Optics and Fluid Dynamics Department annual progress report for 1997

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Publication date:
1998

Document Version
Publisher's PDF, also known as Version of record

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Citation (APA):

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Optics and Fluid Dynamics
Department
Annual Progress Report for 1997

Edited by S.G. Hanson, P.M. Johansen, L. Lading,
J.P. Lynov and B. Skaarup

Risø National Laboratory, Roskilde, Denmark
January 1998
Abstract  Research in the Optics and Fluid Dynamics Department has been performed within the following three programme areas: (1) optical materials, (2) optical diagnostics and information processing and (3) plasma and fluid dynamics. The work is concentrated on combinations of systems, structures and materials. The systems work is focused on sensors, information processing and storage; the structures work is concentrated on pattern formation and diffractive elements; the materials work is centred on the understanding and utilisation of novel materials and nonlinear phenomena for optical components and systems. Scientific computing is an integral part of the work. Biomedical optics is a new activity and the work on polymer optics is enhanced considerably. The activities are supported by several EU programmes, including EURATOM, by research councils and by industry. A summary of the activities in 1997 is presented.

The cover picture shows out-of-plane coupling from a thin-film waveguide comprising a surface-relief grating. Shown is a snapshot of the $H_z$ field component. The wave propagation is simulated using a highly accurate spectral time-domain method.

ISBN 87-550-2339-8
ISSN 0106-2840
ISSN 0906-1797

Grafisk Service · Risø · 1997

Risø-R-1015(EN)
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1. Introduction

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The department performs basic and applied research within optics and nonlinear dynamics, which includes fluids and plasmas. The scope is understanding of physical phenomena as well as development of materials and systems for specific applications. The activities are often carried out in collaboration with other research groups or industry. The training of students at a graduate level is an integral part of the activities and so is the dissemination of results to research and industry.

The work is of importance to the understanding of coherent structures in fluids, plasmas and nonlinear optical systems, as well as to the understanding of optical diagnostic systems and new optical materials. However, the understanding of basic physical phenomena has to be used for devising solutions to problems. This is done in connection with (1) new sensors and measuring systems, (2) the processing of spatial data, (3) devising schemes for novel laser systems and (4) information storage systems. Several results are exploited by industry. The activities are supported by a number of national and international granting agencies. Risø National Laboratory was evaluated in 1997 and so was the department. We operate under a four-year contract with the Ministry of Research and Information Technology. 1997 was the last year under the previous contract. It may be in order here to include some of the main conclusions of the evaluation committee concerning this particular department. The committee recognises that the department has developed good activity in its core areas. It is recommended that prioritised focus is maintained in order to make sure that the rigorous objectives are met within a limited scope of research areas. The industrial collaboration is acknowledged. However, it is questioned whether the research is too far from exploitation and it is stated that reliable facilities are necessary if the department wants to be successful in partnering with industry.

We may put this evaluation in perspective by considering the evolution in (1) publications as illustrated in Figure 1 and (2) income from industry as seen in Figure 2. We find that the two figures are in good accord with two of the main objectives of Risø: to produce good science with industrial applications. The number of submitted patent applications has also increased considerably, but what is probably more important is that the number of initiated contract negotiations and agreements has been considerably larger than ever before. Only research funding from granting agencies did not fulfil expectations.

The activities of the department were thoroughly considered based on the evaluation report. Areas that could enhance the likelihood of exploitation of research results were identified. It was decided that efforts in the following areas would be enhanced:

- polymer optics,
- biomedical optics, and
- microflows.
The department has three programme areas: (1) optical materials (2) optical diagnostics and information processing and (3) plasma and fluid dynamics. There is considerable interaction between the programmes. Several activities are organised in joint projects. An organisational chart is shown in Figure 3.

The work described in this report falls within the following categories:

- **Nonlinear dynamics in plasmas, fluids and optical systems** with novel results on optical turbulence and plasma diagnostics.

- **Optical materials** concentrated on material physics and applications in sensors, information processing and storage with major results on fabrication of diffractive elements and modelling of nonlinear light interaction with polymers.

- **Diagnostics and sensors** for probing physical systems using diffractive optics where new schemes for using speckle dynamics were developed and analysed, and initiatives taken to enhance the work in biomedical optics.

- **Scientific computing** focusing on the application of spectral models to highly nonlinear distributed systems where novel methods for the numerical analysis of systems with waveguides and surface diffractive structures are being developed.

- **Information processing**, both electronic and optical, for pattern recognition and illumination with structured light in industrial systems with new results on memory based neural networks and energy efficient pattern projection.

![Graph of Refereed Publications - Optics and Fluid Dynamics](image)

Figure 1. Number of refereed publications published by the staff of the department per year. The number of publications per scientist has doubled in the period shown here. The minimum in 1992-93 occurred in connection with a reorientation of several of the activities of the department.
Figure 2. Industrial income per year for the department. (Income related to Euratom activities is not included.)

Figure 3. Organisational chart of the Optics and Fluid Dynamics Department. The lower boxes indicate the major areas of activity.
2. Optical Materials

2.1 Introduction

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The year 1997 has been one of considerable challenge to the Optical Materials research programme. The recommendations made in connection with the international evaluation of Risø together with a new performance contract with the Ministry of Research and Technology have called for redirection of the scientific priorities of the research programme and for the scientists to broaden their projects so that they will be able better to cover both the educational aspects and industrial collaboration in the individual research projects that take place within the research programme. This will be an ongoing process in the years to come, since focus will be directed towards the technological impact of the scientific results achieved. Moreover, a new field encompassing the combination of optics and polymers will be sought implemented in close collaboration with the Condensed Matter Physics and Chemistry Department. However, for these activities to be fully implemented substantial funding will be necessary and, hopefully, such funding can be attracted under the cover of the new Danish National Research Strategy to be implemented in 1998.

The projects within the Optical Materials research programme are organised in two main directions covering the interaction of coherent laser light with organic and inorganic materials, respectively. Moreover, activities on manufacturing new materials by means of laser-assisted deposition and by fabrication of various optical elements are taking place.

The significant new results obtained in 1997 can be summarised as follows:

• In the organic research, remarkable, new results on the fabrication of diffractive optics using conventional compact disc technology have been achieved in collaboration with the Danish CD manufacturer, SDC-DanDisc. By this technology it has proven feasible to mass-produce optical elements at low costs and, consequently, to remove a major obstacle for industrial use of such elements. It is worth noting that the results have been obtained without external funding from research councils or other funding bodies. Within the activities on azobenzene side-chain polymers for storage purposes a new model based on so-called mean-field theory has been constructed from which it has been shown that intermolecular forces play an essential role in the understanding of the way in which holograms are formed in the material. Moreover, within the framework of the same model it has been demonstrated that the photoinduced structural changes observed experimentally can also be successfully explained. Furthermore, the anisotropy and topography of the deep surface relief gratings have
been investigated by means of polarised diffraction experiments from which the contributions to the diffraction efficiency from anisotropy and surface relief, respectively, can be separated. Finally, the properties of linear and circular birefringence and linear and circular dichroism have been characterised in these materials.

- The inorganic research has also resulted in a very notable, new result, namely the invention of a mode-locked laser diode array by means of phase conjugate feedback. The resulting high-power single-mode laser system has unique coherence properties and has been patented only recently. A two-photon photorefractive effect has been found in the piezoelectric material of La$_3$Ga$_5$SiO$_{14}$ which makes this crystal particularly interesting for applications in two-colour gated recording and for studying the photorefractive effect in the resonant two-photon absorption regime. When information is stored in photorefractive media, the so-called non-linear cross talk between images becomes important for establishing the fundamental limits of storage capacity. In the context, a new strong index grating stemming from a three-wave recording process has experimentally characterised the rise time that was found to depend strongly on the intensity ratio of the incident recording beams. As regards the excitation of parametric states in photorefractive media, it has been shown theoretically that the simplest case of the central subharmonic is unstable and, hence, cannot exist as an end-state. The transversal state, however, is shown to be stable. The thin film production of ITO thin films by means of pulsed laser deposition has been continued and has resulted in films with remarkably low surface roughness. Holographic gratings have been generated in these films with a laser wavelength of 363 nm, the existence of which has been measured by diffraction of a read-out laser beam. A set-up for measuring the angular distribution of neutrals as well as ions under pulsed UV laser ablation has been constructed. By measuring the ion flux with a probe it has proven possible to deduce the exact position of the incident laser beam on the target which is of importance to practical ablation of materials.

2.2 Organic Materials

2.2.1 Photoinduced anisotropy

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Among the potential materials for reversible optical data storage the liquid crystalline azobenzene side-chain polyesters are especially promising due to their unique optical properties. Holograms of very high diffraction efficiency can be written (and erased) by laser illumination in this material and, equally important, the holograms are exceptionally stable. In order to clarify the mechanism responsible for these remarkable properties we have constructed a mean-field theory of the storage process. It has been shown that the intermolecular forces are essential
for an understanding of the way in which holograms are gradually stored during illumination. An example of the comparison between theory and experiment is shown in Figure 4. In addition, the mean-field theory has provided an explanation for the stability of the holograms. This explanation is based on theoretical results that show that the optical data are stored in entire **domains** rather than in individual molecules. Hence, the superior stability of a large domain in comparison with a single molecule is transferred to the optical hologram.

Figure 4. During illumination by laser light the refractive indices of the azobenzene polymer change and the material becomes anisotropic. The figure shows a comparison between theoretical and experimental results for the time dependence of the phase difference $\Delta \phi$ which is a measure of the degree of anisotropy. In an optical storage system the data are encoded as a localised change of the optical properties via this photoinduced anisotropy.


2.2.2 **Photoinduced surface reliefs**

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Another example of photoinduced structural changes in azobenzene polymers is the formation of surface structures on illuminated films. Experimentally, it has been shown that these structures form even when the material is illuminated by two orthogonally polarised laser beams so that the intensity is completely uniform. Therefore, the formation of surface reliefs cannot be due to thermal effects (a thermal driving force would require the presence of a spatially varying intensity). Instead, we have proposed an explanation\(^1\) based essentially on the mean-field discussed above. The idea follows from the observation that even though the total intensity of the writing beams is spatially constant, the polarisation state of the total electric field varies in space. Thus, according to the mean-field theory, ordered molecular structures with varying orientations and degrees of order are formed. In turn, the
attractive intermolecular forces pull material into regions with a high degree of order and a suitable orientation for the migration of material. The resulting profile is shown in Figure 5.

![Figure 5. Comparison between the experimental and theoretical surface profiles produced under illumination by two orthogonal circularly polarised beams.](image)


2.2.3 An analysis of the anisotropic and topographic gratings in a side-chain liquid crystalline polyester

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Deep surface relief gratings with large aspect ratios have considerable potential as holographic optical elements. We have previously reported the observation of strong surface relief features in a side-chain liquid crystalline azobenzene polyester irradiated with two orthogonally polarised laser beams in a polarisation holographic set-up. The side-chain liquid crystalline polyester denoted P6a12 was synthesised by transesterification of 2-[6-[4-[4-(cyanophenyl)azo]-phenoxy]-hexyl]-1,3-propanediol and diphenyl tetradecanedioate in the melt. Films with a typical thickness of 1.5 μm are spincoated on glass substrates and exposed to two orthogonally circularly polarised beams at 488 nm. Both an anisotropic grating and a surface relief grating are found to result. A weak, plane-polarised HeNe laser beam at 633 nm is used to measure the diffracted power in various orders. The first-order diffracted beam is then passed through a Wollaston prism. Through measurements of the horizontal and vertical polarisation contributions to the diffracted beam, it is possible to separate the contributions to the diffraction efficiency into an anisotropic part and a surface relief part. When the HeNe beam is vertically polarised, the intensities of the two beams after the Wollaston prism are given by:
\[ I_{vv} = \left| a + be^{\delta_0} \right|^2 = a^2 + b^2 + 2ab \cos \delta_0 \]  \hspace{1cm} (2.1)

and

\[ I_{vh} = a^2. \]  \hspace{1cm} (2.2)

In the above equations, \( a = \sin(\Delta \phi)/2 \), and \( b = \cos(\Delta \phi)J_1(\Delta \psi) \). \( \Delta \phi \) and \( \Delta \psi \) are the phase differences due to anisotropy and surface relief in the films. \( J_1(\Delta \psi) \) is the first-order Bessel function of the first kind in \( \Delta \psi \). \( \delta_0 \) accounts for a possible phase shift between the anisotropic and the surface relief gratings. When illuminated with a horizontally polarised probe beam, the intensities are given by:

\[ I_{hv} = a^2, \]  \hspace{1cm} (2.3)

and

\[ I_{hh} = \left| -a + be^{\delta_0} \right|^2 = a^2 + b^2 - 2ab \cos \delta_0. \]  \hspace{1cm} (2.4)

Thus, by measuring the intensities \( I_{vv}, I_{vh}, I_{hh} \) and \( I_{hv} \), we can find the phase shifts \( \Delta \phi \) and \( \Delta \psi \). Figure 6 shows the experimental curves for the different intensities as a function of time of a laser of 75 mW corresponding to an incident intensity of 1060 mW/cm\(^2\), and the calculated values of the anisotropy, \( \Delta \phi \), and the phase difference due to surface relief \( \Delta \psi \). It is seen that the gratings due to anisotropy and surface relief arise at the same time.

![Figure 6. Diffraction efficiency and derived phase shifts as a function of time.](image)

We also find strongly polarisation dependent surface relief patterns. We believe that the surface relief appears due to the modulation of the magnitude and direction of the interfacial tension between regions illuminated with light with different polarisations.

2.2.4 Polarimetric investigation of materials with both linear and circular anisotropy

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We have investigated light propagation through materials with both linear and circular anisotropy and have found the relation of the amplitude and polarisation transfer functions to the four anisotropic characteristics: linear and circular birefringence as well as linear and circular dichroism. In our experiments we have used films of side-chain liquid crystalline azobenzene polyesters. The films are illuminated with elliptically polarised 488 nm radiation from an argon ion laser, with difference ellipticities. The Stokes parameters $S_{j}^{\text{out}}$ ($j = 0, 1, 2, 3$) of a weak HeNe probe beam at 633 nm are measured after passage through the film. We find that when the exciting beam is elliptically polarised, circular anisotropy is induced in the films in addition to linear anisotropy. The following table summarises the results of these measurements:

<table>
<thead>
<tr>
<th>Ellipticity of exciting light (e)</th>
<th>Ratio of circular to linear birefringence</th>
<th>Ratio of circular to linear dichroism</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>0.2</td>
<td>0.17</td>
<td>0.18</td>
</tr>
<tr>
<td>0.7</td>
<td>1.28</td>
<td>1.8</td>
</tr>
<tr>
<td>0.97</td>
<td>2.96</td>
<td>10.00</td>
</tr>
</tbody>
</table>

Table 1.

It is seen that the ratio of circular to linear anisotropy increases with increase in the exciting light ellipticity. The determination of the optical constants of materials with both linear and circular anisotropy is of importance to the design, analysis and synthesis of new optical polarisation elements such as polarisation holographic gratings, beamsplitters and multiplexers.


