Title
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Publication Date
1993-08-20

LBL-34543
UC-410

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UNIVERSITY OF CALIFORNIA

Accelerator & Fusion Research Division

Presented at the Eighth National Conference on Synchrotron Radiation Instruments, Gaithersburg, MD, August 23–26, 1993, and to be published in the Proceedings

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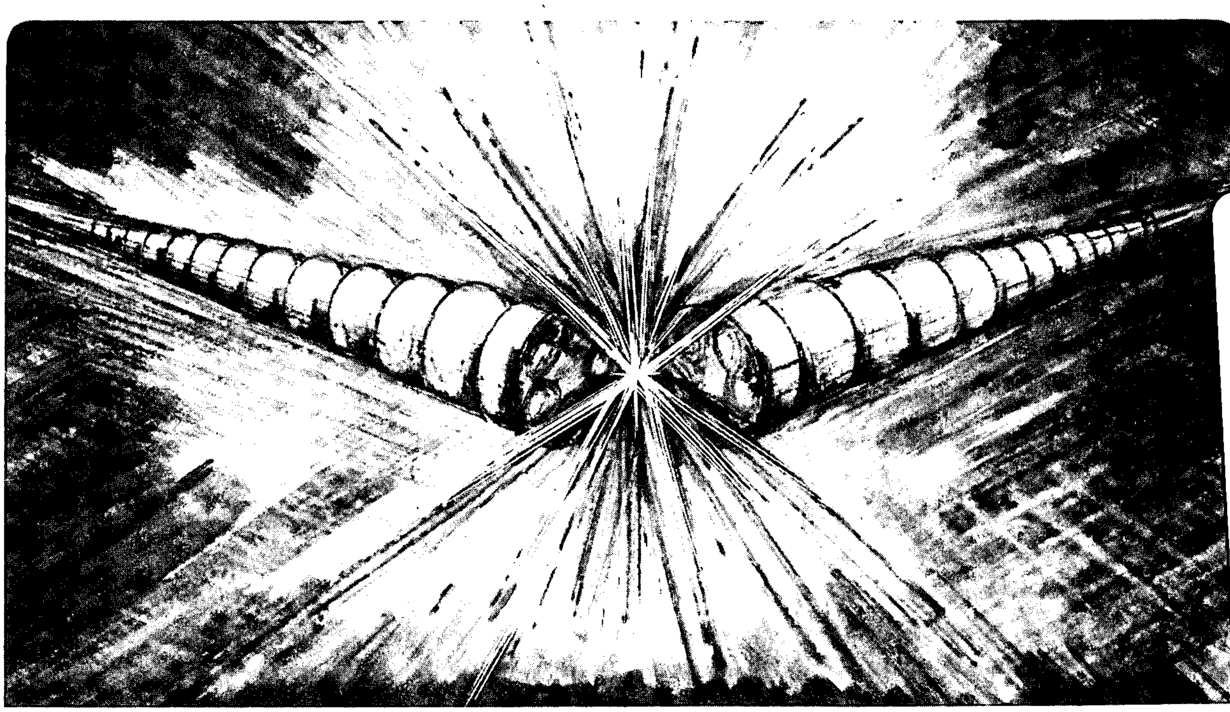

Prepared for the U.S. Department of Energy under Contract Number DE-AC03-76SF00098

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THE DIFFERENTIAL METHOD FOR GRATING EFFICIENCIES IMPLEMENTED IN MATHEMATICA*

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***This work was supported by the Director, Office of Energy Research, Office of Basic Energy Sciences, Materials Sciences Division of the U.S. Department of Energy, under Contract No. DE-AC03-76SF00098.**

The Differential Method For Grating Efficiencies Implemented In Mathematica™

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ABSTRACT

In order to facilitate the accurate calculation of diffraction grating efficiencies in the soft x-ray region, we have implemented the differential method of Nevière and Vincent in Mathematica [1]. This simplifies the programming to maximize the transparency of the theory for the user. We alleviate some of the overhead burden of the Mathematica program by coding the time-consuming numerical integration in C subprograms.

We recall the differential method directly from Maxwell's equations. The pseudo-periodicity of the grating profile and the electromagnetic fields allows us to use their Fourier series expansions to formulate an infinite set of coupled differential equations. A finite subset of the equations are then numerically integrated using the Numerov method for the transverse electric (TE) case and a fourth-order Runge-Kutta algorithm for the transverse magnetic (TM) case.

We have tested our program by comparisons with the scalar theory and with published theoretical results shown in Topics in Current Physics, Vol. 22, chapter 6 for the blazed, sinusoidal and square wave profiles. The Reciprocity Theorem has also been used as a means to verify the method. We have found it to be verified for several cases to within the computational accuracy of the method.

1. THE MATHEMATICAL PROBLEM

We want to calculate the efficiency of a surface whose profile can be described by a periodic function (i.e., a grating) using the expansion of the periodic functions into their Fourier series. Maxwell's equations give us a set of coupled ODEs for the spatial region completely containing the periodic profile. Numerical integration of a finite subset of this set of equations gives us the field amplitudes at $y = a$ (see figure 1).

We make the following assumptions: the incident radiation is a single plane wave with a TE or a TM field; no conical diffraction; the surface is pseudo-periodic (in x) with periodicity d, the grating constant; the grating is of infinite extent in the x directions; the substrate has a known index of refraction; for all y

≤ 0, there exists only the homogeneous substrate; both media are isotropic: the permeability and the permittivity are constants in each medium; both media ($y \leq 0$ and $y \geq a$) have zero net charge; and the permittivity does not vary significantly so we assume it to be a constant equal to that in vacuum, m_o .

2. THEORY

From Maxwell's equations, we find the propagation equation for a TE field is:

$$\nabla^2\mathbf{E} + [i\,\omega\mu_o\,\sigma + \omega^2\mu_o\,\varepsilon]\,\mathbf{E} = 0. \tag{2.0}$$

With $\tilde{\varepsilon}(\mathbf{r}) = \omega^2\mu_o\,[i\,\sigma/\omega + \varepsilon(\mathbf{r})]$, we can write:

$$\nabla^2\mathbf{E}(\mathbf{r}) + \omega^2\mu_o\,\tilde{\varepsilon}(\mathbf{r})\,\mathbf{E}(\mathbf{r}) = 0. \tag{2.1}$$

Similarly, for the a TM field, we have

$$\nabla^2\mathbf{H}\,(\mathbf{r}) + \omega^2\mu_o\,\tilde{\varepsilon}\,(\mathbf{r})\,\mathbf{H}(\mathbf{r}) = 0. \tag{2.2}$$

Let $\mathbf{U}(\mathbf{r}) = \mathbf{E}(\mathbf{r})$ for the TE case and $\mathbf{U}(\mathbf{r}) = \mathbf{H}(\mathbf{r})$ for the TM case. In each case, we work with the field polarized parallel to the z axis (and the grooves). Since the field amplitude is not a function of z but is parallel to $\hat{\mathbf{z}}$, $\mathbf{U}(\mathbf{r}) = U(x, y)\,\hat{\mathbf{z}}$.

