# Characterization of Diffraction Anomalies in 2-D Photonic Bandgap Structures

Marcin Sarnowski, Thomas Vaupel, Volkert Hansen, *Member, IEEE*, Ernst Kreysa, and Hans Peter Gemuend

***Abstract*—This paper deals with transmission anomalies of freestanding two-dimensional bandgap structures, which have found a large application range as filter and guiding structures in communication systems and radioastronomical applications in the far infrared region. The effect appears as a sharp breakdown of the transmission factor in the passband of quadratic patch and slot structures, first revealed by measurements. This paper outlines the numerical confirmation of these effects by computer simulations based on the method of moments combined with the Floquet theorem. The transmission and reflection behavior is examined for different structure geometries, frequency ranges, angle, and polarization of the incident wave also revealing alternative structures suppressing these effects. The modeling with electric and magnetic currents allows the characterization of both patch and slot arrays. Finally, cross shaped structures are examined allowing the complete suppression of this kind of anomalies.**

***Index Terms*—Diffraction anomalies, Floquet theorem, method of moments, 2-D photonic bandgap structures.**

## I. Introduction

DOUBLE periodic arrays of apertures or striplike structures have found a large number of applications as photonic bandgap structures and/or polarization sensitive components. With improved manufacturing capabilities they can be applied from the microwave region over millimeter wave frequencies up to the far infrared region as elements of integrated optics like filters, couplers, resonators, reflectors and guiding structures. Measurements of the properties of freestanding structures with quadratic patches or slots have revealed, that—depending on the properties of the incident wave—sharp breakdowns of the transmission characteristics can appear unfortunately in the passband region. Similar effects observed in optical diffraction gratings were already discovered in 1902 and were called Wood's anomalies [1], since no agreement could be found with the ordinary theory of gratings of this time. The theory of Ulrich, first published in 1970, assumes that these kinds of transmission breakdowns may be caused by interactions of the exciting waves with the inherent leaky waves of the structure at certain frequencies, other theoretical studies are based on a modal expansion [8]. In the present paper our flexible full-wave simulation concept for such structures, which is based on the method of moments (MOM) with arbitrary asymmetric basis functions combined with the Floquet theorem [6], is briefly outlined, afterwards numerical results of the scattering parameters in comparison with measurements of the Max Planck Institute for Radioastronomy in Bonn and with the measurements in [2] are presented. The paper contains comprehensive numerical studies of slotlike and striplike metal meshes depending on various excitation and geometry parameters. Good alternative structures suppressing the observed anomalies are given by appropriate cross-shaped structures like Jerusalem crosses, which also enable a higher package density.

Manuscript received January 5, 2001; revised June 13, 2001.

M. Sarnowski, T. Vaupel, and V. Hansen are with the University of Wuppertal, 42119 Wuppertal, Germany (e-mail: thvaupel@lycos.de).

E. Kreysa and H. P. Gemuend are with the Max Planck Institute for Radioastronomy, Bonn, Germany.

Publisher Item Identifier S 0018-9480(01)08709-9.

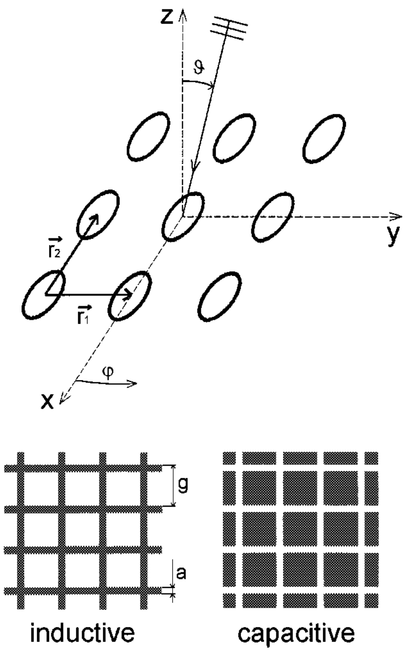


Fig. 1. General grid array consisting of a double periodic arrangement of elementary cells. Inductive and capacitive grids defined by: $a$: strip width or gap width, respectively, and $g$: periodicity.

## II. Mathematical Formulation

A brief summary of the mathematical theory is given as follows, a detailed presentation can be found in [4].