2.2.5 Fabrication of diffractive optics using compact disc technology

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The use of diffractive optics has hitherto been limited mainly because suitable methods for mass fabrication were unavailable. During the past five years one particular technology that can accommodate for this demand has emerged, viz. the compact disc technology. There are a couple of reasons why this production method is particularly suited for mass fabrication of diffractive optics. Firstly, the dimensions of the information bearing pits in the CD are comparable with those of diffractive optics, i.e. $\approx 1 \, \mu m$. Secondly, the process yields a polymer
replica free from stress-induced birefringence. Last, but not least, the
wavefront distortion from the polycarbonate injection moulded disc is
very low. With this technique including simple Fresnel zone plate arrays,
see Figure 7 and Figure 8, and complex elements for use in laser-based
sensors, a number of diffractive optical elements have successfully been
replicated at SDC-DanDisc, a Danish CD manufacturer.1

Figure 7. Atomic Force Microscope (AFM)
image of Fresnel zone plate on compact disc.

Figure 8. Fresnel zone plate mass-produced by CD-
technology photographed by phase-contrast microscopy.

1. L. Lindvold and E. Rasmussen, “Massefabrikation af diffraaktiv optik
med Compact Disc teknologi”, DOPS NYT 4-97, 1997.

2.2.6 The use of elastomer micromoulding to create replicated
diffractive optics from a UV-curable resin

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A facile method1 for replication of diffractive optics has been developed.
The method is based on the techniques that have been developed for
microcontact printing. One of the key elements in this procedure is the
fabrication of a mould made from an elastomer poly (dimethylsiloxane).
This moulding technique yields precision moulds with feature sizes down
to 50 nm and aspect ratios from 1:0.5 to 1:2, which makes it very suitable
for replicating surface relief diffracting structures. Due to the excellent
release properties of the elastomer, direct copies from a photoresist
master can be obtained without damaging the master. The elastomer copy
can be utilised directly to make a polymer replica by sandwiching a UV-
curable resin between the elastomer stamper and a substrate. Irradiating
the UV-resin with UV light hardens the resin in 10 sec. The elastomer
mould is removed and the replica can be postpolymerised. Using this
method the use of time-consuming electroforming procedures can be
avoided.

1. L. R. Lindvold, E. Rasmussen and N. B. Larsen (Risø National
Laboratory); M. Rasmussen and J. B. Rasmussen (Ibsen Micro Structures
A/S), “Use of elastomer micromoulding to create replicated diffractive
optics from a UV-curable resin”, Proc SPIE 3291, to be published in
1998.
2.3 Inorganic Materials

2.3.1 Stationary states of photorefractive parametric oscillation

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The theoretical explanation of photorefractive parametric oscillation has entered a new era. Previously it was only possible to describe the threshold for excitation of the parametric oscillation as a function of various parameters, whereas it is now possible to explain the behaviour of the stationary states reached after the threshold has been exceeded.

Photorefractive parametric oscillation can be observed when a running holographic grating is written in a photorefractive crystal of, e.g., Bi$_{12}$SiO$_{20}$ (BSO). A schematic presentation of the set-up is shown in Figure 9. Two writing beams from an argon-ion laser at a wavelength of 514.5 nm form an interference pattern in the BSO crystal. A slight frequency shift in one of the beams causes the interference pattern to run and for a sufficiently small contrast a holographic grating with the same spatial frequency $K$ and temporal frequency $\Omega$ as the interference pattern is recorded in the material. These frequencies are termed the fundamental frequencies. If the contrast is increased, however, a very beautiful process can appear: new gratings that can be generated with frequencies lower than the fundamental ones. This effect is termed photorefractive parametric oscillation. Experimentally, such gratings can be observed by using a read-out laser Bragg-matched to them. During the last years the thresholds for these excitations have been described, but very recently initiatives have been taken to investigate the stationary state reached after growth of the new gratings.\footnote{It has been shown that the simplest case when the new grating has the frequencies $K/2$ and $\Omega/2$ is actually unstable and, for that reason, cannot exist as an end-state. If, on the other hand, the transversal state in which two new gratings split up transversally to the fundamental grating is analysed, it can be shown that a stable state can be reached.\footnote{This is shown in Figure 10.}} These investigations are purely theoretical, but will be followed up by experimental verifications in the new year.
Figure 9. Schematic set-up for recording and read-out of holographic gratings in photorefractive BSO.

Figure 10. Grating wave vector diagram for the stable end-state in which two new gratings with opposite transversal components are present.


2.3.2 Single-mode laser diode array with phase conjugate feedback

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Single-mode semiconductor lasers provide spectrally and spatially coherent light. High optical power density of quantum-well laser diodes can, however, thermally destroy the sensitive nanostructures of these devices - especially the facets. Consequently, the quantum-well laser diodes are limited to an optical output power of maximally 200 mW. But in many applications much higher output power is needed. One approach to increase the output power is to form an array of laser elements. Such laser diode arrays are now commercially available with output power exceeding 20 W. Unfortunately, these devices suffer from a multimode non-diffraction limited radiation pattern and have a very short coherence length of a few hundred micrometers, which limits the usefulness of the output beam.

We have invented a new high-power single-mode laser system\textsuperscript{1} that has an output beam with unique coherence properties. The system, which
is shown in Figure 11, is based on a high-power GaAlAs laser diode array coupled to a photorefractive phase conjugator. The phase conjugate feedback is made frequency selective by placing a high finesse Fabry-Perot etalon in the external cavity between the conjugator and the laser diode array. The frequency selective feedback system forces the multimode laser diode array to oscillate in a single spatial and a single longitudinal mode with conversion efficiency exceeding 90%. In comparison with the freely running laser diode array, the line width has been reduced to less than 0.02 nm, the coherence length has been increased by a factor of 70 and the output has become diffraction limited. The last-mentioned factor implies that the output beam can be focused to a spot at the size of a wavelength. More than 80% of the total energy provided by the laser diode array can be extracted from the single-mode laser system.

![Figure 11. A GaAlAs laser diode array with phase conjugate feedback from a BaTiO$_3$ crystal. L1, L2, L3 and L4 are lenses, WP is a half-wave plate, SF is a spatial filter and ET is an etalon.](image)


### 2.3.3 Photorefractive information storage

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In the photorefractive information storage research project a new kind of cross talk between holographic information in photorefractive optical memories is investigated. In the optical storage set-up, multiple gratings are induced in the photorefractive material due to the interference between one reference beam and N object beams. Because of the non-linear nature of the photorefractive electric space charge field, the holographic gratings interact and, in specific cases, cause changes in the holographic diffraction efficiency by up to more than 90%.

The cross talk is investigated experimentally and theoretically in different photorefractive materials such as Bi$_{12}$SiO$_{20}$, LiNbO$_3$ and BaTiO$_3$. The purpose of the experimental work is to establish the fundamental nature of the cross talk, i.e. how it is controlled and how it influences the data storage capacity.
We have investigated the effects of non-linear interaction between gratings in Bi$_{12}$SiO$_{20}$ and have shown that even in the limit of low diffraction efficiencies (below 0.1%) strong modifications of the fundamental gratings are present.\(^1,2\) Applying an electric field to the Bi$_{12}$SiO$_{20}$ sample, we have shown that the coupling between gratings can be so pronounced that one grating completely cancels another grating.\(^2\)

Recently, we have shown that higher order combinational gratings play an important role in explaining cross talk between index gratings in photorefractive media. We have presented the first experimental results of the existence of a new, strong combinational index higher order grating in a three-wave mixing experiment.\(^3\) The rise time of the new grating is strongly dependent on the intensity ratio of the incident recording beams as opposed to the first harmonic grating. Furthermore, the spectral dependence of the cross talk has been investigated. Unusually high cross talk has been observed in Bi$_{12}$SiO$_{20}$ at wavelengths of 488 nm and 476 nm.\(^4\)

The data storage project is supported by the Danish Technical Research Council under grant # 9502694.

2. P. M. Petersen, P. E. Andersen and P. Buchhave, "Enhanced nonlinear interaction between gratings in drift dominated photorefractive Bi$_{12}$SiO$_{20}$", CLEO Technical Digest vol. 15 (paper CThI58), Baltimore, USA, 323-326, 1995.

2.3.4 Two-photon photorefractive effect in piezoelectric La$_3$Ga$_5$SiO$_{14}$ crystals doped with Pr$^{3+}$

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In the continuous search for new photorefractive materials for applications in the fields of, e.g., holographic data storage and adaptive optics, we investigate the photorefractive effect in piezoelectric La$_3$Ga$_5$SiO$_{14}$ crystals doped with Pr$^{3+}$ ions.

In a previous investigation\(^1\) the different charge migration processes responsible for the photorefractive effect were investigated and revealed a substantial contribution from the photovoltaic effect. The purpose of this work is to investigate the charge excitation processes leading to the photovoltaic effect.

The absorption spectrum of the crystal is shown in Figure 12. The sharp features of the spectrum can unambiguously be ascribed to transitions of the 4f$^2$ multiplet of the Pr$^{3+}$ ions. Earlier investigations of
the photorefractive effect in the crystal were made at $\lambda = 514$ nm. This wavelength lies just outside the resonance of the absorption spectrum.

![Figure 12. Absorption spectrum for La$_3$Ga$_5$SiO$_{14}$:Pr$^{3+}$.](image)

![Figure 13. Illustration of a resonant two-photon excitation process.](image)

In our experiments the photorefractive effect was investigated at the resonant frequency $\lambda = 488$ nm. This investigation revealed a quadratic dependence of the diffraction efficiency on intensity which indicated that the excitation processes at this frequency are of a two-photon nature. Electrons are first excited from the ground state (G) of the $4f^2$ multiplet to an intermediate (I) metastable state of the multiplet (see Figure 13). From this state electrons are excited to the conduction band of the material giving rise to charge transport leading to the photorefractive effect.

The two-photon nature of the excitation processes makes the crystal an exciting candidate for applications in two-colour gated recording. Also, the material opens for the possibility of studying the photorefractive effect in the resonant two-photon absorption regime.

2.3.5 Electrons emitted from solid deuterium excited by keV electrons

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The solid hydrogens are the most volatile targets that exist in equilibrium with vacuum. These solids show peculiar features during bombardment by charged particles, primarily because of the weak binding of the molecules to the solid. In the past we have studied the erosion of these solids, since pellets of the solid hydrogens play and will play an important role for controlling the particle density in present and future fusion devices.

We have for the first time measured the energy distribution of D$_2$ molecules ejected from solid deuterium. For other volatile solids, the energy distribution has been an important tool to identify the mechanisms that provide the molecules with translational energy for ejection. The spectrum shown in Figure 14 exhibits a peak around a few meV, which may be indicative of a strong component induced by a linear collision cascade. The structure superimposed on the high-energy part of the spectrum originates from ejection processes at the surface. However, the low-energy part of the spectrum comprises a thermal component in addition to the collision cascade contribution. Such a thermal component occurs because of the volatility of solid deuterium and is usually not seen for other solids.

The particles ejected were almost exclusively D$_2$ molecules, but a minor fraction of D$_4$ molecules was detected as well. D atoms are probably also emitted, but cannot be observed due to the relatively high background level.

![Energy distribution of sputtered particles for 0.5 keV electron bombardment at a target temperature of 3.2 K. The linear collision cascade spectrum (dashed line) is shown as well.](image)

Figure 14. Energy distribution of sputtered particles for 0.5 keV electron bombardment at a target temperature of 3.2 K. The linear collision cascade spectrum (dashed line) is shown as well.

2.3.6 Production of transparent, conductive optical films by pulsed laser deposition

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Pulsed laser deposition is a widely used technique for thin film deposition of many types of materials. The advantage of the method is that the chemical composition of a target may be reproduced in a film on a suitable substrate. Another important point is that the target particles typically arrive at the substrate with an energy that exceeds 1 eV. The high energy enhances the surface mobility on the growing film, which generally improves the crystalline quality of the film.

We have studied films of indium tin oxide (ITO), which is a transparent, conductive material. This material is used as electrodes for optical components, but is also being considered as a medium for optical storage.¹

We have measured the specific resistivity for thin films produced in oxygen, neon, argon and xenon ambient gas substrates at room temperature as well as at 200°C and 300 °C. (Figure 15). The lowest specific resistivity is obtained for oxygen with a substrate temperature of 200°C. Nevertheless, one notes that it is possible to produce conductive films within a certain pressure interval during deposition for all gases at room temperature. This is not possible with any other method, which always requires a heated substrate.

Even the room temperature films turned out to have remarkably low roughness. Observations with an atomic force microscope indicate that these films were typically formed with grains up to a diameter of 100-200 nm of less than 0.5 nm roughness. For larger areas of sizes up to micrometers the roughness variation was at most 10-20 nm.
Figure 15. Specific resistivity versus background gas pressure for ITO films deposited in oxygen, neon, argon and xenon, respectively. Measurements are made both for films deposited on non-heated and heated substrates. Film thicknesses are between 25 and 260 nm.


2.3.7 Holographic gratings produced in transparent films made by laser ablation

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Gratings generated by two coherent beams from an ion laser have been observed in an indium tin oxide (ITO) film produced by pulsed laser ablation. Such gratings have earlier been demonstrated to exist in sputter-deposited films produced on hot substrates. We have for the first time demonstrated that holographic gratings can be generated in ITO films produced at room temperature. ITO has the special property that it is a transparent conductor. Therefore, electrodes on optical components are frequently made of ITO and are also often produced by laser ablation.

We have extended earlier studies with a Kr-ion laser to an Ar-ion laser operating at 363 nm. Two coherent beams are adjusted to overlap in the film plane and produce an interference pattern that creates the holographic grating. A weak, diffracted HeNe laser beam confirms the existence of this grating.
Deposition of materials by laser ablation is a standard technique for producing thin films of complicated composition. However, the basic processes in pulsed laser deposition, the interaction of light with a solid and the material transport to a substrate, are not known in any detail. We have, therefore, constructed a set-up to study some of the basic processes in pulsed UV laser ablation: the angular distribution of the neutrals as well as the ions. To simplify the experimental parameters, we have studied an elemental metal target rather than a chemical compound, and a target in vacuum rather than one in a background gas.

The ions produced in the plume of the ablation plasma were collected by a system of 14 Langmuir probes positioned on a semicircular holder with a silver target in the centre and a radius of 8 cm from the probes to the target. The collected current makes it possible to determine the angular distribution of the ions. Since we have previously measured the distribution of the emitted particles, ions + neutrals,\(^1\) we were able to determine the ion fraction of the emitted particles as well. At low fluences, 0.9 J/cm\(^2\), the dominant fraction is neutral, but with increasing energy practically all emitted particles become ionised. In particular, all particles are ionised in the forward directed plume at fluences above 2 J/cm\(^2\).\(^2\)

The probe signal provides us with the current as a function of time for all probe directions. Such a signal can be converted to a time-of-flight spectrum or an energy distribution of the emitted atomic ions. It turns out that there is a high-energy tail with atoms up to more than 500 eV in directions close to the normal and for fluences above 2 J/cm\(^2\) (Figure 16).\(^3\) With increasing angle with respect to the normal the energy as well as the intensity of the emitted ions decrease.

These energy distributions are important because particles with energies exceeding 20 eV can produce defects in films or even sputtering. Both effects are highly undesirable, but are usually suppressed by a background gas that slows down the particles that arrive at a film.
Figure 16. Energy distribution for ions in a log-log plot for a fluence of 2.5 J/cm² (upper figure) and 0.8 J/cm² (lower figure).