The permeability varies only with medium, therefore $\tilde{\varepsilon}(\mathbf{r})$ becomes $\tilde{\varepsilon}(x, y)$. Relating the wave number k, the permeability e, and the (complex) index of refraction $\tilde{n}$, we write:

$$k^2(x, y) = \omega^2\,\mu_o\,\tilde{\varepsilon}_1 = k_1{}^2 \quad \text{if } y > g(x, y) \text{ (in vacuum)}$$

$$k^2(x, y) = \omega^2\,\mu_o\,\tilde{\varepsilon}_2 = k_2{}^2 = \tilde{n}^2\,k_1{}^2 \qquad \text{if } y < g(x, y) \text{ (in the substrate)} \tag{2.3}$$

where $g(x, y)$ describes the interface between the media. With these results, we can write the propagation equation for both cases as:

$$\nabla^2\,U(x, y) + k^2(x, y)\;U(x, y) = 0. \tag{2.4}$$

3. CONTINUOUS QUANTITIES ACROSS THE BOUNDARY

Continuity is crucial in order to match the solutions at the boundaries. Regardless of the polarization, the fields **E** and **H** are continuous across the boundary between the media.

For the TE case, the derivatives of the electric field are continuous across the boundary. In the TM case, the derivative of the magnetic vector is not continuous across the boundary because of the change in the permeability with the change in medium; however, $\dfrac{1}{\tilde{\varepsilon}(\mathbf{r})}\dfrac{\partial\mathbf{H}(\mathbf{r})}{\partial\hat{n}}$ is continuous across the boundary, $\hat{\mathbf{n}}$ being the unit normal to the boundary $g(x, y)$. We will use this quantity to determine the valid propagation equation in $[0, a]$ for the TM case.

4. THE PROPAGATION EQUATIONS

For each region in the TE case, we have:

$$\text{For } y \le 0: \ \nabla^2 E(x, y) + k_2^2 \ E(x, y) = 0 \tag{4.0}$$

$$\text{For } 0 < y < a: \ \nabla^2 E(x, y) + k^2 (x, y) E(x, y) = 0 \tag{4.1}$$

$$\text{For } y \ge a: \ \nabla^2 E(x, y) + k_1^2 \ E(x, y) = 0 \tag{4.2}$$

For each region in the TM case, we have:

$$\text{For } y \le 0: \ \nabla^2 H(x, y) + k_2^2 \ H(x, y) = 0 \tag{4.3}$$

$$\text{For } 0 < y < a: \ \nabla \cdot \{(k^2(x, y))^{-1} \text{grad } H(x, y)\} + H(x, y) = 0 \tag{4.4}$$

$$\text{For } y \ge a: \ \nabla^2 H(x, y) + k_1^2 \ H(x, y) = 0. \tag{4.5}$$

5. THE FOURIER SERIES FOR THE FIELDS

The incident radiation (of unit amplitude) may be described by $U(x, y) = \exp[i\, \mathbf{k_1}.\mathbf{r}]$. If this radiation propogates isotropically with incidence angle θ (measured counterclockwise from the +y axis), then $\mathbf{k_1} = k_1 \sin\theta\, \hat{\mathbf{i}} - k_1 \cos\theta\, \hat{\mathbf{j}}$ and thus $U(x, y) = \exp[i\, \alpha_o\, x - i\, \beta_{1o}\, y]$, where $a_o = k_1 \sin\theta$ and $b_{1o} = k_1 \cos\theta$ To account for the radiation from reflection at y = a, each diffracted order n has an associated plane wave given by

$$U_n (x, y) = A_n \exp[i\, k_1 \ (x \sin \theta_n + y \cos \theta_n)] , \tag{5.0}$$

where θ_n is the diffraction angle and A_n is the field amplitude for the n-th order. Using the grating equation to find θ_n, $n\, l / d = \sin\theta_n - \sin\theta$, (with $k_1 = 2\pi / l$ and $K = 2\pi / d$), equation (5.0) becomes:

$$U_n(x, y) = A_n \exp[i\, k_1 \sin \theta_n\, x + i\, k_1 \cos \theta_n\, y)] = A_n \exp[i\, \alpha_n\, x + i\, \beta_{1n}\, y]. \tag{5.1}$$

In general, there are numerous diffracted orders so the total field can be expressed as the sum of plane waves in all possible orders. Including all possible orders, and setting $A_n = 0$ for nonexistent orders, the total field can be described by:

$$U(x, y) = \sum_{n=-\infty}^{\infty} A_n \exp[i\, \alpha_n\, x + i\, \beta_{1n}\, y] = \sum_{n=-\infty}^{\infty} U_n(y) \exp[\, i\, \alpha_n\, x], \quad y \ge a, \tag{5.2}$$

which is a Fourier series with basis vectors being $\{\exp[i\, \alpha_n\, x]\}$.

6. SOLVING THE PROPAGATION EQUATION FOR y > a AND y < 0

For $y > a$, $\quad \nabla^2 U(x, y) + k_1^2\, U(x, y) = 0 \Rightarrow$

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) \sum_{n=-\infty}^{\infty} U_n(y) \exp[\, i\, \alpha_n\, x\,] + k_1^2 \sum_{n=-\infty}^{\infty} U_n(y) \exp[\, i\, \alpha_n\, x\,] = 0 \Rightarrow$$

$$\sum_{n=-\infty}^{\infty} \{\frac{\partial^2 U_n(y)}{\partial y^2} - \alpha_n^2 U_n(y) + k_1^2 U_n(y)\} \exp[i \alpha_n x] = 0 ,$$

$$\forall n, \quad \frac{\partial^2 U_n(y)}{\partial y^2} + [k_1^2 - \alpha_n^2] U_n(y) = 0. \text{ Letting } \beta_{1n}^2 = [k_1^2 - \alpha_n^2] ,$$

$$\forall n, \quad \frac{\partial^2 U_n(y)}{\partial y^2} + \beta_{1n}^2 E_n(y) = 0. \text{ The solution is:}$$

$$U_n(y) = A_n^{(1)} \exp(- i \beta_{1n} y) + B_n^{(1)} \exp(i \beta_{1n} y) \tag{6.0}$$

$$U(x, y) = \sum_{n=-\infty}^{\infty} \{A_n^{(1)} \exp(- i \beta_{1n} y) + B_n^{(1)} \exp(i \beta_{1n} y)\} \exp[i \alpha_n x], \quad y > a. \tag{6.1}$$