A general array structure consisting of a double periodic arrangement of so-called elementary cells is outlined in Fig. 1. These elementary cells can describe slot geometries within a metallic sheet or metallic striplike structures with arbitrary shapes. The double periodic continuation of the elementary cell is described by the displacement vectors

$$\vec{r}_1 = a_1\vec{e}_x + b_1\vec{e}_y \quad \vec{r}_2 = a_2\vec{e}_x + b_2\vec{e}_y \quad \vec{r}_{pq} = p\vec{r}_1 + p\vec{r}_2 \tag{1}$$

leading to the final structure of infinite lateral extension, with the $pq$th elementary cell addressed by $\vec{r}_{pq}$.

The structures under discussion are arranged in free space, e.g., by a membrane support technique, but the method can also handle structures in different planes embedded in a multilayered medium.

The elementary cell can be modeled by electric or magnetic currents, depending on the case that we want to model the strip or the slot parts of the structure, respectively. The current distribution is represented by a sum over $N$ subdomain basis functions $\vec{f}_n(x, y)$ with unknown current amplitudes $U_n$. This leads in the case of magnetic currents to the expression

$$\vec{M}_{00}(x, y, z) = \sum_{n}^{N} U_n \vec{f}_n(x, y)\delta(z) \tag{2}$$

with the metallization plane located at, e.g., $z = 0$. Considering the phase shift on the $pq$th cell due to the exciting plane wave with arbitrary incident angle, we get the following expression for the overall structure:

$$\vec{M}(x, y, z) = \sum_{p=-\infty}^{\infty} \sum_{q=-\infty}^{\infty} \vec{M}_{00}(x - \Delta x_{pq}, y - \Delta y_{pq}) \cdot \delta(z) e^{j(k_{ex}\Delta x_{pq} + k_{ey}\Delta y_{pq})} \tag{3}$$

with $k_{ex}$ and $k_{ey}$ the wavenumbers of the exciting plane wave. These magnetic currents are directly arranged above and below a metallic sheet with zero thickness in order to model the slot areas [5].

If we model the slot areas of a structure, we have to fulfill the condition for the magnetic field

$$\left[\vec{H}^{+}(\vec{M}) - \vec{H}^{-}(\vec{M})\right]_{\tan, z=0} = -\vec{H}^{\text{inc}}|_{\tan, z=0} \tag{4}$$

within the slot areas with $\vec{H}^{\text{inc}}|_{\tan}$ the resulting tangential field on the metallic sheet due to the incident wave.

In the case of strip or patch metallizations, we have to fulfill the well-known impedance boundary condition [1]

$$\vec{E}_s \Big|_{\tan, z=0} - R^s \vec{J} = -\vec{E}^{\text{inc}}_{\tan, z=0} \tag{5}$$

on the strips which allows the further consideration of metallic losses by means of a surface impedance $R^S$ and a finite thickness $d$ of the metallization due to the relation $R^S = 1/(\kappa d)$ valid for the very thin metallic sheets given in our case (~100 nm, $\lambda/d \approx 3\,000:1$). Due to this thin sheets, no further modal analysis as in [8], [11] is needed, on the other hand, this simplification enables the simulation of much more complicated metallization and aperture geometries. The case of zero thickness is also helpful to numerically demonstrate the duality of inductive and capacitive structures (see Section III-C). From the above conditions integral equations can be formulated for the unknown current amplitudes. The integral equation, discretized by the series representations (3), is solved by the Galerkin MOM, leading to a linear system of equations with the system matrix $[Y]$ and the matrix elements

$$Y_{nm} = \frac{1}{a_1 b_2 - a_2 b_1} \sum_{p=-\infty}^{\infty} \sum_{q=-\infty}^{\infty} \overleftrightarrow{G}^{H}_{M}(k_x(p, q), k_y(p, q)) \cdot \vec{F}_m(k_x(p, q), k_y(p, q)) \cdot \vec{F}_n(-k_x(p, q), -k_y(p, q)) \tag{6}$$

where $\overleftrightarrow{G}^{H}_{M}$ denotes the composite Green's function for the magnetic field above and below the metallic sheet, $\vec{F}_n$ are the Fourier transforms of the basis functions $\vec{f}_n$ and the discrete wavenumbers

$$k_x(p, q) = k_{ex} + 2\pi \frac{b_2 p - b_1 q}{a_1 b_2 - a_2 b_1}$$
$$k_y(p, q) = k_{ey} + 2\pi \frac{a_2 p - a_1 q}{a_1 b_2 - a_2 b_1} \tag{7}$$

in context with the Floquet theorem.