2.3.9 Ion probe measurement of pulsed laser deposition in a reactive atmosphere

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Deposition of materials by pulsed laser ablation is a standard technique for producing films of, e.g., oxides. Pulsed laser ablation of such oxide films is usually performed with an ambient gas at a pressure around 0.01-1 mtorr. The thin oxygen background gas may maintain the stoichiometry of oxide films heated to high temperatures (500-700°C), but has the additional effect that target particles are slowed down to acceptable
energies before the impact on a film. Otherwise, energetic particles from the target produce defects or even sputtering of the film. Both processes reduce the crystalline quality of the film.

A problem of great practical importance is to know the precise position of the laser beam on the target since the flux of emitted particles has very strong directional dependence. The ion flux registered with a Langmuir probe gives instantaneous information about the position of the beam for a known background pressure, laser pulse energy and probe position.

We have performed a series of ion probe measurements as a function of oxygen pressure. A silver target was irradiated with an Nd: YAG laser at 355 nm with pulse energies typical for pulsed laser ablation. A characteristic ion signal with peak splitting is shown in Figure 17. The high-energy peak consists of particles that have passed the background gas without collisions, whereas the low-energy peak contains atoms that have undergone collisions with oxygen molecules from the background gas.

![Figure 17. Ion signal obtained with a probe biased with -40 V as a function of ion flight time.](image_url)
3. Optical Diagnostics and Information Processing

3.1 Introduction

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The second year after the reorganisation of the Optics and Fluid Dynamics Department has been terminated, a year in which a slight change of focus for Risø National Laboratory has been called for: larger emphasis has to be put on programmes and dedicated projects with industrial participation. This demand is taken seriously in the programme on Optical Diagnostics and Information Processing and has already resulted in a series of contacts and agreements with, in particular, Danish industrial partners. The change has not required drastic actions to be taken, but is generally in the line of the ongoing way of selecting projects. The combination of a profound understanding of the basic physics and good knowledge of measurement techniques provides for viable and comprehensive concept design. The manifold fields into which the work in the programme and in the department itself is divided are continuously being viewed as an advantage. Combinations of disciplines offer a fan of opportunities for especially industrial partners - a benefit which is frequently being recognised by our partners.

Basic scientific research in the field of infrared spectroscopy undertaken for the last couple of years has resulted in participation in a large European programme on investigation of exhaust gases from jet engines in collaboration with Deutsche Forschungsanstalt für Luft- und Raumfahrt, British Aerospace and Alfa Romeo Avio. Determination of hot gaseous constituents based on simultaneous measurement of transmitted and emitted radiation through a plume has here been proven feasible and has thus provided a new tool for combustion diagnostics.

A research field in medical optics has been successfully launched with the start of a Ph.D. project. Optical methods may in the future prove to be a valuable tool in non-invasive diagnostics without ionising radiation. Unfortunately, a large project headed by Risø National Laboratory with participation of universities, hospitals and a Danish industrial partner has for political reasons not been supported yet.

Two large projects including memory-based networks for pattern recognition have with great success been concluded in 1997 and will open up for a closer engagement of this group’s expertise in the field of medical optics where the need for data extraction and pattern recognition is imperative.

A one-year participation in a programme headed by Mikroelektronik Centret at the Technical University of Denmark has been terminated. A systematic description of the statistics of light scattered from rough surfaces has been presented with special emphasis on the dynamics of the
speckle patterns. This facilitates stringent analysis of various systems for monitoring of linear and angular velocities and displacements.

Together with the Japanese company Hamamatsu a previous basic patent has been extended to provide future industrial implementation. The aim is to introduce pattern generation using phase filters instead of amplitude filters, thereby uncovering very energy efficient ways of producing patterns for printing, display, etc.

Though the year 1997 has called for a slight change in focus, the momentum of the programme has been kept. During our work in the past year and the accompanying discussions on future projects, we have observed good indications of a robust impact on society in the coming years. The combination of theoretical and practical knowledge provides for a package just as suited for industrial collaboration as for basic scientific work.

### 3.2 Infrared Technology

#### 3.2.1 Diffuse reflectance infrared Fourier transform spectroscopy of mineral powders

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A method for analysing the content of carbonates in precursor powder by diffuse reflectance infrared Fourier transform spectroscopy (DRIFTS) has been developed and is now used routinely to analyse commercial superconductor powders. The detection limit of the carbonates by using this method was determined to be better than 100 ppm (% weight).

Methods for analysing powder samples quantitatively are of great importance since many of the mineral powdery samples are insoluble in water. In addition, IR techniques can be used to determine the crystal structure of the sample and the chemical content of an amorphous sample as well. This makes IR-based spectroscopic techniques attractive and supplementary to, for instance, X-ray diffraction-based techniques. An example of this is shown in Figure 18 where the DRIFTS spectra of quartz and amorphous SiO$_2$ are displayed. Many complex mineral materials of industrial importance can be examined by DRIFTS in the mid-IR spectral range, for instance cements and glasses.

The feasibility of using the DRIFTS technique for mineral powder analysis in a broader sense has been investigated.$^{1,2}$ Next year, the DRIFTS technique will be used to analyse the mineral content in biomass ashes. In this future work the focus will be on the possible detection of potassium salt compounds in order to understand their catalytic behaviour.
Figure 18. FTIR spectra of quartz and amorphous SiO$_2$. It is observed that the crystal structure of the quartz sample results in distinct and sharp spectral bands compared with the smooth spectral bands of SiO$_2$.

A specular reflectance accessory to plug into the FTIR spectrometer will be available next year. By combining mid- and near-infrared detectors it is possible to cover the spectral range from 500-7000 cm$^{-1}$. The specular accessory provides a non-destructive method for measuring the reflectance of material surfaces.


3.2.2 Infrared temperature calibration

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A reference laboratory for calibration of infrared instruments was established at Risø in 1996. Traceable calibration of pyrometers and infrared thermometers is made with blackbodies in the temperature range –50 °C to 1600 °C. The work affects the following five main topics in reducing uncertainties of noncontact temperature measurements:

- calibration service of infrared thermometers for customers;
- temperature measurements for customers;
- research and development of improved methods for infrared temperature measurements;
- measurement of spectral emissivity of samples and coatings (Figure 19);
- consultative service and information.

Risø is involved in the EU project “Trirat” where of laboratories from most of Europe participate. The overall objective of the project is to provide improved, sub-Kelvin accuracy in infrared radiation.
thermometry at industrial levels in the range –50 °C to 800 °C. The traceability is transferred from the highest metrological levels down to the industrial level. We will work towards reaching sub-Kelvin accuracy of our calibration sources at low temperatures in the near future.

With the combination of high accuracy traceable blackbody sources and spectral measurements of infrared radiation Risø has state-of-art calibration capabilities.

Figure 19. Spectral emissivity of a coated aluminium sample.

### 3.2.3 FTIR emission-transmission spectrometry of gases at high temperatures

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The determination of gas temperatures and concentrations in combustion systems, flames, flares and chemical gaseous processes is crucial in order to understand and control the processes that take place in these systems. Fourier transform infrared spectroscopy (FTIR) is used for non-intrusive measurements to provide information about species concentrations and gas temperatures along a line of sight in combustion systems. It proves, however, to be more attractive to implement passive detection methods that are based on the measurements of the emitted thermal radiation from combustion systems that monitor the state of the industrial process in-situ.

To study the possibility of using passive methods we have designed and implemented an experimental set-up optimised for emission measurements that comprises an external blackbody source, a hot gas cell and an FTIR spectrometer (Figure 20). It is our future goal to develop and be able to implement passive methods based on the detection of thermal radiation from large industrial furnaces.
To examine the emissive behaviour of gases, a high-temperature gas cell was designed and tested with CO$_2$ at various concentrations. The gas cell was made of stainless steel and is used to measure the radiative and transmissive behaviour of carbon dioxide at various temperatures up to 1073 K. Figure 21 shows the transmittance spectra of CO$_2$ at three different concentrations.

A detailed analytic expression for the measured thermal radiation from a hot gas enclosed in the gas cell was developed. The expression is more complicated than that for transmittance because the thermal
radiation from heated parts inside the gas cell must be taken into consideration. It was necessary to measure the thermal characteristics of the heated sapphire windows placed inside the gas cell in order to describe the thermal radiance of the enclosed gas quantitatively. Figure 22 shows the measured radiance of a heated CO\textsubscript{2} gas sample. By the use of Planck’s radiation law it is possible to calculate the gas temperature on the basis of the radiance spectrum.

![Figure 22](image)

Figure 22. Calculated CO\textsubscript{2} spectral radiance at T\textsubscript{gas} = 473 K. The spectral bands of CO\textsubscript{2} are compared with a Planckian curve. a: with correction, b: without correction for instrument radiation.

The initiated work with the high gas temperature FTIR facility will be carried on next year in a three-year EU-project under the Brite Euram programme for non-intrusive measurement of gas temperature and chemical species in aircraft exhausts.

3.2.4 Optimisation of furnaces with an infrared fibre-optic probe

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Measurements of gas temperatures and gas concentrations in combustion and industrial processes where hot gases are produced are today carried out using intrusive techniques such as probes and extractive sampling systems with slow response times. Fourier transform infrared (FTIR) emission spectroscopy is a non-intrusive technique for simultaneous fast measurements of gas temperatures and concentrations in combustion systems using the infrared spectral features of the hot gases. The effective measuring time of a single-scan low-resolution spectrum is a few ms, i.e. sufficiently fast to resolve the temporal variations in most combustors. The infrared (IR) emission spectra contain valuable information about the process, e.g. information about the gas composition and temperature as well as the solid phase temperature. It is well known that solid surfaces and particles radiate a continuous spectrum, while gases radiate at characteristic spectral lines of the molecule, e.g. CO$_2$ has strong bands at 2350 and 3700 cm$^{-1}$. Other possible parameters to be measured are water vapour, soot and particle concentrations in the flue gas; unburnt gases can also be detected.

The capability of IR-techniques to operate in a harsh environment with fast response times makes them attractive for active control and regulation of the combustion process in systems where fuel properties vary.

A fibre-optic probe was developed at Risø about three years ago for measurement of local gas temperatures in furnaces and flames. The probe has since been improved and used in many different combustion applications.

Measurements have been performed in a straw-fired furnace, Masnedø Power Plant, located about 90 km south of Copenhagen. Approximately 7.2 tons (dry) of straw per hour are fed with screws into the furnace and are burnt on a vibrating grate. Risø’s water-cooled fibre-optic probe was inserted through an inspection port in the side wall looking across the furnace. The effects and time delays from load variations are shown in Figure 23. The period of fine structure of the gas temperature and water concentration fluctuations is 2 minutes, which is identical to the interval of the grate vibration. The variations in fuel load result in low frequency variations in gas temperature, water concentration and steam production. Approximately 75% of the water content in the flue gas is water formed by combustion of the straw. Water is formed only during pyrolysis of the straw, the early stage of the combustion process, whereas the conversion of the straw char results in the formation of CO$_2$. The following details about the furnace operation can be found from Figure 23:

- There is a fair correlation between the flue gas temperature, the water content, the steam flow and the load (signal from fuel feeding system) variations.
- Fuel load variations are reflected by variations in water concentration. A period with low water concentration is followed by a drop in gas temperature.
Steam flow variations follow the flue gas temperature with approximately a 2-minute delay. These effects might be used to control the fuel feeding system to provide smoother operation of the furnace. This work was carried out for Sjællandske Kraftværker I/S, Denmark.

Figure 23. Correlations between the load, the water content in the flue gas, the steam production and the flue gas temperature. The fuel load, the feeding velocity of the straw bale, was varied approximately 15% during the experiment. The curves on the flue gas temperature and the water concentration are running averages (approx. 50 s) based on 2000 instant measurements with the IR-probe.

The measurement of peak temperatures in flames is another example of the use of infrared spectroscopy (Figure 24). The measurement of instant gas peak temperatures is interesting with regard to understanding the process and the chemical reactions that take place. One example is the formation of nitrogen oxides (NO\textsubscript{x}) in oxygen-rich zones of the flame reaching high peak temperatures, thereby causing increased formation of thermal NO\textsubscript{x}. A second example is that the mixing of hot gas flows, such as the fuel-rich gas and air flows, may be studied by measuring the rapid gas temperature fluctuations.

Figure 24. A gas temperature profile through large-scale flame measured with Risø’s IR-probe. Mean value and standard deviation (i.e., ± 68.3% of measurements) of local gas temperatures are shown with dots and error bars, respectively. The peak temperature in the flame measured at the furnace wall (dashed lines) is in good agreement with measured gas temperatures in the centre of the flame. The y-axis is divided in 100°C. The scale of axes and other details are confidential.

3.2.5 Temperature measurements of burning fuel particles in fluidised bed combustor

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Solid fuels contain a varying amount of elements that affect the melting point of the ash, e.g. potassium, sodium, sulphur and chloride, which may cause significant operational problems in fluidised beds. The most important parameter influencing the bed agglomeration in a fluidised bed is the actual process temperature. It is well known that the temperature of the burning particles exceeds the bed temperature; furthermore, recent experiments performed in a pilot scale fluidised bed indicate that agglomeration starts on the surface of the fuel particles. It appears that the temperature of the burning particles is crucial for understanding and modelling the ash transformations and bed agglomeration process in fluidised beds.

The objective of the present work was to determine the exceeded temperatures of straw and sludge pellets burnt under selected operation conditions of a laboratory fluidised bed at ETC (Energy Technology Centre in Pite, Sweden), i.e. for different oxygen pressures and bed temperatures, with a new ceramic infrared probe developed at Risø.

An uncooled ceramic infrared probe inserted into the reactor (600-1100°C) was designed to transmit thermal radiation from the interior of the bed via an optical fibre to Fourier transform infrared spectrometer. The ceramic probe tip is uncooled to minimise disturbances of the temperature field in the reactor. The set-up allows
measurements of single-scan spectra in the spectral range 1750 to 7000 cm\(^{-1}\) (1.4 to 5.7 m) using an InSb detector with the spectrometer. A detailed drawing of the infrared-probe is shown in Figure 25. Thermal radiation within a 2 mm diameter circle at the sapphire window (90% of energy) is focused with a CaF\(_2\) lens on the end of the optical fibre. The tip of the probe is made of a 100 mm long and 8 mm outer diameter ceramic tube with a 1 mm thick, 5 mm in diameter, sapphire window closing the end of the tube. A high-temperature ceramic glue was used to fasten the window to the ceramic tube. The ceramic tube was chosen with an expansion coefficient similar to sapphire, i.e. about 5.5x10\(^{-6}\) m/K, to obtain a gastight probe tip over a large temperature range, i.e. from ambient to >1000°C. The probe is purged with a small gas flow to avoid gas absorption of CO\(_2\) and H\(_2\)O from atmospheric air that would otherwise enter into the probe. The replaceable ceramic probe tip is locked with two screws to the mount. The mount is water cooled to protect the lens and the optical fibre from heat from the reactor wall and heating elements.

![Design of the infrared probe](image)

Figure 25. Design of the infrared probe. a: sapphire window; b: ceramic tube; c: water cooled mount; d: lens; e: connector for the optical fibre and f: purge gas. The field of view of the probe is illustrated by the dotted lines.