For $y < 0$, the solution is analogous to that for $y \geq a$, except that $k = k_2$ and $\beta_{2n}^2 = [k_2^2 - \alpha_n^2]$:

$$U_n (y) = A_n^{(2)} \exp(- i \beta_{2n} y) + B_n^{(2)} \exp(i \beta_{2n} y). \tag{6.2}$$

Since we are assuming medium 2 extends homogeneously to $y = -\infty$, there are no other discontinuities for $y < 0$ that would cause reflections, so $B_n^{(2)} = 0$ and the field is given by:

$$U(x, y) = \sum_{n=-\infty}^{\infty} A_n^{(2)} \exp(- i \beta_{2n} y) \exp[i \alpha_n x], \quad y < 0. \tag{6.3}$$

7. THE TE CASE: $0 \leq y \leq a$

For $0 \leq y \leq a$, $\nabla^2 E(x, y) + k^2(x, y) E(x, y) = 0 \Rightarrow$

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) \sum_{n=-\infty}^{\infty} E_n(y) \exp[i \alpha_n x] + k^2(x, y) \sum_{m=-\infty}^{\infty} E_m(y) \exp[i \alpha_m x] = 0. \tag{7.0}$$

Because $k^2(x, y)$ is pseudo-periodic (with periodicity d),with $K = 2\pi / d$, we can write:

$$k^2(x, y) = \sum_{n=-\infty}^{\infty} k^2{}_n (y) \exp[i\, n\, 2\pi x / d] = \sum_{n=-\infty}^{\infty} k^2{}_n (y) \exp[i\, n\, K x] \text{ and (7.0) becomes:}$$

$$\sum_{n=-\infty}^{\infty} (\{\frac{\partial^2 E_n(y)}{\partial y^2} - \alpha_n^2 E_n(y)\} \exp[i \alpha_n x] + k^2{}_n(y) \exp[inKx] \sum_{m=-\infty}^{\infty} E_m(y) \exp[i(\alpha_0 + mK)x]) = 0$$

Doing a change of index from n to (n-m) to combine the product of the infinite sums $\Rightarrow$

$$\sum_{n=-\infty}^{\infty} \Big(\{ \frac{\partial^2 E_n(y)}{\partial y^2} - \alpha_n^2 E_n(y)\} \exp[i \alpha_n x]$$

$$+ \sum_{m=-\infty}^{\infty} k^2{}_{n-m}(y) E_m(y) \exp[i(n-m)K x] \exp[i (\alpha_0 + mK) x]\Big) = 0 \Rightarrow$$

$$\sum_{n=-\infty}^{\infty} \Big(\{\frac{\partial^2 E_n(y)}{\partial y^2} - \alpha_n^2 E_n(y)\} \exp[i\alpha_n x] + \sum_{m=-\infty}^{\infty} k^2{}_{n-m}(y) E_m(y) \exp[i(\alpha_0 + mK + nK - mK)x]\Big) = 0$$

$$\sum_{n=-\infty}^{\infty} \Big(\frac{\partial^2 E_n(y)}{\partial y^2} - \alpha_n^2 E_n(y) + \sum_{m=-\infty}^{\infty} k^2{}_{n-m}(y) E_m(y) \Big) \exp[i\alpha_n x] = 0$$

$$\frac{\partial^2 E_n(y)}{\partial y^2} = \alpha_n^2 E_n(y) - \sum_{m=-\infty}^{\infty} k^2{}_{n-m}(y)\, E_m(y) = 0, \ \forall\, n \tag{7.1}$$

We want to solve for $A_n^{(1)}$ and $B_n^{(1)}$, the amplitudes of the field at y = a (see (5.2)). Numerical integration of (7.1) yields $E_n(y{=}a)$, where the boundary conditions to start off the integration at y = 0 come from the solutions to the propagation equation for y < 0:

$E_n(y) = A_n^{(2)} \exp(-i\,\beta_{2n}\, y) \quad \Rightarrow \quad E_n(0) = A_n^{(2)}$ and

$dE_n(y)/dy = -i\,\beta_{2n}\, A_n^{(2)} \exp(-i\,\beta_{2n}\, y) \quad \Rightarrow \quad dE_n(0)/dy = -i\,\beta_{2n}\, A_n^{(2)}$, see (6.2).

The continuity of the electric field and its first derivative across the discontinuity of the boundary provide us with two equations for the two unknowns $A_n^{(1)}$ and $B_n^{(1)}$ (see §9).

8. THE TM CASE: $0 \leq y \leq a$

For $0 \leq y \leq a$, $\quad \mathrm{div}\{\frac{1}{k^2(x, y)} \mathrm{grad}\, H(x, y)\} + H(x, y) = 0 \Rightarrow$

$$\frac{\partial}{\partial x}\left(\frac{1}{k^2}\frac{\partial H(x, y)}{\partial x}\right) + \frac{\partial}{\partial y}\left(\frac{1}{k^2}\frac{\partial H(x, y)}{\partial y}\right) + H(x, y) = 0. \tag{8.0}$$

To match the solutions at the boundaries, we work with the continuous quantities in (8.0). Let $\widetilde{E} \equiv \frac{1}{k^2}\frac{\partial H(x, y)}{\partial y}$, where

$$\nabla \times H(x, y)\,\hat{z} = [s - i\, w\, e(\mathbf{r})]\, \mathbf{E}(\mathbf{r}) \Rightarrow \frac{1}{k^2}\frac{\partial H(x, y)}{\partial y} = \frac{1}{i\,\omega\,\mu_o} \mathbf{E}(\mathbf{r}).\hat{\mathbf{i}} = \frac{1}{i\,\omega\,\mu_o} E_x \tag{8.1}$$