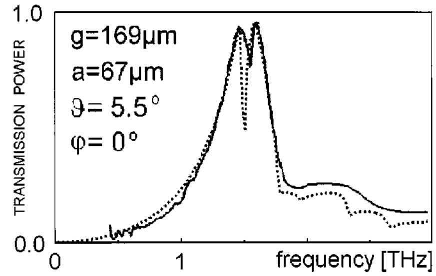


Fig. 2. Transmission power of an inductive grid. Solid line: measurement, dashed line: calculation of a superposition of TE and TM modes.

## III. Experimental Results

The diffraction anomalies in context with freestanding two-dimensional (2-D) photonic bandgap structures have been found by recent measurements made by the Max Planck Institute for Radioastronomy. It could be observed a sharp breakdown of the amplitude of the transmitted wave within a very small frequency range. On the other hand, we could confirm these anomalies by computer aided calculations based on the method outlined above. So far, no satisfactory explanation for this kind of effects can be given, and it is obvious, that structures (e.g., filters) with such a distorted transmission characteristic in the passband cannot be practically used. Due to these facts it seems important to investigate such anomalies in more detail.

In Fig. 1, so-called inductive and capacitive grids are outlined with periodicity $g$ and a metal strip (or gap) width a which is excited by a plane wave with incident angles $\vartheta$ and $\varphi$. Fig. 2 (solid line) shows the measured transmission behavior of a grid with $a = 67$ $\mu$m, $g = 169$ $\mu$m. The transmission breakdown in the range 1.5 THz is very significant. The comparison with the simulated characteristic (Fig. 2, dashed line) shows a good agreement with the measurement. Differencies mainly arise from the measurement principle, based on a nonpolarized conical incident beam applied within the Fourier spectrometer of type BOMEM DA 3.26, which is focused on a circular probe area with a diameter of about 4 cm. Due to the lens arrangement

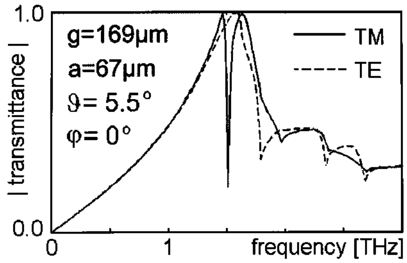


Fig. 3. Calculated transmission factors of an inductive grid with polarization TM and TE, $6 \times 6$ segmentation for the magnetic currents.

within the spectrometer, the incident angle varies with $\Delta\vartheta$ of about $\pm 3^{\circ}$, around an average angle $\vartheta = 5.5^{\circ}$. Furthermore the input beam is nonpolarized, since a thermic radiation source without polarisators is used so far. The nonpolarized input beam is simulated by the equal superposition of two calculations with a transverse magnetic (TM) and a transverse electric (TE) incident wave (see also Fig. 3), respectively, which seems to be a good compromise assuming an equal distribution of all polarization directions within the input beam. Despite of these differences, the good agreement between measurements and simulations rules out the assumption, that the transmittance breakdown could be an error in the measurements or the numerical calculations.

### *A. Magnetic Current Modeling of the Electric Fields Within the Slots*

At first, we have modeled the electric fields within the slot areas of inductive grids by means of magnetic currents using a suited set of basis functions. If we have only rectangular slots, we can apply a uniform discretization of the fields with the well-known symmetric rooftop functions [4].