![Graphs](image)

Figure 26. Experiment on ETC’s reactor at 740°C bed temperature, 200-250 μm sand particles and 3% oxygen. The probe was inserted 80 mm above the distributor plate. Example of data extracted from infrared spectra. It is observed that the emissivity of particles is close to 1 (blackbody radiation). The surface temperatures of the burning straw particles are up to 120°C higher than the bed temperature.
The probe has been used to investigate rapid temperature fluctuations in a laboratory fluidised-bed reactor with burning straw pellets, see Figure 26. Particle temperature measurements made in ten experiments with the bed operated at different bed temperatures, oxygen concentrations and size of sand particles will be compared and reported in the near future. Preliminary results surprisingly indicate that the operation conditions of the fluidised bed play a minor role.

3.3 Medical Optics

3.3.1 Biomedical optics and new laser systems

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The framework programme “Biomedical Optics and new Laser systems” (BiOL) is a new Danish initiative where engineers, physicists, chemists and physicians collaborate on the development of new biomedical applications based on the most recent progress in lasers and optical measurement techniques. Three universities, two university hospitals, one commercial company and one national research laboratory are represented. The aim is to conduct research in advanced laser systems and optical measurement technologies and to apply these systems in dermatology, ophthalmology and biosensing. The competence of the participating institutions includes advanced laser and femtosecond laser facilities, semiconductor laser growth facilities, microfluidics fabrication and handling, and experimental as well as clinical facilities at the hospitals. Finally, the BiOL programme establishes the foundation for education of young scientists in optics, medical science and biotechnology.

Purpose and research activities

The use of optics as a diagnostic tool offers several advantages over existing methods: (i) non-invasive procedures, (ii) use of non-ionising radiation and (iii) high spatial resolution imaging. Optics, thus, has the potential of providing unique clinical applications. The eye and the skin are immediately accessible for non-invasive optical procedures. The ongoing development of optical materials and laser systems with improved features facilitates the development of novel non-invasive diagnostic and therapeutic procedures, including high-precision imaging. However, there are major challenges that remain to be solved.

BiOL is an interdisciplinary collaborative effort, where engineers, physicists, chemists and physicians work closely together on developing non-invasive diagnostic procedures for specific biomedical uses. The main purpose of the BiOL framework programme is to develop biomedical applications within dermatology, ophthalmology and biosensing. The specific research topics include:

• novel imaging systems with high spatial resolution based on fast tunable laser sources for premature detection of skin cancer,
• non-invasive procedures for early detection of eye diseases based on autofluorescence of the lens and retina,
• integrated InGaAsP twin-laser sensors for detection of specific cell types and measurement of active biochemicals,
• improvement of existing imaging systems using a new theoretical model for light propagation in human tissue.

The common aspect in the above biomedical applications is the need for specially designed laser systems with properties that are currently unavailable. Therefore, BiOL enhances research in advanced laser systems and optical measurement techniques. The research topics within new laser systems include:
• fast tunable, single-frequency laser systems based on optical parametric oscillators,
• compact femtosecond lasers,
• high-power single-mode phase locked laser diode arrays,
• novel, integrated InGaAsP laser systems,
• new measurement techniques involving modelling the propagation of coherent optical fields in human tissue with emphasis on the coherence properties.

The BiOL programme comprises several collaborative efforts. The activities are displayed in Figure 27 illustrating the collaborative activities in the frame:
1. Non-invasive ocular spectroscopy and autofluorescence.
2. Systems for high-resolution imaging in turbid media.

![Figure 27. Collaborative activities in the BiOL programme.](image-url)
Participants in BiOL
Seven institutions and companies as well as one subcontractor participate in the BiOL frame:

- Optics and Fluid Dynamics Department, Risø National Laboratory, Roskilde, Denmark.
- Department of Chemistry, University of Aarhus, Aarhus, Denmark.
- Institute of Physics, The Technical University of Denmark, Lyngby, Denmark.
- GIGA A/S, Skovlunde, Denmark.
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Perspectives
Biomedical optics is a research field that is experiencing tremendous growth in terms of research activities and applications. The main reason is that optics has the potential of providing non-invasive diagnostic procedures leading to novel and improved methods, which may replace existing clinical procedures.

In the short term BiOL will provide novel biomedical applications such as high-resolution imaging in human tissue and highly sensitive affinity sensors for quantification of specific biochemicals. A key component to ensure this development is the light source. BiOL enhances research in advanced laser systems and simultaneously points out new areas for applications of lasers. In the long term new diagnostic and therapeutic procedures will result from the joint efforts of this collaboration. Furthermore, it provides the foundation for the education of young scientists highly specialised in optics, medical science and biotechnology.

3.3.2 Complex ambiguities in diffuse reflectance data obtained from multilayered structures

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Human skin consists of bounded layers with distinct optical properties. In applications it may be necessary to distinguish between these layers. A commonly used method in modelling light-tissue interactions is the so-called diffusion theory.\(^1\) Using this theory, the diffuse reflectance \(R(r)\) as a function of the source-detector separation \(r\) is calculated. This is also referred to as the reflectance profile.

For a single-layer or a semi-infinite medium, it is possible to extract the optical absorption coefficient \(\mu_a\) and the reduced scattering
coefficient \( \mu_\gamma = \mu_s (1 - g) \), where \( \mu_s \) is the scattering coefficient and \( g \) is the asymmetry parameter, from the shape of the reflectance profile. In this case, it has been shown that the following simple ambiguity exists:

\[
\mu_{s,1} = \mu_{s,1} (1 - g_1) \rightarrow \mu_{s,2} = \mu_{s,2} (1 - g_2).
\] (3.1)

Thus, it is possible to choose two different combinations of scattering coefficients and asymmetry parameters that yield the same reduced scattering coefficient. Keeping the absorption coefficient constant, this results in identical reflection profiles \( R(r) \).

We have modelled the light-tissue interaction on a three-layered structure using diffusion theory. In Ref. 2 we showed that the functional forms of the radial dependence of the diffuse reflectance \( R(r) \) from multilayer and single-layer models are identical. Hence, from a three-layer model \( R(r) \) may be substituted with a reflectance profile calculated from a single-layer structure.

The above hypothesis has been verified in the following way: a feedforward neural network making use of PLS (Partial Least Squares regression) data reduction has been trained to provide estimates of the optical absorption and reduced scattering coefficients for a single-layer structure. Then it is tested with a set of reflectance profiles calculated for a three-layer structure yielding two (effective) optical parameters for the test profiles. The effective optical parameters obtained were thereafter used to calculate \( R(r) \) for the single-layer structure, which showed a perfect match to \( R(r) \) for the three-layer case. Hence, this leads to a complex ambiguity between single- and multilayer diffuse reflectance profiles.

In practical cases the skin structure is not well defined and the determination of optical properties often has to rely on a single-layer model. It is plausible that changing a coefficient in any layer in the three-layer structure may be interpreted as a change in the corresponding effective coefficient in the single-layer model. We have, however, carried out a preliminary analysis that suggests that another ambiguity exists: in the case that the scattering parameter of the third layer is changed, this is interpreted as a change in the effective absorption coefficient in the single-layer model obtained by the neural network. Simultaneously, the effective reduced scattering coefficient does not change. We are currently pursuing a more complete description of this complex ambiguity.

3.3.3 Optical coherence tomography with ultrahigh resolution for non-invasive medical diagnostics

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The optical coherence tomography (OCT) system being developed in the present project is a combination of two well-known techniques, i.e. confocal microscopy and low coherence interferometry. The former ensures that a specific depth is selected in the tissue. Human tissue is, however, strongly scattering and, therefore, imaging of structures at a certain depth is blurred due to scattered (diffuse) light adding to the measured signal. By using the latter, i.e. an interferometer with a low coherence source, only light from the volume with thickness corresponding to the source coherence length contributes to the desired interferometric signal. Hence, the low coherence provides high spatial longitudinal resolution imaging, i.e. of the order of 15 µm in human tissue. The above description is, however, a crude approximation of the practical system. For example, it is assumed that light can be focused through a strongly scattering medium. This assumption implies that in practical systems only a small fraction of the reflected light is utilised: only the retroreflected part of the light.

In Figure 28 the OCT system is shown. It consists of a fibre-optic Michelson interferometer. Light from the low coherence source (a superluminescent diode) is split into two paths: one going into the reference arm with a movable mirror, the other going to the object of investigation. The reflected light is collected through the same fibres and is directed to the detector, where the interference signal is obtained. Longitudinal scans of the object are performed by scanning the reference mirror, and 2D or 3D images may be obtained by scanning the object laterally.

In the Optics and Fluid Dynamics Department we have developed and contributed to the field of light propagation in stochastic media including human tissue. Based on this firm knowledge we are currently pursuing an adequate description of the OCT system including light scattering and the focusing of the light. The theoretical modelling is based on the extended Huygens-Fresnel formulation that describes light propagation in highly scattering media taking into account its coherence properties. Based on this model, we expect (i) improved imaging capabilities of the OCT system, and (ii) an increased penetration depth.

In the near future, a portable OCT system will be developed based on a source at 800 nm, 1300 nm or 1500 nm, since the light penetration in tissue is maximised in these wavelength regions. The system should be modified in accordance with the theoretical investigation. Different configurations will be investigated, including a multimode configuration and a so-called in-line reference configuration.
The portable system will then be taken into a preclinical investigation in collaboration with Marselisborg Hospital. The purpose is to assist in diagnosing skin diseases. In particular, skin cancer will be investigated. Images are acquired by the OCT system and these are subsequently compared with traditional histology. Using various image processing techniques, a database is formed, which may then be used to assist diagnostic assessments.

The present research project is supported financially by The Danish Technical Research Council under grant no. 9601565.

1. The theoretical modelling is carried out in close collaboration with Dr. H. Yura, Electronic Technology Center, The Aerospace Corporation, Los Angeles, CA, USA.

### 3.3.4 Local diffuse reflectance from three-layered skin tissue structures

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A new model describing light propagation in a highly scattering, layered structure based on diffusion theory has been developed. Using this model, the diffuse reflectance or transmittance may be calculated in the steady state regime.

Human skin consists of bounded layers with distinct optical properties. Depending on the specific diagnostic application it may be necessary to distinguish between these layers when light-tissue interactions are modelled. Diffusion theory\(^1\) and Monte Carlo simulations\(^2\) (MCS) are commonly used for describing the light propagation in tissues. Time-domain, frequency-domain and continuous
wave (CW) measurement techniques may be modelled using the above models. In the present work, we are considering CW measurement techniques only.

The diffusion approximation to transport theory has been widely used to describe light propagation in turbid media for a variety of geometries and source functions. For example, Takatani and Graham\(^3\) investigated the diffuse reflectance and transmittance from a two-layer tissue structure illuminated by a collimated beam. The localised diffuse reflectance from single- and multilayer structures may also be obtained by MCS.\(^2\) This is a purely numerical method with the major advantages that it is valid for all values of the albedo and is valid close to sources and at boundaries. Naturally, it lacks the capability of providing analytical expressions for the reflectance and transmittance. One important assumption is commonly made in MCS: the single scattering phase function \(p(\cos \theta)\) is assumed to follow the Henyey-Greenstein approximation.\(^2\) Nevertheless, the method agrees well with experiments for most tissues.

In our work,\(^4\) we are primarily concerned with measuring the glucose content of skin tissue \textit{in vivo} from CW diffuse reflectance measurements. In this geometry, we obtain the local diffuse reflectance \(R(r)\), known as the reflectance profile, as a function of the source-detector separation \(r\). We model different skin structures depending on the geometry of our experimental set-up. Structure #1 consists of an epidermal layer, a dermal/blood layer and a subcutaneous tissue layer. This structure may be used to model the operation of devices with small source-detector separation, e.g. fibre-optic devices. Structure #2 consists of an epidermal/dermal/blood layer, a fat layer and a layer of muscle-like tissue. Such a structure is suitable for modelling devices with relatively large source-detector separation. Our calculations are carried out at a single wavelength. However, the wavelength range may easily be extended by including the spectral dependence of the optical properties.

We have used diffusion theory to derive a novel expression for the diffuse reflectance from a three-layer structure. The functional forms of \(R(r)\) from a single-layer and a multilayer structure are identical.\(^4,5\) Hence, practical experiments are made cumbersome by this fact. We have compared our computations using diffusion theory with MCS and obtained good agreement.

In these calculations, all three layers have the same refractive index: \(n_0 = n_1 = n_2 = 1.4\). The layered structure consists of an epidermal layer, a dermal/blood layer and a subcutaneous layer. The thickness of each layer is 0.12 mm, 1 mm and 10 mm, respectively. The asymmetry parameter is assumed constant in these calculations: \(g_0 = 0.92\), \(g_1 = 0.88\) and \(g_2 = 0.85\). The absorption coefficients of the first and third layers are: \(\mu_{a0} = 0.02\) mm\(^{-1}\) and \(\mu_{a2} = 0.01\) mm\(^{-1}\). The scattering coefficients of the first and third layers are: \(\mu_{s0} = 35\) mm\(^{-1}\) and \(\mu_{s2} = 15\) mm\(^{-1}\). The scattering coefficient \(\mu_{s1}\) of the middle layer is varied with values: 10 mm\(^{-1}\), 15 mm\(^{-1}\) and 25 mm\(^{-1}\). In this case the absorption coefficient is \(\mu_{a1} = 0.05\) mm\(^{-1}\). In Figure 29a the comparison between MCS (solid lines) and the corresponding diffusion theory calculations (dashed lines) is shown. The comparison between MCS and the diffusion theory with varying absorption of the middle layer is shown in Figure 29b. The scattering
coefficient is $\mu_{a1} = 20 \text{ mm}^{-1}$. The absorption coefficient $\mu_{a1}$ is varied with values: 0.02 mm$^{-1}$, 0.05 mm$^{-1}$ and 0.10 mm$^{-1}$. Qualitatively we observe good agreement between the two methods.

In our data analysis, we use a novel expression to fit the reflectance data leading to enhanced determination of the optical properties. For both skin structures we investigate the sensitivity of $R(r)$ on changes in the optical properties according to physiological changes in blood volume and glucose concentration. Using the multilayer diffusion theory model and the improved data analysis, we have simulated representative tissue glucose concentration changes and blood volume changes. Typically, the change in the fitting parameters due to glucose changes was smaller than the corresponding change due to blood volume changes.

Hence, we have demonstrated that the demands for accurate determination of various biological interferences, e.g. blood volume changes, are high. Finally, we have established the complicated relationship between the reflectance profile $R(r)$ (or the fitting parameters) and the underlying optical properties.

Figure 29. The reflectance profile $R(r)$ as a function of the source-detector separation $r$ from a three-layer structure. (a) variation of the reduced scattering coefficient in the second layer (parameters in text). (b) variation of the absorption coefficient in the second layer (parameters in text).
3.3.5 Evanescent field sensing: a new intracavity method

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A new concept for the detection of very small changes in the refractive index of a small sample of transparent material is being investigated. This is of great interest in connection with affinity sensors for biomedical applications. The concept is based on measuring the frequency difference between two modes of a laser (possibly a twin-laser), where the evanescent field of one mode is affected by small refractive index changes. Intracavity sensing allows for orders of magnitude greater sensitivity than external sensing. The frequency difference is obtained by light beating of the two modes. An imbedded diffractive element ensures proper mode matching of the light beating. The relative frequency change is equal to the relative change in refractive index properly averaged over the waveguide. The performance of the intracavity system is compared with a system based on a Mach-Zender interferometer. The intracavity system may achieve a resolution that is $10^4$-$10^6$ higher than the sensitivity of a system based on an external interferometer. A number of problems related to the practical implementation are currently being investigated. An implementation based on III-V materials with a waveguide configuration and Bragg mirrors appears possible with existing technologies. A concept based on a polymer configuration (see Figure 30) may be very attractive where disposable sensors are required.