Substituting $\widetilde{E}$ in to (8.0),

$$\frac{\partial H(x, y)}{\partial y} = k^2\, \widetilde{E} \tag{8.2}$$

$$\text{and} \quad \frac{\partial \widetilde{E}}{\partial y} = -\frac{\partial}{\partial x}\left(\frac{1}{k^2}\frac{\partial H(x, y)}{\partial x}\right) - H(x, y) \tag{8.3}$$

We can write a Fourier series for our new function $\widetilde{E}$ because it is related to **E** by a constant quantity. The Fourier series expansions for the fields and the wave number are:

$$\widetilde{E}(x, y) = \sum_{n=-\infty}^{\infty} \widetilde{E}_n(y) \exp[\, i\, \alpha_n\, x\,], \quad H(x, y) = \sum_{n=-\infty}^{\infty} H_n(y) \exp[\, i\, \alpha_n\, x]$$

$$k^2(x, y) = \sum_{n=-\infty}^{\infty} k^2{}_n\,(y) \exp[inKx] \quad \text{and} \quad \frac{1}{k^2(x, y)} = \sum_{n=-\infty}^{\infty} \left(\frac{1}{k^2(y)}\right)_n \exp[i\, n\, K\, x] .$$

Inserting the appropriate expansions into (8.2), we have:

$$\frac{\partial}{\partial y}\sum_{n=-\infty}^{\infty} H_n(y) \exp[i\, \alpha_n\, x] = \left(\sum_{n=-\infty}^{\infty} k_n^2(y) \exp[i\, \alpha_n\, x]\right)\left(\sum_{m=-\infty}^{m} \widetilde{E}_m(y) \exp[i\, \alpha_m\, x]\right)$$

A change of index from m to (n-m) to combine the product of the infinite sums gives us:

$$\sum_{n=-\infty}^{\infty} \frac{\partial H_n(y)}{\partial y} \exp[i\,\alpha_n\,x] = \sum_{n=-\infty}^{\infty} \sum_{m=-\infty}^{\infty} k^2_{n-m}(y)\,\widetilde{E}_m(y)\exp[i\,(\alpha_{n-m}+\alpha_m)\,x]$$

$$\text{where } \alpha_{n-m}+\alpha_m = \alpha_o + (n-m)K + \alpha_o + m\,K = \alpha_o + n\,K = \alpha_n\,,$$

$$\frac{\partial H_n(y)}{\partial y} = \sum_{m=-\infty}^{\infty} k^2_{n-m}(y)\,\widetilde{E}_m(y),\ \forall n. \tag{8.4}$$

Inserting the appropriate expansions into (8.3), we have:

$$\frac{\partial}{\partial y}\sum_{n=-\infty}^{\infty} \widetilde{E}_n(y)\exp[i\,\alpha_n\,x] =$$

$$-\frac{\partial}{\partial x}\left(\sum_{n=-\infty}^{\infty}\left(\frac{1}{k^2(y)}\right)_n \exp[i\,n\,K\,x]\frac{\partial}{\partial x}\left(\sum_{m=-\infty}^{\infty} H_m(y)\exp[i\,\alpha_m\,x]\right)\right) - \sum_{n=-\infty}^{\infty} H_n(y)\exp[i\,\alpha_n\,x]$$

$$\sum_{n=-\infty}^{\infty}\left(\frac{\partial \widetilde{E}_n(y)}{\partial y} + H_n(y)\right)\exp[i\,\alpha_n\,x] = -\frac{\partial}{\partial x}\left(\sum_{n=-\infty}^{\infty}\left(\frac{1}{k^2(y)}\right)_n \exp[i\,n\,K\,x]\left(\sum_{m=-\infty}^{\infty} i\,\alpha_m\,H_m(y)\exp[i\,\alpha_m\,x]\right)\right)$$

Differentiation and a change of index from n to (n-m) on the product of the infinite sums yields:

$$\sum_{n=-\infty}^{\infty}\left(\frac{\partial \widetilde{E}_n(y)}{\partial y} + H_n(y)\right)\exp[i\,\alpha_n\,x] = -\left(\sum_{n=-\infty}^{\infty}\sum_{m=-\infty}^{\infty} \alpha_m^2\left(\frac{1}{k^2(y)}\right)_{n-m} H_m(y)\exp[i\,\alpha_n\,x]\right),$$

$$\frac{\partial \widetilde{E}_n(y)}{\partial y} = -\sum_{m=-\infty}^{\infty} \alpha_m^2\left(\frac{1}{k^2(y)}\right)_{n-m} H_m(y) - H_n(y),\ \forall n \tag{8.5}$$

Numerical integration of (8.4) and (8.5) yields $H_n(y{=}a)$; §9 shows us how to solve for $A_n^{(1)}$ and $B_n^{(1)}$. The boundary conditions to start off the integration at y = 0 come from the solutions to the propagation equation for y < 0 (see (6.3)):

$$H(y=0) = A_n^{(2)} \text{ and } \widetilde{E}(y=0) = \frac{1}{k_2^2}\frac{\partial H_n(0)}{\partial y} = -\,i\,b_{2n}\,A_n^{(2)}\,/\,k^2{}_2 \tag{8.6}$$

$$\text{where } \widetilde{E}(y=0) \text{ in (8.2) gives us } \frac{\partial H_n(0)}{\partial y}.$$

9. MATCHING SOLUTIONS

The numerical integration yields $U_n(a)$. Matching this with the solution for y > a:

$$U_n(a) = A_n^{(1)}\exp(-\,i\,\beta_{1n}\,a) + B_n^{(1)}\exp(i\,\beta_{1n}\,a) \tag{9.0}$$

$$dU_n(a)/dy = -\,i\,\beta_{1n}\,A_n^{(1)}\exp(-\,i\,\beta_{1n}\,a) + i\,\beta_{1n}\,B_n^{(1)}\exp(i\,\beta_{1n}a) \tag{9.1}$$

Then solving these for $A_n^{(1)}$ and $B_n^{(1)}$:

$$A_n^{(1)} = \frac{1}{2}[U_n(a) + \{1/i\ \beta_{1n}\}\ dU_n((a)/dy\ ]\ \exp(-\ i\ \beta_{1n}\ a\ ) \tag{9.2}$$

$$B_n^{(1)} = \frac{1}{2}[U_n(a) - \{1/i\ \beta_{1n}\}\ dU_n(a)/dy\ ]\ \exp(\ i\ \beta_{1n}\ a\ ) \tag{9.3}$$

10. THE LINEAR ALGEBRA PROBLEM

We have assumed that the $A_n^{(2)}$, the transmitted field amplitudes, are known. We have ignored the fact that we have an infinite set of coupled ordinary differential equations. We truncate the sum to $\pm N$. We now have a finite basis (and sum) with dimension 2N+1; we choose a set of basis vectors, $\{\exp[i\ \alpha_n\ x]\}$, that completely spans our finite space. Each basis vector corresponds to a unique diffraction order. Once we find how this basis transforms under transmission and reflection, we can generate a matrix that will tell us how any vector in that space will be transformed.

