by different colors. The structure was in this case sliced to sublayers; a selected one is emphasized by thin dashed horizontal lines. The internal modes of each sublayer are not shown. Vertical cross-section of a sliced three-layer structure with texture applied to the bottom layer Jump to Figure 1 To carry out reliable and accurate simulations of solar cell structures with RCWA, it is of prime importance to study the role of input settings first. In our analysis, we focus on the role of the number of sublayers and the number of modes used in simulations. A higher number of sublayers improves the geometrical description of the structure. The maximum mode number, M, defines where the discrete Fourier spectrum of is cut and at the same time how many diffraction modes directions of light we consider in our calculation some might also be evanescent. A higher number of modes leads to both a better description of the actual light propagation and diffraction, as well as improved structure accuracy distribution by taking more Fourier components. However, it also leads to an increase of the size of the system of equations, so it is desirable to use as low number of modes as possible, while maintaining suitable accuracy of simulations. Furthermore, thin coherent and thick incoherent layers are included. The realization of high efficiency solar cells requires the capability of modeling such optical structures [26]. The results will be published elsewhere, whereby the focus of this paper is firstly a detailed analysis of RCWA simulation applicability and accuracy, and secondly to use RCWA for optimization of the inverted-pyramid nanotexture, and thirdly, integration in CMA and applicability of CMA for simulation of a fully encapsulated silicon heterojunction solar cell. For the combination of RT and TMM we employed the previously developed optical simulator CROWM [13,28,29] , which was previously tested and experimentally verified on different solar cell structures, including thick macrotextured layers RT simulation and thin-film layers TMM simulation. Whereas RCWA is used for detailed description of optical situation in thin nanometer-textured stacks, raytracing and TMM are utilized to define the optical situation in the region of micro- or macrotextured thick or thin layers. The incoherent nature of light in thick layers is assured by the RT algorithm, while coherent RCWA requires wavelength averaging to eliminate interference fringes. Principle of the coupled modeling approach CMA. RCWA is applied to the parts of the structure where nanotextures are present to produce scattering matrices. By applying iterative coupling, the optical situation in the region of nanostructures, microstructures, thin and thick layers can be simulated in an effective and accurate way. RCWA is applied to the parts of the structure whe The intensities are divided into transversal electric TE and transversal magnetic TM polarization components. The RCWA waves can be simply transformed into rays and back, as the phase is not needed when propagating in incoherent parts of the cell. This makes the combination of the methods very suitable to couple, as there is no need for additional transformations, unlike the combinations of raytracing with other methods. However, the phase can also be considered in the presented CMA if, e. One should note that in general, the polarization of a wave with respect to the normal of the interface can change from TE to TM or vice versa. This is unlike in locally flat interfaces considered with ray optics or TMM, where local TE and TM polarization persist after reflection or refraction. This difference in 3D wave simulations is caused by the diffracted waves, which may not propagate in the same plane as the incident wave. Significant errors are produced if polarization changes are not considered properly. In CMA simulation, RCWA results for the assigned sub-structure are calculated in advance for various predefined discrete incident angles. For discretized directions and wavelengths, a scattering matrix of outgoing waves modes is generated â€” an individual scattering matrix is generated per each discretized direction. In comparison of the presented CMA to the OPTOS simulation tool [29] which generates scattering matrices for all layers and stacks them together, we are able to trace rays throughout the structure at their exact angles and positions, which gives us greater versatility in structure we are able to consider. Additionally, similar to the approach of Rothemund et al. The CMA enables simulation of single and multi-junction solar cells and photovoltaic modules, such as perovskite-crystalline silicon tandem solar cells [31] including nano, micro and combined textures. In this paper, we focus only on heterojuction silicon solar cells. CMA simulations were performed for different discretization steps in the polar and azimuth angle to determine the proper input settings for the simulations. Even these parameters lead to approximately 25, RCWA simulations for the complete wavelength range of interest, resulting in a total of approximately three days for a simulation of the complete wavelength spectrum on a desktop PC. The same set of RCWA-generated scattering matrices with given nanotexture was then used for all presented CMA simulations of the given structure, leading to significant timesaving. Schematic representation of the simulated HJ Si solar cell structure including illustration of the front and rear textures. Schematic representation of the simulated HJ Si solar cell structure including illustration of the Jump to Figure 3 The front of the basic solar cell structure consists of transparent conductive oxide e. H layer for electrical passivation, a slightly n-doped crystalline Si c-Si wafer absorber , and an intrinsic and n-doped a-Si: In our model, thin layers follow the applied wafer textures. The complex refractive indices of the layers used as input for optical simulations were taken from the PV Lighthouse database [32] and correspond to measurements of realistic layers [18,]. In our analysis, two types of textures were included and applied to either the front or rear interfaces: We intentionally focus on the two textures that are commonly applied in HJ Si solar cells. The first one can be experimentally realized on the nanometer scale by UV nanoimprint lithography NIL in combination with dry and wet etching of the wafer [6]. The second, the random pyramid texture, is typically used as a microtexture in c-Si solar cells and can be obtained by wet etching with KOH [36]. The corresponding front thin layers are indicated by different colors. Besides these parameters, the pyramid fraction PF is defined as the ratio between the area of the inverted pyramid red square and the area of the unit cell green square and is 0. The depth is dependent on the PF as the pyramid facets are defined by the slow-etching crystallographic plane [6]. A similar approach was also taken in [3]. The micropyramid faces are also defined by the slow-etching crystallographic plane, leading to the same The vertical span of the random micropyramids is 9. The top and cross-sectional views of the simulated partial structures, applied to the front part of the solar cell. The pixilation observable in the thin layers in c is a result of sublayer discretization in RCWA equivalently thick sublayers for the texture are shown. In a , the area of the pyramid is marked with red square, while area of the unit cell is marked with a green square. The PF factor, defined by the ratio of these two areas, is 0. The top and cross-sectional views of the simulated partial structures, applied to the front part of The combination assumes a nanotexture including thin layers superimposed on the random micropyramid texture in the direction normal to the random micropyramids.

6: OSA | Rigorous coupled-wave analysis of planar-grating diffraction

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