![Intracavity Affinity Sensor Diagram]

Figure 30. An intracavity affinity sensor. The laser is designed to be capable of oscillating in two spatial modes. One mode may be subjected to small changes of the propagation constant that affect the frequency of that mode. The difference frequency is obtained by light beating on the photodetector at the output of the laser.
3.4 Optical Measurement Techniques

3.4.1 Optical flow measurement

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From an industrial point of view, flow sensors are interesting for calculations of consumption in, e.g., district heating, drinking water and gas systems. The aim of the work is to investigate whether it is possible to produce an optical flow sensor that is smaller, more robust, more accurate and cheaper than the existing sensors.

In this work a flow sensor based on a laser time-of-flight system is being developed. This has previously been utilised for a surface velocity sensor. The laboratory flow set-up is shown in Figure 31. It consists of the flow chamber (to the right) with windows for optical access to the fluid and the optical sensor (on the left-hand side of the chamber).

![Figure 31. Laboratory set-up of optical flow sensor.](image)

The transmitter and receiver optics are integrated into a single holographic optical element (HOE) which is seen in the centre of Figure 31. The HOE is illuminated by a plane wave from the near-infrared laser diode (upper left corner) and produces two focused spots in the flow with a well-defined spacing. The backscattered light from particles in the fluid is imaged by the HOE onto two photodiodes (left-hand side). The flow velocity is determined by measuring the time of flight of particles moving from one illuminated spot to the other.

By using surface relief HOEs we have the possibility of cheap large-scale fabrication of the optics by injection molding. Tests of the sensor
are to be carried out at Kamstrup, in laboratory flow benches as well as in district heating systems.


3.4.2 Laser anemometry for wind turbines

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Wind turbines are becoming an important source of electric energy. The majority of wind turbines are connected to the electric grid. As the number of large turbines increases, the need for reliable local wind measurements for power curve determination and for advanced control becomes more important. We have investigated laser anemometry for this application.

Laser anemometers for wind measurements have been investigated in a number of different contexts. We have identified several configurations that have been experimentally verified and also configurations that so far are purely conceptual. The most convincing systems for long-range applications have proved to be of the so-called backscattering reference-beam detection configuration. The detection is done by mixing backscattered light with a reference beam usually derived from the same laser that provides the transmitted light. The basic layout of such a configuration is shown in Figure 32 although the actual implementation may be quite different. CO$_2$ lasers and, more recently, also solid state lasers have been used for these configurations. A set of design goals were established and different configurations, lasers and detectors have been investigated in relation to cost, compactness, robustness, efficiency, effective scattering cross-section, propagation effects (wavefront distortions - as well as effects of rain and fog). Our overall conclusion is that for the present application a reference beam configuration based on a CO$_2$ laser with a photoconductor as light detector is preferable.
The spatial and temporal averaging was investigated in relation to characteristic wind turbine parameters and the noise processes of the laser anemometer (particles and photons). Averaging over a length of 20 m and a time given by the convection time over that length, a lower limit of the statistical uncertainty appears to be a fraction of a percent of the mean velocity.

As an alternative to the configuration shown in Figure 32 we have investigated a so-called autodyne or self-mixing configuration. Here the backscattered light is fed back into the laser. This perturbs the laser and for small perturbations the intracavity power will exhibit oscillations given by Doppler shift of the backscattered light. A system based on a tapered waveguide laser (Figure 33) is very simple in terms of layout and number of components. However, a properly designed laser is currently not available. For high-gain lasers (like CO$_2$ lasers) the performance may be equal to or even better than a system based on external mixing.
3.4.3 Autodyne detection

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The detection of low-level light fluctuations may be done by mixing with a reference beam. This is a well established technique and is, e.g., used in certain types of laser anemometers. The detection may also be carried out by feeding the low light level into a laser and measuring the perturbation of the intracavity power. Optical feedback into the laser is - especially for semiconductor lasers - often a problem because the feedback perturbs the laser oscillation. However, in some cases this can be utilised advantageously. The concept is well known but, to our knowledge, no rigorous analysis of the statistical performance of an autodyne - or self-mixing - system relative to a system with external mixing has been given. (The principles are illustrated in Figure 32 and Figure 33, respectively, in connection with Doppler anemometers that measure the axial velocity component.)

We have investigated this in connection with distributed feedback semiconductor lasers. The conclusion is that for low light levels there may be an advantage, and the optical layout is certainly much simpler if no frequency shift of the reference is needed in order to determine the sign of the velocity.

The concept is currently being investigated in connection with CO$_2$ lasers for atmospheric wind measurements. Also in the case of the high gain CO$_2$ laser does there appear to be an advantage in applying the autodyne mode of operation. The optical layout is greatly simplified and is less sensitive to mechanical vibrations within the anemometer.

3.4.4 Measurement of angular deflection

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Measurement of one-dimensional (1D) angular displacement between two states is important in many industrial processes for condition monitoring. This usually calls for the use of coded targets or the application of some kind of contacting pick-up probe on the target. In order to overcome these limitations a new concept has been investigated. Advantage is here taken of the random speckle pattern produced when coherent light is scattered off the surface of a rough or semi-rough surface. The speckle pattern yields a unique “fingerprint” of the surface. An optical layout has been investigated in which the scattered field off the surface from a plane incident wave is collected by a lens and subsequently Fourier transformed, i.e. the detector(s) is/are placed in the back focal plane of the collecting lens. The speckle patterns before and after an angular displacement will show a translation which is independent of any linear translation of the object as well as of the wavelength and the target distance. Calculating the crosscovariance between the two detector signals and finding the value at which the
crosscovariance attains its maximum provide the angular displacement. Figure 34 shows the intensity distribution of two speckle patterns from a linear CCD-array placed in the Fourier plane and the resulting crosscovariance. The crosscovariance is a measure of the displacement one speckle pattern has to undergo to make it overlap a second speckle pattern.

An angular resolution of 0.3 mdeg has been demonstrated with a standard set-up. Large angular deflections may cause speckle decorrelation thus reducing our ability to ascertain the peak of the crosscovariance precisely with subsequent lack of precision in the measured angular displacement. An approximate maximum angular displacement of 300 mdeg has been found in the system presented here.

![Figure 34. Two linearly displaced speckle patterns before and after an angular displacement of 50 mdeg (shown to the left) and the corresponding crosscovariance (shown to the right).](image)

Inserting a standard CCD-camera in the Fourier plane instead of a linear CCD-array facilitates determination of the direction of the out-of-plane angular displacement as well as of the magnitude of the deflection. Figure 35 shows the two-dimensional crosscovariance for a deflection of 200 mdeg along a direction having an inclination of approximately 50° with respect to the x-axis.
Figure 35. Two-dimensional crosscovariance of the intensity patterns recorded by a CCD-array (left) with the corresponding contour plot shown to the right.

A system for measuring the linear distribution of angular deflections may be implemented by Fourier transforming the scattered field along the horizontal axis while imaging along the vertical axis. This is facilitated by inserting a cylindrical lens adjacent to the spherical lens performing the Fourier transformation. Figure 36 shows a measurement of the vertical distribution of angular displacement for a vertically placed steel beam with torsion of 200 mdeg and 400 mdeg applied at the top. The recordings were made at the bottom point of fixation and clearly show the uneven distribution of bending.
The use of two-dimensional CCD-arrays may improve the resolution and thus increase the sensitivity below the 0.3 mdeg.

Systems for measuring the torsional twist of rotating shafts have been investigated and will provide for wider dissemination of the ideas previously presented.


3.4.5 Measurement of linear velocities

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Measurement of linear velocities has attracted increased interest after the advent of cheap laser diodes and low-cost integrated optical elements. Combining these elements will provide for robust - yet inexpensive - optical systems with a variety of applications ranging from stand-off measurement in the steel industry to non-invasive measurement of blood flow in human tissue.
A compact system based on *Vertical Cavity Surface Emitting Laser Diodes (VCSELs)* is depicted in Figure 37. The emitted light from the diodes will be focused by the microlens array and the two illuminated spots are subsequently imaged onto the two detectors. The transit time for the speckles or the surface structures to move from one spot to the next will provide the instantaneous target velocity.

![Microlens array diagram](image)

**Figure 37.** Compact laser-based velocimeter based on two adjacent VCSELs, a microlens array, detectors and an imbedded signal processor.

The importance of investigating the behaviour of laser-based systems on various materials with varying surface properties is therefore obvious. The information carrying surface structure may be the microscopic surface indentations or the large-scale reflection structures. The perceived sizes of these structures are of vital importance for the accuracy of the sensor and are highly dependent on the optical implementation.\(^1\)

The determination of linear and angular velocities of solid surfaces will to a large extent involve the same processing objectives. Mutual benefit can thus be achieved with these two sensor systems. Furthermore, the optical schemes have similarities which may provide for a versatile optical set-up that can form the basis for a generic system.\(^2\)

Implementation of this concept in a miniaturised version has been considered\(^3\) where special emphasis has been placed on the aspect of reducing any bias error. Systematic errors may occur if systems are not properly designed. Such errors may prevent the use of this kind of measurement systems in industry where length determination of moving objects is based on integrating the measured velocity.

3.4.6 Dynamic speckle statistics

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Coherent light scattered from surfaces will usually give rise to a granular intensity pattern, named a speckle pattern. In case the surface roughness is larger than the wavelength and the illuminated spot is larger than any scale in the lateral surface elevation distribution, the speckle pattern will solely be given by the optical parameters. This case is named fully developed speckles. The surface structure will here have little impact on the intensity distribution. In many situations the scattering surface will have a surface roughness or a lateral scale that does not allow for obtaining fully developed speckle, and the spatial field and the intensity correlation functions will reflect the surface properties. Analysis of systems for measurement on polished or semirough materials such as shafts and partly reflecting surfaces thus relies on a theoretical analysis including this aspect.

Within the limitations of the generalised ray-matrix method, analytical expressions for the first-order intensity moments are obtained for arbitrary cylindrically symmetric ABCD optical systems, assuming beam illumination of reflective targets with arbitrary values of surface roughness whose heights are a Gaussian process.1 In contrast to previous work, the results presented here are valid for an arbitrary number of correlation areas of the target that contribute to the observed intensity. In addition, analytic closed-form results, as well as a highly accurate approximation based on elementary functions, are presented for the heterodyne signal-to-noise ratio in situations where the scattered light is mixed with a strong local oscillator.

3.4.7 Improvement of the axial response in 3D light focusing by use of dynamic phase compensation

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The axial response of a high numerical aperture optical system is known to be very sensitive to any mismatch in refractive index between that of a specimen and that of an immersion medium. Light focused deeply into the specimen is usually strongly degraded by spherical aberration resulting from the refractive index mismatch. Even a small amount of spherical aberration is known to be sufficient to produce substantial degradation of the point spread function far more in the depth than in the lateral direction. Various approaches to correcting these aberrations have been proposed in the literature. However, most approaches are limited to considering first-order aberration correction and/or the proposed methods only work for a given and fixed focusing depth. We have investigated the possibility of dynamically compensating for all orders of spherical aberration resulting from refractive index mismatch by use of a phase-only spatial light modulator.  

A generic optical system is shown in Figure 38. Light is focused by the objective lens into the three-layer configuration with refractive indices: $n_0$ (immersion), $n_1$ (cover glass) and $n_2$ (specimen). Assuming the objective lens is optimised and aberration corrected for a focusing depth just below the cover glass, we can derive an expression for the accumulated phase for a given plane wave component with angle of incidence $\theta$ and for any given stage movement $z_0$. A dynamic phase function that can compensate for all orders of spherical aberration due to the accumulated phase error has been found analytically. By use of a compensating phase function
displayed on the SLM it is possible to improve the axial point spread function significantly as shown by the example in Figure 39.

Figure 39. Calculated axial responses for different stage movements: (a) \( Z_0 = 0 \), (b) \( Z_0 = 25 \), (c) \( Z_0 = 50 \) and (d) \( Z_0 = 150 \), where \( \lambda_0 \) is the free-space wavelength of the focused light. \( I_1 \) : continuous phase compensated, \( I_2 \) : binary phase compensated and \( I_3 \) : original non-compensated axial response.

Comparing the three graphs for the continuous phase compensated (\( I_1 \)), binary phase compensated (\( I_2 \)) and non-compensated (\( I_3 \)) it is evident that a remarkable improvement can be achieved for the axial response. \( I_1 \) has been perfectly aberration corrected but perhaps more interesting is the fact that it is possible to achieve a rather nice compromise by using binary-only phase compensation (compare \( I_2 \)). Binary phase modulation is by far the most robust and simple modulation scheme to implement, and several binary-only phase modulating liquid crystal SLMs are now commercially available. A wide range of optical systems could benefit from a dynamic phase compensation technique: e.g., 3D bit-oriented memory systems, 3D photonic microfabrication, ophthalmology and confocal microscopy.

3.4.8 Lossless projection of light

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Imaging of phase objects, i.e. visualising and projecting the information imprinted by a non-absorbing object into the phase of a transmitted light beam has always been a subject of considerable interest in optics. From a theoretical point of view it is a fundamental challenge to devise new phase-only imaging methods that provide the most efficient, simple and robust use of available photons radiated from a given light source. From an application point of view, a phase-only imaging technique is attractive for at least two reasons: firstly, the majority of the emitted photons will not be dissipated whereby heat generation and resulting damaging effects in the optical hardware are prevented; secondly, photons that are not absorbed by the optics can be efficiently utilised and transferred to a desired target projection. Consequently, one can use a weak light source to generate a desired light projection with strength comparable with that generated by a much stronger light source combined with conventional amplitude modulating optics. On the other hand, one can apply a strong light source in a phase-only modulating system without having to be concerned about deteriorating effects due to absorption. Applications are plentiful. Here we will mention a few: high-power laser machining, marking and labelling in parallel, large-screen projection, beam shaping, laser guidance, photo-litography and structured light.

The scheme is grounded on an extension of the well-known Zernike phase contrast method into the domain of full range \([0;2\pi]\) phase modulation breaking the small-phase-angle limitation of Zernike’s method. By careful and continuous control of the spatial average value of the input phase modulated light combined with specific pre-estimated phase retardation at the phase contrast filter, a pure phase based image formation can be achieved. In comparison with previously known phase-only imaging techniques, this dramatically simplifies the synthesis of arbitrary intensity patterns, and the requirements of the space bandwidth product (number of resolution elements) are also significantly reduced compared with those of, e.g., phase-only holography because we apply a simple pixel-to-pixel imaging operation. For these reasons our method renders it more feasible to utilise a dynamic and relatively coarsely grained spatial light modulator as input phase modulating device. Experimental results verifying the new approach have been demonstrated based on the optically addressed phase-only PAL-SLM from Hamamatsu Photonics (see Figure 40).
Figure 40. Experimental examples with binary read-out patterns obtained with the PAL-SLM from Hamamatsu Photonics. The intensity levels of the binary patterns are on average 3.5 times stronger than the intensity level of the original read-out beam shown in the top-left corner which indicates that approximately 90% of the photons in the read-out beam are in use in the synthesised binary intensity patterns.