We have simulated the transmission behavior of the structure in Fig. 2 (inductive rectangular grid). Fig. 3 shows the calculated transmission for the incident angles $\varphi = 0^{\circ}$ and $\vartheta = 5.5^{\circ}$ for both TM and TE polarization. Obviously, the sharp breakdown only appears for the TM polarization. We could observe, that already a coarse discretization of $3 \times 3$ subdomains leads to reliable results whereas an increased resolution of up to $6 \times 6$ only exhibits slight differences compared with the coarser resolutions. A discretization of about eight subdivisions per wavelength and $10 \times 10$ Floquet modes is sufficient in nearly any case and can be given as a simulation guideline. For a quick comfirmation, we perform some calculations with this rule and vary the current discretization and number of Floquet modes, thus often also a coarser discretization and a smaller number of Floquet modes leads to reliable results.

### *B. Modeling of the Electric Currents on the Strips*

Instead of modeling the apertures with magnetic currents, we are also able to model the electric currents on the metallic strips. For an efficient modeling we have applied a nonuniform discretization of the left and the lower side of an elementary cell. With additional overlapping basis functions, a consistent modeling with current continuity at the cell boundaries is achieved. This modeling method allows a further insight in the electromagnetic behavior of the structure and enables, e.g., the consideration of metallic losses. The good agreement of the results of this modeling (Fig. 4) with Fig. 3 yields to a further confirmation for the sharp transmittance breakdown as a real physical effect.

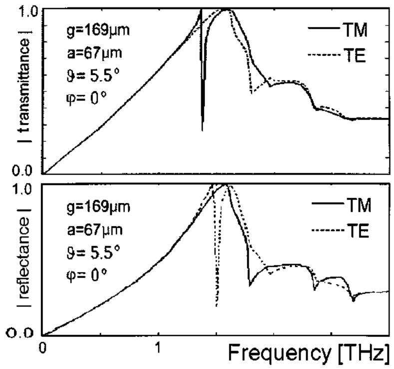


Fig. 4. Calculated transmission factors of the inductive grid by modeling the electric currents of the strips (top) and reflection factors of a capacitive grid (bottom). $6 \times 6$ segmentation for the electric currents.

### *C. Duality of Inductive and Capacitive Grids*

On the other hand we can also consider rectangular metallic patches—so-called capacitive grids (see Fig. 1)—by modeling the electric patch currents. Inductive and capacitive grids in free space are dual to each other with regard to their transmittance and reflection behavior as well as for the polarization, what becomes obvious by a comparison of the inductive grid results with the behavior of the dual capacitive structure (Fig. 4, bottom). This numerical proof of Babinet's principle is a further confirmation of the numerical accuracy and reliability of the applied methods.

### *D. Cross Shaped Structures With Orthogonal and Nonorthogonal Displacement Vectors*

In addition to the simple patch structures we have also examined cross shaped structures with orthogonal and nonorthogonal displacement vectors. We have considered two values for the angle $\varphi$ ($0^{\circ}$ and $45^{\circ}$) and both polarizations TM and TE. The results for the reflection factors are given in Fig. 5. In contrast to the orthogonal arrangement of the crosses with the breakdown at $\varphi = 0^{\circ}$ for the TE case, we observe the breakdown for the nonorthogonal structure for the TM case and vice versa for the incident angle $\varphi = 45^{\circ}$. This is due to the fact, that the orthogonal structure appears nonorthogonal for $\varphi = 45^{\circ}$ and vice versa for the nonorthogonal structure. Similar results are also obtained for nonorthogonal grids with rectangular patches or slots.

### *E. Comparison With Results of Other Publications*

Thus far, only a few papers dealing with these anomalies in context with freestanding grids can be found. In [2], an inductive grid was investigated with periodicity $g = 101$ $\mu$m and a width of the metallic strips $a = 14$ $\mu$m. In this paper, the measured transmission power of this structure shows two deep breakdowns and a further slight breakdown at about 3.4 THz (Fig. 6, solid line). Our numerical simulations of this structure (Fig. 6, dashed line) are in good agreement except of the