Define the following column vectors: the n-th element is the n-th order field amplitude:

$\Psi_A^{(1)}$ (incoming plane waves) = $\{A_{-N}^{(1)}, A_{(-N+1)}^{(1)}, \ldots, A_0^{(1)}, \ldots, A_N^{(1)}\}$

$\Psi_B^{(1)}$ (diffracted plane waves) = $\{B_{-N}^{(1)}, B_{-(N+1)}^{(1)}, \ldots, B_0^{(1)}, \ldots, B_N^{(1)}\}$

$\Psi_A^{(2)}$ (transmitted plane waves) = $\{A_{-N}^{(2)}, A_{(N+1)}^{(2)}, \ldots, A_0^{(2)}, \ldots, A_N^{(2)}\}$

Our basis vectors are: $\{\Psi(j)_A^{(2)} = \{\delta_{-N,j}, \delta_{(N+1),j}, \ldots, \delta_{0,j}, \ldots, \delta_{N-1,j}, \delta_{N,j}\}: j \in [-N, N]\}$.

See figure 2 for Nevière illustration of the problem. Define the square transformation matrices M_A and M_B with (2N+1) rows and columns as follows:

$$\Psi_A^{(1)} = M_A \cdot \Psi_A^{(2)}$$

$$\Psi_B^{(1)} = M_B \cdot \Psi_A^{(2)}$$

There exists some matrix R such that $\Psi_B^{(1)} = R\ \Psi_A^{(1)}$

$R\ \Psi_A^{(1)} = R\ M_A\ \Psi_A^{(2)} \Rightarrow M_B\ \Psi_A^{(2)} = R\ M_A\ \Psi_A^{(2)} \Rightarrow R = M_B\ (M_A)^{-1}$

For the transmission matrix, T: $\Psi_A^{(2)} = (M_A)^{-1}\Psi_A^{(1)} \Rightarrow T = (M_A)^{-1}$

The columns of M_A are $\Psi_A^{(1)}$, the incoming images of the $\Psi(j)_A^{(2)}$. The columns of M_B are $\Psi_B^{(1)}$, the outgoing images of the $\Psi(j)_A^{(2)}$, where j ranges from -N to +N.

11. THE CALCULATION OF THE GRATING EFFICIENCIES

The diffraction efficiency of the surface is the ratio of the reflected energy to the incident energy. We begin with the average of the Poynting vector [2] for time-harmonic radiation, denoted by $\langle\overline{S}\rangle$. Let i denote incident radiation and r denote reflected radiation.

$$\langle\overline{S}_i\rangle = \mathrm{Re}[\ (\mathbf{E}_i)^* \times \mathbf{H}_i] \quad \text{and} \quad \langle\overline{S}_r\rangle = \mathrm{Re}[\ (\mathbf{E}_r)^* \times \mathbf{H}_r]$$

Let e_n denote n-th order efficiency. The efficiency, looking down in $-\hat{y}$, is given by $e_n = <\overline{S}_r>\cdot(dA)_r / <\overline{S}_i>\cdot(dA)_i$, where $(dA)_i = -\,dA\,\hat{y}$ and $(dA)_r = dA\,\hat{y}$ give us:

$$e_n = -<\overline{S}_r>\hat{y} \;/\; <\overline{S}_i>\cdot\hat{y} \tag{11.0}$$

The fields are $U_i = \exp[i\,\alpha_o x + i\,\beta_{1o}\,y]\,\hat{z}$ and $(U_n)_r = B_n^{(1)}\exp[i\alpha_n x + i\,\beta_{1n}\,y]$.

Starting with the TE case,

$$<\overline{S}_i> = \mathrm{Re}[\,(E_i)^* \times H_i] = \mathrm{Re}[\,(E_i)^* \times \frac{1}{i\,\omega\,\mu_o}\nabla \times E_i] = \frac{1}{\omega\,\mu_o}\mathrm{Re}[\,\alpha_o\,\hat{x} - \beta_{1o}\,\hat{y}\,]$$

$$<\overline{S}_i>.\,\hat{y} = -\frac{1}{\omega\,\mu_o}\beta_{1o} = -\frac{1}{\omega\,\mu_o}k_1\,\mathrm{Cos}\,\theta.$$

$$<\overline{S}_r> = \mathrm{Re}[\,(E_r)^* \times H_r] = \mathrm{Re}[\,(E_r)^* \times \frac{1}{i\,\omega\,\mu_o}\nabla \times E_r] = |B_n^{(1)}|^2\frac{1}{\omega\,\mu_o}(\alpha_n\hat{x} + \beta_{1n}\,\hat{y})$$

$$<\overline{S}_r>\cdot\hat{y} = |B_n^{(1)}|^2\frac{1}{\omega\,\mu_o}\,\mathrm{Re}[\beta_{1n}\,] = |B_n^{(1)}|^2\frac{k_1}{\omega\,\mu_o}\mathrm{Re}[\mathrm{Cos}\,\theta_n]$$

$$e_n\,(TE) = |B_n^{(1)}|^2\;\mathrm{Re}[\mathrm{Cos}\,\theta_n]\,/\,\mathrm{Cos}\,\theta. \tag{11.1}$$

For the TM case, we write the Poynting vector in terms of **H**:

$<\overline{S}_i> = \mathrm{Re}[\,(E_i)^* \times H_i] = \mathrm{Re}[\left(\frac{1}{\sigma - i\,\omega\,\varepsilon}\right)^*(\nabla \times H_i)^* \times H_i] = \mathrm{Re}[\frac{1}{\omega\,\varepsilon}(\,\alpha_o\,\hat{x} - \beta_{1o}\,\hat{y})]$, where in vacuum, the conductivity is zero and the permittivity is a real number,

$$<\overline{S}_i>\cdot\hat{y} = -\frac{1}{\omega\,\varepsilon}\beta_{1o} = -\frac{1}{\omega\,\varepsilon}\mathrm{Cos}\theta$$

$$<\overline{S}_r> = \mathrm{Re}[\,(E_r)^* \times H_r] = \mathrm{Re}[\left(\frac{1}{\sigma - i\,\omega\,\varepsilon}\right)^*(\nabla \times H_r)^* \times H_r] = \frac{1}{\omega\,\varepsilon}|B_n^{(1)}|^2\mathrm{Re}[\alpha_n\,\hat{x} + \beta_{1n}\,\hat{y}]$$

$$<\overline{S}_r>\cdot\,\hat{y} = \frac{1}{\omega\,\varepsilon}|B_n^{(1)}|^2\;\mathrm{Re}[\beta_{1n}]$$

$$e_n\,(TM) = |B_n^{(1)}|^2\,\mathrm{Re}[\mathrm{Cos}\,\theta_n]\,/\,\mathrm{Cos}\theta. \tag{11.2}$$