3.5 Knowledge Based Processing

3.5.1 Robot navigation by shape and object recognition

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Image processing and learning algorithms are essential techniques for performing automatic shape and object recognition in images. Handling these tasks is relevant to applications such as machine vision, visual navigation of robots and automatic surveillance. This year we finished an ESPRIT project dealing with automatic recycling of old TV sets. Our contribution to the project was an image processing unit than can be trained to recognise different components within a TV set. The information sources are 2D data from a colour video camera in combination with depth data obtained from a chirped laser radar developed by Siemens, see Figure 41. Examples of tasks for the shape recognition system are to locate attachment regions on the rear panel, the printed circuit boards and the electron gun. A traditional model-based image processing technique will not suffice as the components may vary considerably from one TV set to another. It is therefore necessary to have a robust detection scheme. In order to handle the variations it is sensible to introduce a learning-based approach. A learning-based approach is also necessary to be able to incorporate new types of TV sets on a continuous basis. Furthermore, any kind of available a priori information must be used to facilitate the task; for instance, the deflection unit will always be close to the centre of a given TV set (use of this knowledge limits the potential search area). The different kinds of a priori information are handled by a model building tool. This model builder is also the basis for the disassembly controller which controls the disassembly strategies based on expectations and information from the shape recognition module.

The availability of depth information together with 2D information is valuable and will probably be more essential in future inspection and supervision systems. Exploitation of this concept, however, calls for low-cost 3D sensing devices that can easily be integrated into industrial vision systems.

In collaboration with the Technical University of Darmstadt and FZK in Karlsruhe we have finished a project on incineration control funded by the EU Environmental & Climate programme. The main purpose of the project was to improve the incineration control in order to keep the flue gas clean and to optimise the incineration process. Knowledge of the incoming waste will facilitate the incineration control process as one can then predict the behaviour of the incineration process for different choices of the control parameters. Today, information about the incoming waste at the plant in Darmstadt is restricted to an ad hoc value (obtained by visual inspection) reported to the control system.
In order to automate the visual classification process we have investigated the possibility of using video data recorded at the waste entrance funnel. Image processing routines together with expert systems are used to classify the waste images into different groups. The output classes must necessarily be grouped according to visual features such as colour composition and granularity size. The group labels can thereafter be fused with density information to obtain better separability. The idea is to have classes that correlate with specific ranges of heating values. Image processing software and a classification module were developed to process the visual information of the incoming waste. Colour and granularity size information is extracted. A classifier has been built that can classify a waste image into a cluster with characteristic visual features. This class information can be used together with information on the water contents to estimate the heating value.

An infrared (IR) camera was used to record images within the kiln chamber of an incineration plant in Darmstadt. The IR camera monitored the drying/ignition zones. The measured intensities reflect the surface temperature of the burning waste in combination with the temperature of the soot particles. By studying temperature profiles over time (corresponding to monitoring the drying process) one can deduce the heating value. We developed image processing software to analyse the burning behaviour in the drying zone.

3.5.3 Example-based learning
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There exist a number of paradigms for implementing machine intelligence. Some of the most widespread concepts are statistical decision theory, artificial neural networks and memory-based reasoning. The different paradigms originate from different traditions, but all of them aim at producing proper geometrical decision boundaries in the input space. Accordingly, one often sees models that combine techniques originating from different paradigms.

An essential task in machine intelligence is to learn from examples, i.e. one tries to come up with a model that maps or classifies the training examples satisfactorily according to a suited quality measure. A sensible quality measure normally corresponds to a trade-off between a small model variance and acceptable fitting accuracy.

Artificial neural networks have become a popular tool for learning. A couple of years ago there was a tendency to consider artificial neural networks as adequate black box algorithms that could be used without having to understand the problem in question in greater detail. In reality, it is not that simple. It is essential to have the possibility of extracting information on how a specific problem is being learned and, furthermore, to control the learning algorithms using existing a priori knowledge.

At Risø National Laboratory we have focused on a neural network architecture that belongs to the memory-based reasoning category. This type of architecture stores more specific information on the training examples than most of the other neural network architectures.
Accordingly, it is possible to come up with confidence measures that express how much support a decision has from the training distribution. On the other hand, the traditional architecture may have problems with noisy examples as well as skewed class distribution. We have therefore been working on eliminating these problems with the architecture while still keeping its traditional benefits. This work includes novel pruning techniques; the results have been very encouraging as we have been able to obtain state-of-the-art results over a range of different classification problems. As a result there are at present plans for transferring the technology to Danish industry.


3.6 Calibration

3.6.1 Temperature Calibration

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For more than 30 years the thermometry laboratory in the department has calibrated temperature sensors for use in Risø's own test facilities.

The laboratory was accredited in 1978 and is approved in the Danish Accreditation Scheme, DANAK, to issue certificates for calibration of temperature measurement equipment. DANAK certificates are the only Danish certificates that are accepted in connection with ISO-9000 certification.

The instruments in the laboratory are traceable to international standards. The reference thermometers are regularly calibrated at National Physical Laboratory (NPL) in London to secure accordance with the International Temperature Scale, ITS-90.

Accredited calibrations can be made in the temperature range 150 °C – 1100 °C with an uncertainty better than ±0.008 °C - 0.018 °C up to 550 °C and ±0.5 °C further up to 1100 °C. Available in the laboratory is a set of liquid bath thermostats and electrical furnaces to establish any temperature in the accredited temperature range.

An electrical high temperature furnace has been installed and tested in the laboratory. The max. temperature is 1600 °C. Calibrated type R thermocouples have been purchased at NPL to secure traceable measurements. This new installation will be used to expand the accredited temperature range from the present 1100 °C to 1600 °C.
Facilities for calibration of infrared thermometers have been established. Thermostated black bodies covering the temperature range from 50 °C to 1100 °C are now available in the laboratory. The intention is to extend the temperature calibration accreditation to cover infrared calibrations too.

3.6.2 Temperature measurements

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Temperature measurements are made in situ in waste incineration plants, furnaces, power plants, autoclaves, etc. If the plant instrumentation has electrically available outputs, these signals can be collected simultaneously with the signals from Risø’s sensors by Risø’s computer based data acquisition system. This allows a direct comparison of Risø's measurements and the readings of the plant instruments.
4. Plasma and Fluid Dynamics

4.1 Introduction

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A unifying theme for the research performed under the Plasma and Fluid Dynamics programme is the dynamic behaviour of continuum systems. The continuum systems under investigation cover fluids, plasmas and optical media. Both linear and nonlinear problems are addressed in a combination of experimental, numerical and theoretical studies. Scientific computing in a broad sense plays a major part in these investigations and includes theoretical modelling of the physical phenomena, development of accurate and efficient numerical algorithms, visualisation and animation of the computed results and last, but not least, validation of the numerical results by detailed comparisons with carefully conducted experiments.

Due to the broad approach to the problems, the various projects are scientifically overlapping, not only in the programme, but to a large extent also with projects in the rest of the department as well as in other departments at Risø. This overlap is considered a strength since it gives rise to considerable synergy between different parts of the laboratory.

The goals of the scientific studies are two-fold: on the one hand the investigations aim at achieving a deeper understanding of the fundamental behaviour of complex physical and technical systems; on the other hand the acquired knowledge is sought utilised in the definition and design of solutions to specific technological problems. Examples of new projects launched in 1997 and targeted towards the solution of technological problems include the development of numerical algorithms for the design of novel diffractive optical sensors and the combined experimental and numerical investigations of microflows.

The main results obtained during 1997 can be summarised as follows:

- **Fusion plasma physics.** The studies conducted in this area form the physics part of the research unit under the Association Euratom - Risø National Laboratory. In collaboration with the Max Planck Institute for Plasma Physics in Garching, Germany, the first successful measurements with Risø’s laser diagnostic on the Wendelstein 7-AS stellarator of two-point correlations in plasma turbulence have been carried out. These experimental investigations were supported by a number of theoretical and numerical studies. Theoretical studies have been carried out on the spectral analysis of plasma turbulence time series, and fully three-dimensional numerical simulations of various types of plasma turbulence have been conducted. New results have also been obtained on particle diffusion in electrostatic turbulence and on the theoretical description of inward transport via the concept of ‘Turbulent Equipartition’.
• **Fluid dynamics.** Detailed experimental and numerical investigations of the influence of a spatially varying Coriolis force on the nonlinear dynamics of vortices have been carried out. These studies have direct applications to geophysics but are also used to simulate nonlinear transport processes in magnetised plasmas - processes that are impossible to measure directly. The scientific activities in fluid dynamics have been extended to include numerical and experimental studies of microflows with special emphasis on the dynamic behaviour of macroscopic particles, e.g. biological cells.

• **Optics.** Several detailed experiments on various aspects of nonlinear pattern formation and soliton dynamics have been carried out. In particular, the world’s first demonstration of control of ‘optical turbulence’, or ‘optical chaos’, has been performed. The optical experiments have been supplemented by several theoretical and numerical studies of the dynamic properties of various nonlinear, optical systems. For the design of new optical sensors, a project aimed at accurate numerical modelling of diffractive optical elements has been initiated. This project is based on a new, spectral algorithm which is superior to existing numerical methods for this type of problem.

• **Biophysics.** During 1997, scientific studies of various complex problems in biophysics have been carried out. In parallel to the scientific research, investigations were conducted on how these studies are best integrated in the overall research strategy of Risø. It was decided that from 1998 the Materials Physics and Chemistry Department will organise all the biophysics research at Risø.

### 4.2 Fusion Plasma Physics

#### 4.2.1 Collective scattering turbulence measurements at the W7-AS stellarator

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Work continued on collective scattering turbulence measurements on the W7-AS stellarator experiment at the Institute for Plasma Physics in Garching. The instrument, which is based on a two-point correlation measurement technique, has been designed to give enhanced spatial resolution of large-scale turbulence.\(^1\) Relatively small-scale turbulence is measured at two points in the plasma. When looking at small scales, the spatial extent of the measurement volume can be reduced, which improves the spatial resolution. The two points are separated by a distance corresponding to the large-scale turbulence that is important for transport in the plasma. Measuring the cross-correlation of the signals from the two measurement points allows the group velocity at large scales to be inferred. The limitation to the spatial resolution that can be achieved depends on the presence of measurable fluctuations in the plasma at small scales.
Initial attempts were made at measuring fine-scale turbulence with wave number, $k > 100 \text{ cm}^{-1}$. Results obtained during the first six months of 1997 indicated that such measurements were only possible at isolated events when the plasma was strongly perturbed. In order to obtain a continuous, or quasi-continuous turbulence spectrum, the optical set-up was changed in order to probe smaller wave numbers. Results obtained when measuring turbulent fluctuations centred at $k > 36 \text{ cm}^{-1}$ are shown in the following figures.

![Figure 42. W7-AS plasma discharge number 40774 of 29 September 1997. From top to bottom: diamagnetic energy [kJ], electron temperature [eV], line integrated electron density [$10^{-19} \text{ M}^{-2}$], and neutral beam injection power [kW].](image)

At these wave numbers the spatial extent of the measurement region corresponded to a long pencil with a diameter of 4 mm, and a characteristic length of the order of one meter.

Some parameters for a typical plasma discharge with neutral beam injection at W7-AS are shown in Figure 42. The discharge lasts about 400 msec, with the highest temperatures and densities obtained in the latter part of the discharge. Measurement results from the discharge are shown in Figure 43. The measuring points were placed in the upper half of the plasma and were separated by 13.8 mm, along a line parallel to the radial coordinate. At each measuring location, fluctuations centred at $k = 36 \text{ cm}^{-1}$, and with a spread in $k$ of about 10 cm$^{-1}$ were detected. The beams were orientated to measure fluctuations travelling in the poloidal direction. The left-hand side of Figure 43 illustrates the temporal development of the measured power spectrum in the two channels. A strong signal is obtained at the end of the discharge. The strong central peak in the power spectrum is due to a small parasitic leakage between the local oscillator and primary beams. The right-hand side of Figure 43 shows the H-alpha diagnostic signal which is an indicator for the particle and energy flow out of the plasma. The sharp peak in the H-alpha signal indicating a burst of energy out of the plasma occurs at the time when the collective scattering turbulence signal is largest.
The power spectrum has a maximum at about -250 kHz as seen in Figure 44. This corresponds to a poloidal phase velocity of about 450 M/sec in the electronic diamagnetic drift direction.

Figure 43. Measured power spectrum vs. time (left) and H-alpha signal (right).

Figure 44. Power spectrum measured at t = 370 msec.

Figure 45. Normalised cross-correlation of the data shown in Figure 45.
The correlation of the two channels is shown in Figure 45. The correlation has a displaced peak at a delay time of about 0.25 msec, which corresponds to a group velocity of about 55 M/sec.

Work in progress is aimed at measuring the distribution of fluctuations at various regions in the plasma cross-section.


4.2.2 Spectral analysis of plasma turbulence time series

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A hybrid Doppler/time-of-flight laser anemometer has recently been developed at Risø, and has been installed at the Wendelstein 7-AS stellarator. The experiment yields time series of the fluctuating plasma density at two neighbouring measurement volumes. The subsequent data analysis and interpretation have prompted the development and implementation of a new spectral data analysis technique.

The spectral analysis has been applied to model time series, obtained by numerically solving the Hasegawa-Mima equation for plasma drift wave turbulence as shown in Figure 46. Model data are useful for an initial test and verification of the basic mathematical machinery. Noise and other experimental effects can be added to the data and their influence on the analysis can be studied. In particular, the effect of scattering geometry (e.g. the size, shape, alignment and distance of measurement volumes) in the actual experiment can be investigated. From the model simulation, time series \( x(t) \), \( y(t) \) of the plasma density at two probe positions are obtained. A preanalysis step involves decomposing each series into an ensemble of elementary series, weighted by a window function that minimises amplitude leakage. The data are subsequently fast Fourier transformed to frequency space, where the actual analysis is performed.

The cross-power spectrum and cross-correlation are first computed. The two-point correlation is used to estimate the time-of-flight of density fluctuations between the two probes and, hence, to estimate their typical propagation speed. A more refined correlation analysis, applied to each individual frequency component, yields the frequency-dependent phase velocity \( w/k \) and thus the dispersion relation \( k = k(w) \). In combination with the power spectrum we can then estimate the wave number spectrum. Therefore, the two-probe systems allows us to resolve and identify oscillations in both frequency and wave number space, and to find their interrelation.

Nonlinear wave dynamics is identified by bispectral analysis. The bispectrum directly measures the nonlinear coupling between wave triplets and vanishes for uncorrelated waves. It is found to be a useful indicator of nonlinear effects, by studying the transition from linear to strongly nonlinear wave dynamics in the Hasegawa-Mima model. Bispectral analysis can consequently detect and identify nonlinear effects
such as three-wave coupling, spectral cascades and formation of coherent structures.

The spectral techniques outlined here are now being employed in the analysis of W7-AS fluctuation data.