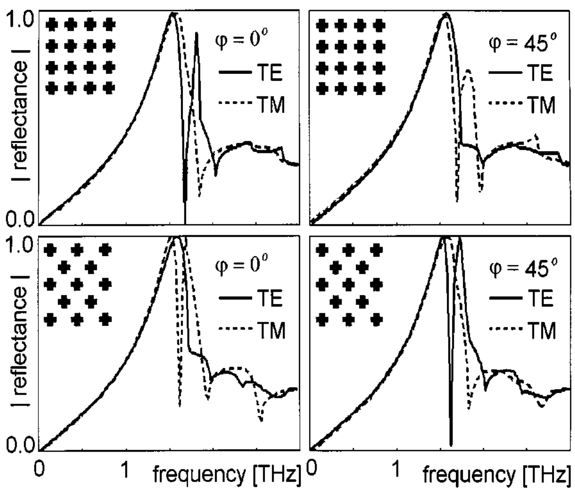


Fig. 5. Calculated reflection coefficients of capacitive grids with $g = 162.6\ \mu$m (top) and $g = 230\ \mu$m (bottom), $a = 102.96\ \mu$m, $b = 22.5\ \mu$m, $\vartheta = 5.5°$.

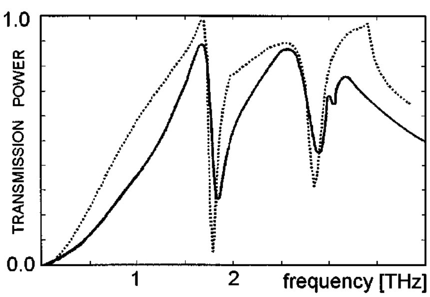


Fig. 6. Measured (solid line) and calculated (dashed line) transmission power of an inductive grid. Width of the strips $a = 14\ \mu$m, periodicity $g = 101\ \mu$m, polarization TM, angles of incidence: $\varphi = 0°$ and $\vartheta = 30°$.

different amplitudes which are mainly due to the finite lateral dimensions, metallic losses and additional influences of wavy and/or rough surfaces and local variations of the grid constant. The theory of Ulrich for these kinds of breakdowns deals with the forced excitation of leaky waves leading to strong reflections if the wavenumber of the incident wave is close to the (complex) wavenumber of the corresponding leaky wave. First investigations in context with such phenomena, generally called "Wood's anomalies," are already presented in [1] and are continued in [3].

Since the theory of Ulrich [2] is partly based on phenomenological considerations [7], it would be very desirable to find the dispersion characteristics of the leaky waves directly by the appropriate formulation and solution of the corresponding eigenvalue problem forming the main part of our ongoing investigations.

### *F. Avoidance of Diffraction Anomalies by the Use of Jerusalem Crosses*

Comprehensive studies of further geometries have shown, that Jerusalem crosses probably form the best alternative geometry for the use in freestanding grids with one metallization plane. Thus no diffraction anomalies could be observed for both polarizations TM and TE for all considered incidence angles and the transmission properties can be adjusted in a wide range by the special shape and the package density of

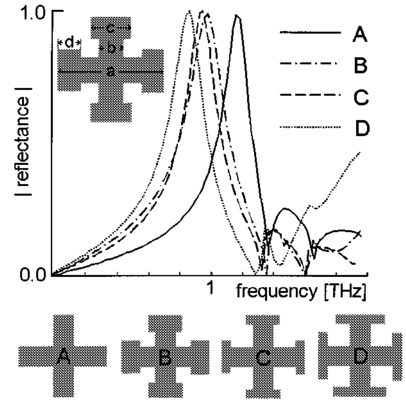


Fig. 7. Calculated reflection coefficients of orthogonal capacitive grids with periodicity $g = 200\ \mu$m, angle of wave incidence $\vartheta = 5.5°$, $\varphi = 0°$. Polarization TE. Dimensions of the crosses: (A) $a = 120\ \mu$m, $b = 24\ \mu$m (B) $a = 120\ \mu$m, $b = 24\ \mu$m, $c = 48\ \mu$m, $d = 24\ \mu$m (C) $a = 120\ \mu$m, $b = 24\ \mu$m, $c = 48\ \mu$m, $d = 12\ \mu$m (D) $a = 120\ \mu$m, $b = 24\ \mu$m, $c = 72\ \mu$m, $d = 12\ \mu$m.