We have assumed an incident plane wave of unit amplitude, $\exp[i\,\alpha_o\,x - i\,\beta_{1o}\,y]$. In our Fourier basis of $\{\exp[i\,\alpha_n\,x]\}$, it is represented as {0, 0, ..., 0, 1, 0, ..., 0}, where the 1 is in the space corresponding to n = 0, denoted by v_i. Let v_r denote the vector of reflection. Then $v_r = R.v_i$ and v_r is now a column vector: the n-th element is $B_n^{(1)}$, the field amplitude for the n-th diffracted order. To calculate the reflection efficiencies for all orders in [-N, N], we use the following for both polarizations:

$$\mathbf{e} = |v_r|^2\;\mathrm{Re}[\mathrm{Cos}\,\theta_n]\;/\;\mathrm{Cos}\theta \tag{11.3}$$

where **e** has 2N+1 elements, the n-th element being the n-th order efficiency.

12. NUMERICAL METHODS

For the TE case, we want to solve (7.1), for each n (from -N to +N). Write the set of 2N+1 equations in terms of matrices by making the following definitions to arrive at (12.0):

$\Psi(y) = \{E_{-N}(y), E_{-(N+1)}(y), ..., E_0(y), ..., E_{(N-1)}(y), E_N(y)$ and

$V(y)$ is a square matrix of dimension $2N+1$: $V(n, m) = \alpha_n^2 \delta_{nm} - k^2{}_{n-m}(y)$.

$$\frac{\partial^2\Psi(y)}{\partial y^2} = V(y).\Psi(y) \tag{12.0}$$

(12.0) is a second order ODE which Nevière solves using the Numerov[3] method.

Let $\xi(y) = \Psi(y) - \frac{h^2}{12}\frac{\partial^2\Psi(y)}{\partial y^2} = \Psi(y) - \frac{h^2}{12}V(y)\cdot\Psi(y) \Rightarrow \xi(y) = [\,I - \frac{h^2}{12}V(y)\,]\cdot\Psi(y)$ (12.1), where I is an identity matrix of the same dimensions as the matrix $V(y)$, h is the integration step size and both $\xi(y)$ and $\Psi(y)$ are column vectors. The Numerov integration formula is:

$$\xi(y + h) = [\,2\,I + h^2\,V(y) + \frac{h^4}{12}V(y)\cdot V(y)]\,\xi(y) - \xi(y - h) + O(h^6) \tag{12.2}$$

We need $\xi(0)$ and $\xi(h)$ to start the numerical integration; these are calculated with a second order Runge-Kutta algorithm, and then (12.1) gives us $\xi(h)$:

$$\Psi(h) = [I+\frac{h^2}{6}V(0) + \frac{h^2}{3}V(h)+\frac{h^4}{24}V(0)\cdot V(h)]\cdot\Psi(0)+h[\,I+\frac{h^2}{6}V(h)]\frac{\partial\Psi(0)}{\partial y} + O(h^5) \tag{12.3}$$

Then (12.2) gives us $\xi(a)$. To compute $\Psi(a)$, where $1 >> \frac{h^2}{12}V_{nm}(y)$, $\forall$ n, m, we invert (12.1) and use a binomial expansion:

$$\Psi(a) = [I - \frac{h^2}{12}V(a)]^{-1}\cdot\xi(a) \Rightarrow \Psi(a) = [\,I + \frac{h^2}{12}V(a) + \frac{h^4}{144}V(a)\cdot V(a)]\cdot\xi(a) \tag{12.4}$$

Equations (9.2) and (9.3) also require the first derivative of the electric field at $y = a$. Using the Raynal [4] method:

$$\frac{\partial\Psi(a)}{\partial y} = [\,10\,\xi(a - 7h) + 28\,\xi(a\text{-}6h) - 485\,\xi(a\text{-}5h) + 1778\,\xi(a\text{-}4h) - 3325\,\xi(a\text{-}3h)$$

$$+ 3740\,x(a\text{-}2h) - 3150\,x(a\text{-}h) - 360\,x(a)]\,/\,(720\,h) + 147\,Y(a)/\,(60\,h) + O(h^6) \tag{12.5}$$

we now have all we need to solve for the grating efficiency for TE polarization.

For the TM case, we want to solve two sets of coupled ODEs, (8.4) and (8.5). We define the column vector $Y(y)$ and the square matrix V as follows:

$$\Psi(y) = \{\widetilde{E}_{-N}(y), \widetilde{E}_{-(N+1)}(y), ..., \widetilde{E}_0(y), ..., \widetilde{E}_N(y), H_{-N}(y), H_{-(N+1)}(y), ..., H_0(y), ..., H_N(y)\}$$

$$V_{nm} = k^2{}_{n-m} \quad \text{for } 1 \le n, m \le 2N+1 \text{ and}$$

$$V_{nm} = \alpha_n\,\alpha_m \left(\frac{1}{k^2}\right)_{n-m} - \delta_{nm} \quad \text{for } 2N+2 \le n, m \le 2(2\,N+1).$$

$\Psi(y)$ has $2(2N+1)$ elements and V has dimension $2(2N+1)$. We can rewrite (8.4) and (8.5) as:

$$\frac{\partial\Psi(y)}{\partial y} = V(y)\cdot\Psi(y) \tag{12.6}$$

Numerical integration of (12.6) using a fourth order Runge-Kutta algorithm gives $\Psi(a)$. The last 2N+1 elements of $\Psi(a)$ are the amplitudes, $H_n(a)$. The first 2N+1 elements of $\Psi(a)$ are the $\widetilde{E}_n(a)$, which give us $dH_n(a)/dy$. Then (9.2) and (9.3) give us the field amplitudes for TM polarization.