Figure 46. Example output of spectral time series analysis. The Hasegawa-Mima equation was solved to yield an ensemble of 256 plasma density time series to be analysed. Left (top): typical plasma density fluctuations, (middle) ensemble average power spectrum showing the presence of linear modes with minor peaks due to nonlinear wave coupling, (bottom) probe-pair coherence spectrum detects oscillations coherent over distances exceeding the probe separation to be included in the correlation analysis. Right: bicoherence spectrum reveals nonlinear wave triplet interactions at the dominant 200 kHz range.

4.2.3 Full three-dimensional simulations of the Hasegawa-Wakatani model

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Drift wave turbulence is believed to be a good explanation for the anomalous transport of particles out of a fusion plasma. A model describing these drift waves is the Hasegawa-Wakatani model. In this model the drift waves are linearly unstable and are driven by the density gradient at the edge of the plasma. The model is described by two partial differential equations in the perturbations of the density, \( n \), and the electrostatic potential, \( \phi \). The equations are coupled through a term of the form \( \frac{\partial^2}{\partial z^2} (\phi - n) \), where \( z \) is parallel to the magnetic field.

Previous simulations have been performed using this model in a two-dimensional geometry. Since it is assumed that the motion of the particles is only due to \( \vec{E} \times \vec{B} \)-drift (i.e. in a plane perpendicular to the magnetic field), this was believed to be a fairly good assumption. The coupling between the equations has thus been done under the assumption of only one significant wave number, \( k_z \). Recent simulations showed, however, that full three-dimensional solutions of the equations were
necessary. A full three-dimensional code has now been developed using accurate spectral methods in a tripple periodic geometry, and an example of the results is shown in Figure 47. The resolution of the fields has naturally been smaller than in the two-dimensional case, but as many as 16 modes in the z-direction have been used. The difference from the two-dimensional case is significant. After an initial phase of exponential growth due to the linear instability, the system saturates into a quasi-stationary turbulent state. The total energy is nearly constant and is mainly transferred into the $k_z = 0$ mode. This corresponds to the formation of so-called convective cells. In the present model/geometry these reduce the particle flux. The convective cells are large coherent structures and are apparently formed irrespective of the initial conditions.

Figure 47. A plot of isosurfaces of the potential perturbation after saturation in the quasi-turbulent state. The simulation was started with low level noise as initial condition. The structures are parallel to the z-axis corresponding to very low $k_z$. 
4.2.4 Numerical simulations of drift and flute modes in cylindrical and toroidal geometry

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Simple numerical simulations of plasma turbulence do not consider the influence of boundaries on the flow. Indeed, the frequent use of periodic boundary conditions makes it impossible also to describe any backreaction of the turbulence onto the background quantities. However, such a backreaction can only be described in a fully three-dimensional context; otherwise, the simultaneous distinction between background and fluctuations and their description are not possible. To attack these problems, whose understanding is crucial for the construction and design of fusion machines, effective parallel codes have to be developed. Preliminary results with a code that only describes the fluctuations, a system comparable with the well known Hasegawa-Wakatani equations, show that the dynamics change significantly with the imposed boundary conditions. The nonlinear polarisation drift organises a charge separation along the density background density gradient. Thereby a poloidal shear flow develops, a feature connected to the L-H transition in tokamak machines. Figure 48 shows a typical result of one of these early simulations.

Figure 48. Density and potential fluctuations in a section of a cylindrical plasma.

4.2.5 Diffusion of ideal particles in electrostatic turbulence and the relation to coherent structures

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The diffusion of particles in the presence of self-organised vortical structures capable of trapping them is a long-standing problem. Here we look at ideal particles in a 2D model of electrostatic turbulence. The motion of charged particles in this situation is not only important for the understanding of the observed anomalous transport in fusion machines, but also for the diagnostic of fast alpha particles leaving the reaction zone of a fusion device. Furthermore, this problem is strongly connected to
transport in the oceans and the atmosphere. The reason for using numerical simulations is that within that framework it is easy to distinguish between regions that contain particles trapped in a vortical structure and regions with particles being convected by the fluctuating, turbulent velocity field. Particles trapped in moving structures thus show a superdiffusion type, while for the free particles we find normal diffusion after a short ballistic phase. When the structures themselves move in a chaotic pattern, there is a second ballistic timescale after which the transport is again of the diffusion type. Recently\(^1\) this type of “diffusion” has also been used to explain unexpectedly high concentrations achieved during mixing processes.


4.2.6 Models of dynamics of plasmas confined by curved magnetic fields

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Magnetically confined plasmas exhibit plasma turbulence with intermittent, large, coherent structures. While the modes with a vanishing parallel component are driven by, e.g., the interchange instability, which is due to magnetic field curvature and a density gradient, drift waves with parallel wave number different from zero are driven unstable by density and/or temperature gradients in combination with finite parallel resistivity. Models for flute modes as for resistive drift waves are well established. Here we are developing a three-field model that describes the evolution of the electrostatic potential, the plasma density and the electron temperature. As limiting cases the two simpler models mentioned above are included. Thus, we will be able to describe fluctuating quantities as well as the evolution of the background profiles. Moreover, by formulating this extended model, the range of validity of the various reduced models can be investigated. A proper reduction describing a given experimental set-up can then more easily be found.

A second problem one can only access with this kind of model, as it describes the plasma not only locally as the reduced models do but globally, is the investigation of the influence of boundary conditions on the plasma dynamics. Even though a vast amount of work has been performed as regards the evolution of sheets, the backreaction of the walls onto the plasma turbulence has not yet been considered in detail.
4.2.7 Turbulent equipartition and plasma transport

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Cross-field transport is one of the most important and most difficult areas of fusion research. Even basic transport phenomena, such as the L-H transition, the profile resilience and the particle pinch, have no generally accepted explanations. Turbulent transport driven by low frequency electrostatic fluctuations is recognised to be of significant importance and may account for the major part of the transport, in particular in the edge region of the plasma. Whereas classical collisional transport is generally down the gradients (of temperature and density) and tends to bring the plasma towards thermal equilibrium, turbulent transport may be directed up-gradiently. This type of transport, which is directed inwards from the edge of the plasma to the centre, leads to peaking of the density and temperature profiles and is referred to as the pinch flux. Recently it has been suggested that such inward transport can be explained by Turbulent EquiPartition (TEP). This is based on the existence of Lagrangian invariants in the presence of the turbulence. The system relaxes towards equipartition of these quantities in the accessible phase space.

In order to test the equipartition hypothesis in a simplified system we have derived a two-dimensional model that describes the nonlinear evolution of pressure driven electrostatic flute modes in an inhomogeneous magnetic field. The model consists of a set of partial differential equations that couple fluctuations in density and electron temperature with the fluctuations in the electrostatic potential. Using a quasi-linear approach we found that the turbulence driven by the Rayleigh-Taylor instability may give rise to a pinch flux. Further, the conditions for marginal stability coincide with the profiles predicted by the TEP.

The equations have been solved numerically on a two-dimensional domain bounded in the direction of the gradient of the magnetic field and periodic in the other direction. We have investigated different ways of driving the system, i.e. with a localised temperature or a density source in the interior. In the cases investigated we observe a clear pinch flux of both temperature and density, and the saturated profiles tend to approach the profiles predicted from TEP.

In Figure 49 we show an example of the saturated temperature and density profiles for the case where the plasma is driven by the temperature source. The inhomogeneity of the magnetic field is modelled by a 1/x dependence. The boundary conditions in the x-direction are that the temperature is fixed at both boundaries, while the density flux is set to zero at the boundaries. It is observed that the profiles are close to the ones predicted by the TEP; i.e. n/B and Te/B are roughly constant in the outer region where the flute modes are unstable, whereas in the inner region the dynamics is dominated by simple diffusion.
Anomalous cross-field transport of mass and energy due to low frequency, electrostatic fluctuations is known to influence the formation of equilibria in magnetically confined plasmas. It has not been generally recognised, however, that anomalous cross-field current plays a similar role in some plasma discharges. By simple physical arguments and simulations based on a fluid model we have shown\textsuperscript{1} that low frequency, electrostatic, flute-mode fluctuations can sustain a cross-field plasma current in addition to transport of mass and energy. The results show that this current determines essential features of the fluctuating plasma equilibrium, and explain qualitatively the experimental equilibria and the coherent flute-mode structure observed in a simple magnetised torus.

4.2.9 Model of cold pulse propagation with sign inversion in tokamaks

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The phenomenon of cold pulse propagation with sign inversion is a well known example of anomalous behaviour of transport in tokamak plasmas. In these experiments the plasma response to local cooling of the plasma electrons near the edge of the tokamak was investigated. The temperature pulse was observed to propagate very rapidly through the edge region of the plasma and the temperature increased promptly in the inner third part of the plasma column. Thus, a cold heat pulse propagates inwards and inverses its sign as it approaches the centre of the column. This effect can certainly not be modelled by standard transport models. In these models the transport can be expressed as the sum of the products of transport coefficients and thermodynamic forces related to the gradients of density and temperature, where the coefficients are functions of the local thermodynamic variables as density and temperature. The phenomenon was simulated numerically by an ad hoc introduced variation of thermal conductivity with radius.

We have suggested a transport model that is based on the idea that turbulent transport drives the plasma towards a state of Turbulent EquiPartition (TEP). This state appears as the relaxed state in which Lagrangian invariants that are not destroyed by the turbulence are uniformly distributed. We have thus expanded the fluxes near the TEP state, and by solving the obtained transport equation we reproduce the cold pulse propagation and the sign inversion. It should be emphasised that the aim is not to construct a predictive transport model, but rather to demonstrate the essential importance of the underlying physical model, where the main ingredient is the non-local response of the effective turbulent diffusion coefficient and its relation to the marginally stable profiles of temperature and density, the TEP state.


4.2.10 Ion temperature gradient vortices in shear flow

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Recent tokamak experiments have shown improved stability and confinement properties in plasma regions with high velocity shear. A sheared plasma flow caused by an inhomogeneous perpendicular electric field may have strong influence on the generation and evolution of vortical structures. The shear field may tear the structures apart and may result in smaller scales of the coherent structures, thereby limiting their contribution to the transport.
To investigate the influence of velocity shear on coherent structures we have studied the evolution of monopolar and dipolar vortices in an ITG-model. The equations were solved numerically by a spectral method in a two-dimensional domain with periodic boundary conditions. Monopoles or dipoles are used as initial condition superimposed on the shear field. The dipoles used are stationary solutions to the equations without shear.

![Figure 50](image)

Figure 50. The evolution of the potential (upper row) and the pressure (lower row) versus time.

In Figure 50 the evolution of the potential (upper row) and the pressure (lower row) versus time is shown. A dipole is initialised in a strong shear field, but in a region where the mean velocity is zero. By its own vorticity field it starts moving in the negative $y$-direction, but it is slowly turning around because of the shear field and it moves into the region where the background velocity is in the $y$-direction. Therefore, the dipole eventually moves in the $y$-direction. Although the dipole itself keeps together, new vortices of opposite sign are created where the positive one becomes the strongest. At this stage the total structure resembles a tripole. Theoretical investigations have indicated that tripoles could be stationary solutions to the equations including velocity shear.

For a case where the initial condition consists of a row of monopoles close together in the $y$-direction, vortices of opposite sign are created between the monopoles. These new vortices are stretched out between the original monopoles by the vorticity field and a row of new monopoles is created on each side. The row of original monopoles located along the line of maximum shear seems to be rather stable for a long time. However, investigations of single monopoles have shown that they are normally very unstable in the shear field.
4.2.11 Equilibrium and movement of ideal MHD plasmas in magnetic fields

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A detailed study of the physics governing ideal MHD plasmas which are acted upon by external forces and confined in magnetic fields has been initiated. It is shown that some of the arguments commonly used to explain the physics of how equilibrium is obtained are misleading. It is further shown that the concept of magnetic stresses and the equations of ideal MHD together constitute a good basis for a physical understanding of the interaction between plasmas and magnetic fields.

4.2.12 Relations to authorities, the higher education, the press and the public

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The activities within these fields include:

- Membership of a standing reference group for fusion research formed by the Ministry of Research and Technology to advise Danish representatives in various committees dealing with the European fusion programme.
- Education at university level in fusion research. During 1997 two courses in Fusion Plasma Physics have been taught at the Technical University of Copenhagen.
- Meetings with a number of journalists from technical journals and newspapers, who write about fusion, in order to educate and advise them on the fusion programme.
- Writing of articles on fusion research for various Danish publications. Some ten articles on fusion have been written for Den Store Danske Encyklopaedi (The Great Danish Encyclopedia). A special elementary textbook on fusion plasma physics for high school teachers is in preparation.
- A selected number of the articles written for Den Store Danske Encyklopaedi have been modified and now appear on the world wide web home page of the Fusion Research Group.
- A seminar on fusion research for high school teachers to be held in the autumn of 1998 at the Elmuseum in Bjerringbro with lecturers from the European Fusion Programme is in preparation.
- Membership of the EFIN group and of the FUSION EXPO group.
4.3 Fluid Dynamics

4.3.1 Shear flow instability in a parabolic vessel

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The instability of a forced, circular shear layer in a rotating layer of water has been studied experimentally and numerically. The experiments have been carried out in a rotating parabolic vessel with a differentially rotating inner section. As the water in the vessel adapts to the velocity of the bottom, the rotating central part of the bottom induces a circular shear layer in the layer of water. Above a critical value of the inner rotation, this shear layer becomes unstable and evolves into a number of equally signed columnar vortices (see Figure 51). The final mode number of the instability has been measured as a function of the differential rotation and the water depth. For all depths, the number of vortices decreases with increasing shear. If the vessel rotates faster (more slowly) than the rotation rate corresponding to the parabolic curvature, the depth of the water layer increases (decreases) from the centre to the periphery. This results in a so-called topographical beta effect. A situation with a faster background rotation is characterised by analogous dynamics as geophysical flows at the North Pole or the South Pole and is referred to as $\beta > 0$; the case with slower rotation has no geophysical equivalent and is referred to as $\beta < 0$. Both the number of vortices and the steadiness of the final vortex pattern appear to be influenced by the beta effect. In particular, the vortex chain becomes less susceptible to instability if an observer moving with the vortices has the deeper water on his right-hand side, and tends to become unsteady in the opposite case. Furthermore, the angular velocity of the vortices around the centre of the vessel has been measured. This quantity appears to be much lower than the average of the inner disk and the outer part of the vessel, an effect that can be explained in terms of nonlinear advection of vorticity by the vortex chain. The angular velocity of the vortices is also affected by the beta effect, as can be seen in Figure 52. The vorticity distribution inside a vortex becomes more positive in the deeper part and less positive in the shallower part, adding a dipole moment that affects the velocity of the vortices.

The numerical results consist of the spectral solution of the quasi-geostrophic equation in a geometry similar to the experimental situation and with a term modelling the experimental forcing. The simulations confirm the instability mechanism that is considered to be responsible for the evolution of the shear layer into a chain of vortices, and provide data about the velocity and vorticity fields that would be difficult to obtain experimentally. In particular, the simulations show a modulation of the vorticity field caused by the beta effect (see Figure 52). This modulation is consistent with the conservation of potential vorticity and the additional drift of the vortices measured in the experiments.
Figure 51. Dye visualisation of a stationary vortex distribution with five vortices.