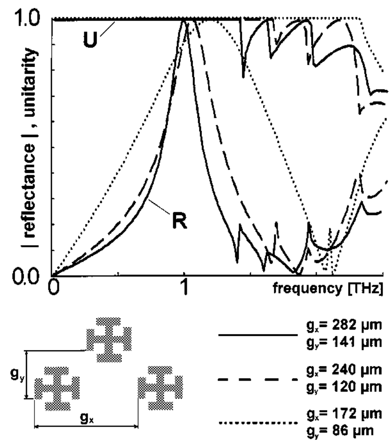


Fig. 8. Calculation of the crosses [see Fig. 7(d)] with nonorthogonal grids and different package density.

the crosses. Due to our description with basis functions on arbitrary rectangular subdomains we can model arbitrary shape variations, as shown in Fig. 7(a)–(d), with a minimum of discretization effort in contrast to a mainly entire domain approach in [9]. Even for the critical TE polarization, we cannot observe any anomalies. The passband behavior for TM polarization is nearly the same. For simple crosses, we get a quite small passband curve which drops down sharply close to the onset of the grating lobes at about 1.37 THz. If we simulate different kinds of Jerusalem crosses, we can recognize a shift of the passband curves to lower frequencies and furthermore we get nearly symmetrical passband curves. The frequency shift is due to the fact, that the overall electrical length of the simple crosses is increased by the additional arms, partly also due to capacitive couplings between the arms. An essential advantage is given by the fact, that this increase of the electrical length is not combined with an increase of the elementary cell dimensions. The use of cross shapes furthermore enables a larger package density compared with rectangular patch structures. This can be performed by using nonorthogonal displacement vectors similar as in Fig. 5. The results with an increasing package density are depicted in Fig. 8, where the cross of Fig. 7 type D was applied. With the quite low package density we get a similar passband curve as with an orthogonal grid (solid line). If we increase the package density, we can observe a successive widening of the passband curve (dashed line), furthermore the onset of the grating lobes is shifted to corresponding higher frequencies. This becomes visible by the unitarity relation. The dotted line corresponds to about the largest possible package density with this structure. In this case we can already observe a part of the second passband curve without distortions due to the onset of grating lobes. Due to these properties a large modeling flexibility without the risk of anomalies is given by such cross structures.

## IV. Summary

In this paper, we have presented the analysis of 2-D photonic bandgap (PBG) structures by modeling them as aperture or striplike double periodic structures with the subsequent application of a numerical approach based on the MOM combined with the Floquet theorem. For certain sets of parameters we can observe a very complex scattering behavior with sharp breakdowns in the passband region which could also be confirmed by measurements. We could outline the dependency of these anomalies of various parameters comprising the excitation and the geometry of the structures. Based on these investigations also alternative structures suppressing these anomalies could be presented.

## References

[1] R. W. Wood, "On a remarkable case of uneven distribution of light in a diffraction grating spectrum," *Phil. Mag. J. Sci.*, ser. 6th, vol. 4, no. XXI, p. 396, Sept. 1902.

[2] R. Ulrich, "Modes of propagation on an open periodic waveguide for the far infrared," in *Proc. Opt. Acoust. Micro-Electron. Symp.*, New York, Apr. 16–18, 1974.

[3] A. Hessel and A. Oliner, "A new theory of Wood's anomalies on optical gratings," *Appl. Opt.*, vol. 4, no. 10, Oct. 1965.

[4] H. Aroudaki, V. Hansen, H. P. Gemünd, and E. Kreysa, "Analysis of low-pass filters consisting of multiple stacked FSS's of different periodicities with applications in the submillimeter radioastronomy," *IEEE Trans. Antennas Propagat.*, vol. 43, pp. 1486–1491, Dec. 1995.

[5] H. Aroudaki, T. Vaupel, V. Hansen, and F. Schäfer, "Full-wave analysis of CPW fed slot antennas for the submillimeter wave region by the spectral domain method," in *Progress Electromag. Res. Symp.*, Noordwijk, The Netherlands, 1994, pp. 1437–1440.

[6] V. Hansen, "Radiation of finite and infinite arrays in multilayered media," in *URSI Int. Electromag. Theory Symp.*, Stockholm, Sweden, 1989, pp. 464–466.

[7] R. Ulrich, "Efficiency of optical-grating couplers," *J. Opt. Soc. Amer.*, vol. 63, no. 11, Nov. 1973.

[8] L. C. Botten, R. C. McPhedran, and J. M. Lamarre, "Inductive grids in the resonant region: Theory and experiment," *Int. J. Infrared Millim. Waves*, vol. 6, no. 7, pp. 511–575, 1985.