13. THE RECIPROCITY THEOREM

We are using substrates with finite conductivity. The differential method does not allow for an accurate calculation of the energy lost to Joule heat in the modulated region, which means that we cannot use energy conservation to check our results. However, we can use the Reciprocity Theorem [5], which says that the efficiency for radiation incident at θ and diffracted at θ_n is the same as the efficiency for radiation incident at $-\theta_n$ and diffracted at $-\theta$.

We verified the Reciprocity Theorem for the cases done by Nevière et. al. in Topics in Current Physics, page 208. See tables 1 and 2.

14. PROGRAMMING

The programming was done with a Mathematica front end and a remote kernel on a RISC 6000. The front end links with ANSI-C programs sitting on the RISC to do the numerical integrations. The programs also compute the scalar theory predictions for the efficiencies in the case of symmetrical square waves. Figure 3 is a flowchart of the program.

Figures 4-7 compare our results with those of Nevière. Our main concerns were: (1) making sure we agreed with Nevière; (2) minimizing the computational time (see figure 8 for the relationship of the time and the number of diffracted orders); and (3) observing the effects of the variation of the results as we changed the total number of diffracted orders as well as the number of evanescent waves (see figure 9). We recommend that you choose a wavelength (or energy) with fairly predictable efficiency (in the case of a blazed profile, we chose the blaze wavelength), and choose a computational time that gives you a desirable accuracy. Figure 10 shows how the efficiency begins to converge with increasing number of orders. Note that for comparisons of efficiencies to have meaning, the same number of orders, 2N+1, as well as the same number of evanescent orders, must be used for the different cases. However, figure 9 shows that varying the number of evanescent orders has a larger effect than varying 2N+1, the total number of orders. It is interesting to note that as we move further from the zero-th order, we are in effect varying the number of evanescent orders used in the calculations which in turn effects the symmetry of the calculation and we find that the ratio e(p)/e'(p) moves away from 1.

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[1] Wolfram, Stephen, Mathematica, Addison-Wesley Publishing Company, 1991.

[2] Stern, Frank, *Elementary Theory of Optical Properties of Solids*, Chapters I and II, Solid States Physics, Volume 15, Academic Press, 1963.

[3] Melkanoff, Michel, Sawada, Tatsuro and Raynal, Jacques, Nuclear Optical Model Calculations, pg 15.

[4] Raynal, Jacques, Seminar Course on Computing as a Language of Physics, ICTP, Trieste, August, 1971.

[5] Petit, R., A Tutorial Introduction, Topics in Current Physics, Volume 22, pg 12.

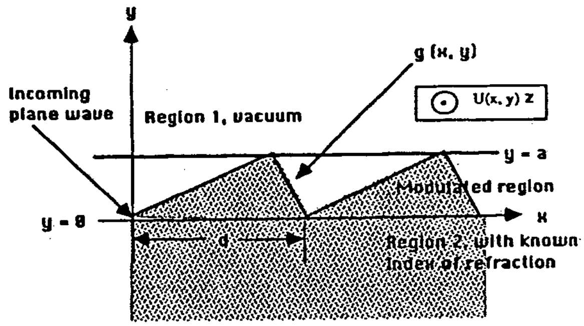


FIGURE 1: BLAZED PROFILE
REGIONS 1 & 2 ARE HOMOGENEOUS AND ISOTROPIC
$U(x, y) = E(x, y)$ for TE and $U(x, y) = H(x, y)$ for TM

FIG. 1. Coordinate System

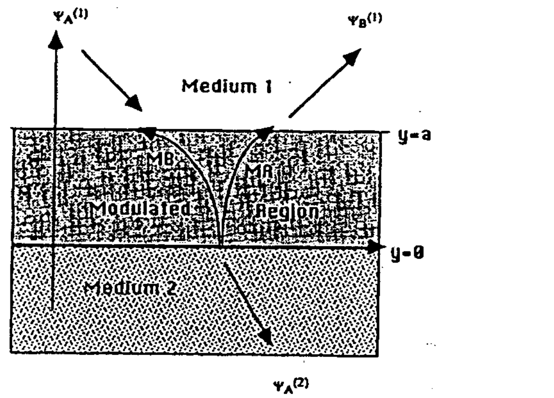


FIGURE 2: NEVIERE'S ILLUSTRATION OF THE LINEAR ALGEBRA PROBLEM

FIG. 2. Nevière's Illustration of the Linear Algebra Problem.

TE/TM PROGRAM FLOWCHART

USER PARAMETERS

CALCULATED PARAMETERS

DISPLAY VALUES

DETERMINE NUMBER OF EXISTING ORDERS

DETERMINE GROOVE PROFILE

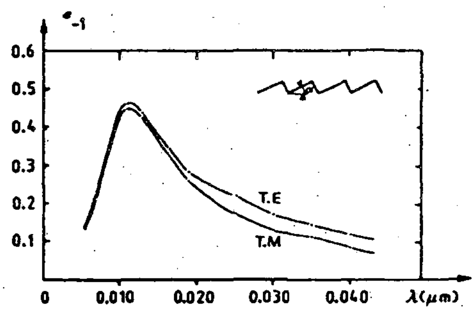
NUMERICAL APPROXIMATION OF $k^2(x, y)$
(AND OF $\frac{1}{k^2(x,y)}$ FOR THE TM CASE) FOR $y \in [0, a]$

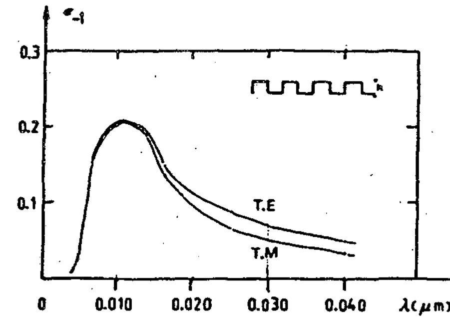
CONSTRUCTION OF THE V MATRICES

SPECTRUM ANALYSIS:
CALCULATION OF EFFICIENCIES

PLOTTING TE/TM SPECTRA:
WAVELENGTH (Angstroms) vs EFFICIENCY
ENERGY (eV) vs EFFICIENCY

FIG. 3. Program Flowchart





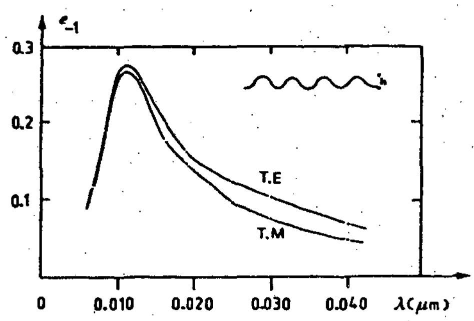


Fig. 6.87. Efficiency of a gold echelette grating in XUV domain, as a function of the wavelength: $\alpha = 1.624^{\circ}$

Fig. 6.88. Same as Fig.6.87 but for a sinusoidal grating: h = 302 Å

Fig. 6.89. Same as Fig.6.87, but for a symmetrical lamellar grating: h = 198 Å

FIG. 4. Results from Topics in Current Physics, Maystre, Petit and Nevière, Vol. 22, p. 208.