[9] C.-H. Tsao and R. Mittra, "Spectral domain analysis of frequency selective surfaces comprised of periodic arrays of cross dipoles and Jerusalem crosses," *IEEE Trans. Antennas Propagat.*, vol. AP-32, pp. 478–486, May 1984.

[10] R. C. McPhedran and D. Maystre, "On the theory and solar application of inductive grids," *Appl. Phys.*, vol. 14, pp. 1–20, 1977.

[11] D. Maystre, "General study of grating anomalies from electromagnetic surface modes," in *Electromagnetic Surface Modes*, A. D. Boardman, Ed. New York: Wiley, 1982.

**Marcin Sarnowski** was born in Wloclawek, Poland, in 1974. He received the M.S. degree in microwave technique and optical telecommunication from the Technical University of Gdansk, Gdansk, Poland, in 1998.

Since 1999, he has been a Research Assistant at the Chair of Electromagnetic Theory, Bergische Universität-Gesamthochschule Wuppertal, Wuppertal, Germany. His research interests include complex electromagnetic-field problems in planar structures.

**Thomas Vaupel** was born in Bochum, Germany, in September 1963. He received the Dipl.-Ing. degree in electrical engineering from the Ruhr-Universität Bochum, Bochum, Germany, in 1992, and the Dr.-Ing. degree from the Bergische Universität-Gesamthochschule Wuppertal, Wuppertal, Germany, in 1999.

In 1993, he was a Research Assistant with the Institute for High Frequency Technology, Ruhr-Universität Bochum. Since the end of 1994, he has been a Research Assistant at the Chair of Electromagnetic Theory, Bergische Universität-Gesamthochschule Wuppertal. His current research interests cover the development of analytical and numerical methods for the analysis of complex microstrip and coplanar structures and antennas.

**Volkert Hansen** (M'82) received the Dipl.-Ing. degree in electrical engineering from the Technische Hochschule Darmstadt, Darmstadt, Germany, in 1969, and the Dr.-Ing. degree from the Institute for High Frequency Technology, Ruhr-Universität Bochum, Bochum, Germany, in 1975.

He then joined the Institute for High Frequency Technology, Ruhr-Universität Bochum, where he was a Research Assistant. In 1985, he habilitated at the Faculty of Electrical Engineering of the Ruhr-Universität Bochum. In 1990, he was appointed a Professor. Since 1994, he has been a Full Professor of theoretical electrical engineering at the Bergische Universität-Gesamthochschule Wuppertal, Wuppertal, Germany. His main research interests are the development of theoretical and numerical methods for antennas and scattering problems with applications to planar circuits and antennas, focusing antennas, frequency- and polarization-selective screens, antennas for geophysical prospecting, and the evaluation of the potential health effects of electromagnetic fields.

Dr. Hansen is member of the International Scientific Radio Union (URSI) and the ITG.

**Ernst Kreysa** received the Ph.D. degree in physics and astronomy from Bonn University, Bonn, Germany, in 1979.

After joining the Max-Planck-Institute for Radioastronomy (MPIfR) in 1974, he was initially involved in the development of astronomical infrared photometers. Since 1980, his interest shifted to millimeter/submillimeter wavelengths, concentrating on the development of single-beam continuum radiometers and latter arrays on the basis of bolometers. At the MPIfR, he is the Leader of the Bolometer Group. As coinvestigator of ISOPHOT, he led the development, fabrication, and qualification of far-infrared filters for that space experiment. His current research concentrates on the development of large-format arrays of bolometers.

**Hans Peter Gemuend** received the Diplom degree in physics and engineering and the Dr.-Ing. degree from the Technical University of Berlin, Berlin, Germany, in 1974 and 1979, respectively. His doctoral dissertation concerned the investigation of the dynamics of the magnetic switching in thin films at low temperatures.

He is currently a Senior Scientist at the Max-Planck-Institute for Radioastronomy (MPIfR), Bonn, Germany. Since 1980, he has been involved with the MPIfR's Submillimeter Technology Division. His main research is the development of filters for millimeter to infrared wavelengths and the implementation of such filters to radioastronomical instruments.