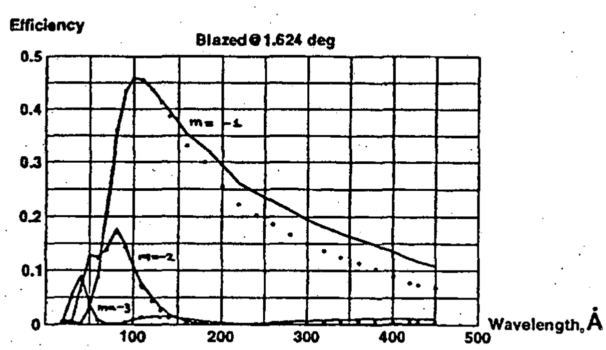


FIG. 5. Blazed profile @ 1.624°

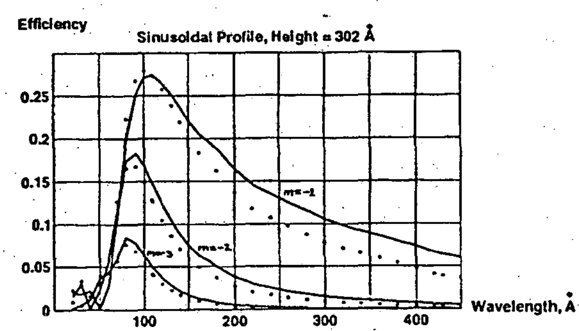


FIG. 6. Sinusoidal Profile

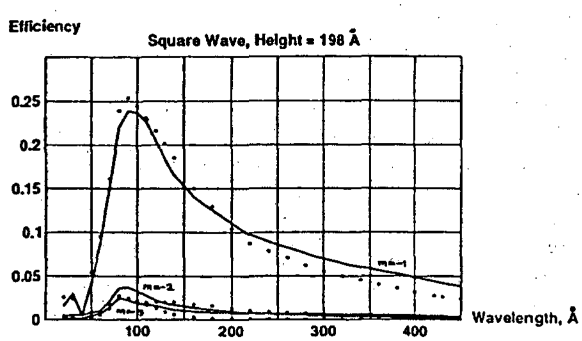


FIG. 7. Square Wave Profile

FIGS. 5-7 are the same case as in figure 4, where Nevière uses a Gold substrate with an incidence angle of 85 degrees, all of which have 600 lines per mm. The solid lines are for TE and the dotted line are for TM.

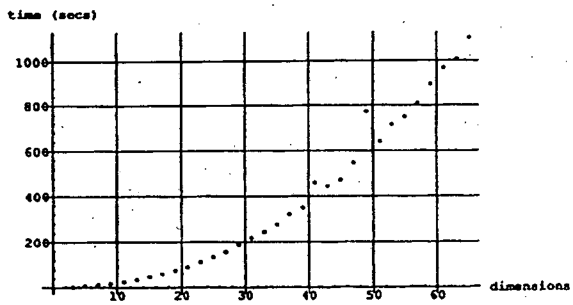


FIG. 8. The computational time increases with the number of orders, 2N+1.

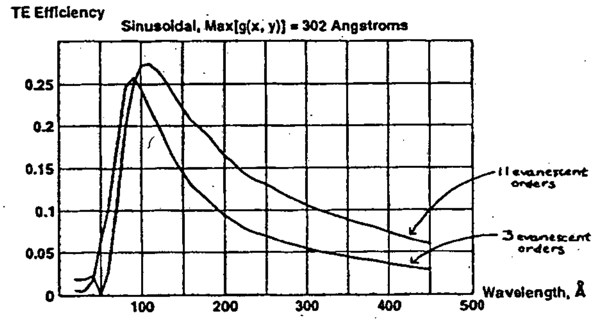


FIG. 9. Comparison of the TE efficiency for the -1 order of the sinusoidal profile shown in fig. 6. The lower values for the efficiency use 3 evanescent orders for calculations, while the higher values use 11.

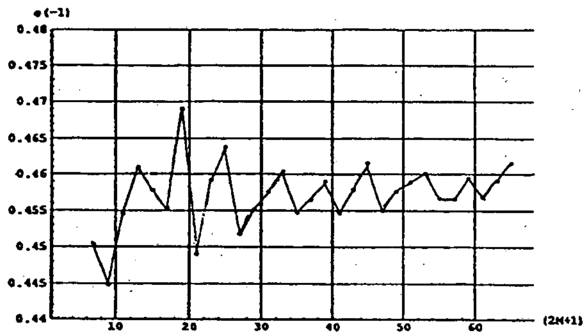


FIG. 10. The behavior of the efficiency (first inner order) for the blazed profile of fig. 5, at λ = 108.972 Angstroms. The efficiency begins to converge as we increase the number of dimensions.

□ TABLE 1
TE: VERIFICATION OF RECIPROCITY
BLAZED @1.624 Degrees, Gold Substrate, 600 gr per mm

p	θ	θp	e(p)	θ'	θp'	e'(p)	e(p)/e'(p)
0	85	85	0.212621	-85	85	0.212906	0.998661
-1	85	81.752	0.45052	-81.752	85	0.438741	1.026847
-2	85	79.4571	0.103649	-79.4571	85	0.105	0.987
-3	85	77.5753	0.009950	-77.5753	85	0.009805	1.014815

□ TABLE 2
TM: VERIFICATION OF RECIPROCITY
BLAZED @1.624 Degrees, Gold Substrate, 600 gr per mm

p	θ	θp	e(p)	θ'	θp'	e'(p)	e(p)/e'(p)
0	85	85	0.221448	-85	85	0.221451	0.999986
-1	85	81.752	0.45929	-81.752	85	0.455943	1.007341
-2	85	79.4571	0.072868	-79.4571	85	0.070964	1.026831
-3	85	77.5753	0.014743	-77.5753	85	0.014008	1.052470

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