Figure 52. Angular velocity of the vortices around the centre of the tank as a function of their number. The data represent cases with and without beta effect. The terms cyclonic and anticyclonic denote a rotation sense in the same and in the opposite direction as the background, respectively.
4.3.2 Particle tracing in a circular shear layer

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As an extension of the study described in the previous section, the trajectories of particles in the vortex chain are presently under investigation. In the experiments, a small number of floating tracer particles are released in the shear region, and a video recording with a camera in the corotating system is made. Subsequently, the trajectories of these particles are determined by a computer program running on a PC equipped with a frame grabber. A typical example of such a trajectory, represented in a system corotating with the vortex chain, is shown in Figure 53. The particle follows the streamlines of the flow, and the trajectory shows an asymmetric state with two satellite vortices around the central vortex. However, due to slight unsteadiness in the velocity field, the particle can move between qualitatively different orbits, and one can observe trapping and detrapping of the particle by one of the vortices. Determination of considerably longer particle traces and their chaotic properties is the subject for further investigation; moreover, studies of the effect of different sizes of particles will be carried out.

In order to study particle trajectories in a shear layer numerically, the numerical code has been extended with a module that is capable of following individual particles with spectral accuracy. Apart from tracing a single particle over a long time, the numerical method is suited for studying the dispersion of a large number of particles. In general, one finds that particles released close to a vortex centre remain trapped indefinitely, but that particles released at the edge of a vortex show an irregular motion corresponding to trapping and detrapping.

Figure 53. Two fragments of a single particle trajectory in a state with two satellite vortices. In the left figure, the particle orbits both vortex centres in a horseshoe-like trajectory; in the right figure, the particle is trapped by one of the vortices.
### 4.3.3 Formation of Taylor columns from horizontal jets

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A new, slowly rotating turntable with a programmable rotation profile has been built. The set-up is designed with a large motor torque compared with the mass of the table so that step-like velocity changes can be obtained. The set-up has been used for preliminary studies of the self-organisation into two-dimensional vortical structures after inlet of a horizontal, dyed water jet into a circular tank with a diameter of 38 cm. The water depth varied between 5 and 20 cm, the background rotation between 3 and 18 rpm.

It is well established that background rotation tends to stabilise two-dimensional structures in fluid systems. It is also generally found that localised initial disturbances develop into vortical structures aligned along the axis of rotation. Taking the disturbances to the limit of three-dimensional turbulent patches with dipolar momentum (in the corotating frame), fluid has been injected horizontally into a rotating tank through a nozzle. Due to instability, the jet breaks up into a highly complicated structure, a structure that comprises the wanted turbulent patch. This initial perturbation has been observed to develop into a dipolar vortex column. However, the time $T_f$ for these columns to form has not been investigated in detail. It must depend on the physical parameters: height $H$ and rotation rate $\Omega$. Measurements show that $T_f$ scales linearly with $H$ and scales reciprocally with $\Omega$, as might be expected from simple arguments. Inertial waves with a vertical component will disperse during a transition time in which the waves travel from the nozzle to the surface and the bottom of the tank; this transition time is closely related to the formation time of the vortex columns.

### 4.3.4 Set-up for investigations of microflows

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Microflows are flows on submillimeter of even micrometer scales. Microflows are considered to have future technological applications ranging from small-scale analysing equipment to instruments for manipulating individual cells in biotechnological applications. Measuring flows on such small scales provides a technological challenge. As a pilot study, an experimental set-up is under construction to test the feasibility of measuring microflows with particle tracking. The set-up consists of a long glass channel composed of three parallel joining sections of 2 x 2 cm each. In order to obtain the low Reynolds numbers encountered on small scales, the channel will be filled with silicon oil with high viscosity. This fluid will be seeded with small particles and will be illuminated with a light sheet. The velocity profile will then be determined from a large number of these particles. The results will be compared with numerical data obtained by a finite-volume method and
will be used as a guide to future experimental investigations on submillimeter flows.

4.3.5 Preparation of fluorescent particles for tracing in the rotating paraboloid

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The transport mechanisms in two-dimensional flows as those in the rotating paraboloid can be revealed by the trajectories of passive tracer particles. The statistical behaviour of the tracer particles characterises the diffusion mechanisms. Tracking of normal reflective particles is disturbed by reflections at the parabolically shaped water surface. By means of fluorescent tracer particles the reflections of the illumination can be filtered away before the corotating video camera is entered. The particles have to be bright and small in order to be detectable by a normal video camera and closely passive particles following the fluid.

The tank is illuminated by six commercial 9 W black-light-blue tubes. The tubes, 16 mm in diameter and 27 cm long, are mounted at the outer periphery of the tank 10 cm above the upper edge of the tank. The tubes are supplied by high frequency transformers (25 kHz) in order to reduce the effect of intensity oscillations during the exposure time of the low frequency video camera (25 Hz).

The fluorescent particles are prepared by doping polystyrene particles (Bangs Laboratories Inc.: Particles P6490002PN, diameter 0.65 mm (297 - 1000 µm) 1.062 g/cc) with fluorescent yellow 3G. The technique used ensures that the fluorescent dye is absorbed in the polystyrene particle rather than being adsorbed to the surface of the particle. In this manner, the dye is not washed out into the fluid during the flow experiments. The dyed particles are prepared by immersion in a 1:1 v/v mixture of ethylethoxypropionate and acetone. This mixture swells the polystyrene particles and allows the dye to penetrate; the mixture also contains the fluorescent dye 1% w/v. The dye contains an aliphatic chain that facilitates the absorption of the dye into the polymer sphere. Subsequent washing in ethanol removes excess dye and solvents. The dyed particles show no appreciable fading during excitation with UV-light.

4.3.6 Numerical studies of monopolar vortex interaction with a continental shelf

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Studies of oceanic monopolar vortex interaction with a continental shelf are studied numerically using an accurate spectral computer scheme in a bounded domain. This study has just begun in cooperation with the Vortex Dynamics Group at University of Technology in Eindhoven. Knowledge of the time evolution for these monopoles is essential for a
better understanding of transport processes in large-scale geophysical flows and for their role in environmental issues.

An essential parameter for the dynamics of vortex flows at intermediate latitudes is the gradient of the Coriolis parameter with respect to the latitude, the so-called $\beta$-effect. A characteristic dynamic feature of the present $\beta$-effect is that, on the northern hemisphere, monopolar vortices move to the northwest. Oceanic vortices can thus meet and interact with bottom topographies or boundaries of a basin, resulting in strong horizontal mixing.

The Vortex Dynamics Group at Eindhoven has been studying such phenomena experimentally in a rotating water tank as well as using a finite different scheme. To study the transport properties of these flows, a bounded pseudospectral code, developed in the Optics and Fluid Dynamics Department, is being modified so that it solves the shallow water equations where the effects of bottom topographies and background rotation are taken into account. Using a highly accurate passive particle solver, detailed information about the transport can consequently be extracted.

4.3.7 Vortex merging in two-dimensional turbulence

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For two-dimensional turbulence it is well established that the energy is cascading towards larger scales resulting in the build-up of large-scale structures. This inverse cascade is believed to be mediated by merging of like-signed vortices. The enstrophy (mean squared vorticity), on the other hand, cascades directly towards smaller scales. To provide detailed understanding of this cascading process we have investigated simple cases of the interaction of a limited number of two or three monopoles with Gaussian or patch-like distributed vorticity by numerically solving the Navier-Stokes equations by a high-resolution double-periodic spectral code.

The temporal evolution of the vorticity for three interacting monopoles is shown in Figure 54. The monopoles were given strengths and initial positions so that three-point vortices with the same strengths and positions would collapse into a single point. In this way we may expect the interaction to be very strong. During the evolution the weak negative monopoles are stretched into filaments by the straining field from the two other structures and parts of the filaments are absorbed by the strong negative monopole. Investigating the energy spectrum reveals that a Kolmogorov-like spectrum has developed at high wave numbers, $E(k) \approx k^{-3}$. For the case of two equal sign monopoles we observed$^1$ a spectrum of: $E(k) \approx k^{-4}$.
Figure 54. Computer simulation of the interaction of three monopoles with Gaussian distributed vorticity but with different sizes and amplitudes. Red colours correspond to positive vorticity; blue colours to negative vorticity. A resolution of 1024 x 1024 Fourier modes was used but only a part of the full computer domain is displayed in the figure.


4.3.8 Transport properties of vortices on the beta plane

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The dynamics of large-scale coherent vortical structures in the oceans and the atmosphere is described by the Charney equation in the quasigeostrophical approximation. In this equation, the ordinary Navier-Stokes equations have been extended to include effects due to the free surface and to planetary rotation (the beta effect).

Smooth monopolar structures will be stationary in the ordinary Navier-Stokes equations. However, when the influence of the beta effect is taken into account, these structures start to drift in the northwestern direction (in the cyclonic case), depending on the ratio of the strength of the vortex to the beta term. It is well known that Rossby waves always drift towards the west, which implies that significant transport of material (in the northsouth direction) can only be conducted by strictly nonlinear, coherent structures. Further, it is quite well established that coherent structures in uniform rotating systems trap material, and that no mixing between the interior and the exterior takes place. However, the vortices
that move on the surface of the earth are quite slow (below the maximum phase speed), leading to a coupling to the linear Rossby waves. Thus, while drifting westwards the vortices emit Rossby waves and thereby they decay, which results in a loss of material that is left behind in the wake and is mixed with exterior fluid due to the emitted Rossby waves.

The detrapping mechanism is not smooth; it seems to be more like oscillatory behaviour where lobes of material are shed off ("lobe shedding") in a region northeast of the core. Then material is transported southwards due to a jet in the wake before it finally reaches a latitude where it terminates, with a slow easterly drift. Introducing a finite Rossby radius, which corresponds to a free surface, in the system seems to stabilise the monopolar vortices significantly. They drift more westerly and are less distorted, decreasing the loss rate of material. It is consequently an open question whether the free surface effect ultimately leads to a more effective transport in the northern direction because the lengths of the trajectories of the vortices are increased.

4.3.9 Numerical studies of the dynamics of macroscopic particles in microflows

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In a large number of technical applications of microflows in biomedicine, narrow channels with widths of the order of 10-100 μm are used to transport, sort and analyse biological cells with dimensions only slightly smaller than the width of the channel. The purpose of these narrow channels is to make it possible to manipulate and analyse the cells one at a time. While the flow of the suspending fluid by itself is fairly simple to analyse due to a very low Reynolds number, the dynamic behaviour of the particles is not trivial, since it is not realistic to consider the particles’ ideal, i.e. of zero mass and extent.

A large-scale numerical study of this problem has been initiated in collaboration with UNI-C, Denmark’s Computer Centre for Research and Education. For this study, the STAR-CD fluid code has been implemented on the IBM-SP parallel supercomputer at UNI-C and a realistic test problem has been identified which will allow for detailed validation of the numerical results against results from the new laboratory experiments described in Section 4.3.4.
4.4 Optics

4.4.1 Selection of unstable patterns and control of optical turbulence by Fourier plane filtering

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The spontaneous formation of periodic spatial patterns is a common feature of a range of physical systems that are excited beyond an instability threshold. The symmetry properties of the emerging spatial structures depend on both bulk and boundary characteristics of the system. In two spatial dimensions hexagonal structures are generic. Analysis of the bifurcation structure of a mean field model of pattern formation reveals that other, nonhexagonal symmetries are valid solutions, yet they generally have smaller growth rates than the observed hexagonal structures.

Particularly from the point of view of the usefulness of pattern formation in the realm of optical information processing it is of interest to extend the range of possible spatial structures, as well as to control which structures the system selects. There are two broadly complementary approaches to the control of optical patterns. In the first, the geometrical structure of the system is modified such that other, nonhexagonal symmetries are preferred. Modifying the basic interaction geometry in a variety of ways leads to a rich spectrum of spatial structures.

A second approach is to stabilise the additional solutions that in principle exist in the original interaction geometry. Several recent works have considered techniques for stabilisation and selection of optical patterns. The proposed techniques have been based on variants of spatially and temporally filtering of the field in an optical feedback loop. A unique feature of optical pattern formation systems is that one has immediate access to the spatial power spectrum of the generated pattern, simply by looking in the back focal plane of a lens. This makes spectral control techniques particularly attractive in optical systems. On the basis of experiments and numerical analysis we demonstrate in this work that a simple implementation of phase independent Fourier filtering techniques in an optical feedback loop provides effective selection of unstable periodic patterns (see Figure 55. Demonstration of pattern selection by Fourier plane filtering. The selected patterns are hexagons (a), rolls (b), rhombic symmetry (c) and squares (d). The figure shows experimental far field, numerical near field and numerical far field, from left to right,, as well as stabilisation of optical turbulence that occurs far above the threshold for pattern formation. When the desired pattern is selected, or the optical turbulence is stabilised, the energy removed by the filter tends to a small level, such that it becomes effectively nonintrusive.
Figure 55. Demonstration of pattern selection by Fourier plane filtering. The selected patterns are hexagons (a), rolls (b), rhombic symmetry (c) and squares (d). The figure shows experimental far field, numerical near field and numerical far field, from left to right.

4.4.2 Optical patterns in quadratically nonlinear media

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A substantial amount of work has been done on pattern formation in nonlinear optics. So far most work has been carried out with cubic nonlinearities which have proved to be well-suited, although they also have serious drawbacks. A limitation, for instance, of photorefractive materials is the slow timescale of the nonlinearity. Quadratic nonlinearities are much faster and less noisy and this gives rise to new effects. Furthermore, the faster timescales may be a great advantage in information processing applications.

A price paid for the better performance of quadratic materials is a slightly more complicated experimental set-up. We have constructed a doubly-resonant cavity intended for second harmonic generation (SHG). The basic principles in the experimental set-up are shown in Figure 56. An Ar-ion laser is used to pump a Ti:Sapphire laser operating at 860 nm. The Ti:Sapphire laser drives a nonlinear cavity consisting of two independent arms for the fundamental frequency (FF) and second harmonic (SH), respectively. The two modes can be tuned independently with piezo mounted mirrors. Also the cavity can be locked to resonance by applying a servo feedback loop.

![Experimental set-up for pattern formation in optical second harmonic generation.](image)

Figure 56. Experimental set-up for pattern formation in optical second harmonic generation.
The described system has also been investigated theoretically. The scaled equations for intracavity SHG are given by:

\[
i\frac{\partial A_i}{\partial T} + \nabla_i^2 A_i = E - \left(\Delta_i + i\right) A_i - A_i^* A_2
\]  

\[
i\frac{\partial A_2}{\partial T} + \frac{1}{2} \nabla_i^2 A_2 = -\left(\Delta_2 + i\gamma\right) A_2 - A_i^2.
\]  

where \(A_i\) and \(A_2\) are the amplitudes for the FF and SH, \(E\) is the field used to pump the cavity, \(\Delta_i\) is the detuning of the cavity from resonance and \(\gamma = \gamma_2/\gamma_1\) is the ratio between the loss rates of the SH and FF. Various types of instabilities can occur and the threshold conditions have been studied by linear stability analysis. Above threshold, numerical simulation shows, for example, hexagonal patterns as illustrated in Figure 57. Numerical simulation of Eqs. (4.1, 4.2) showing hexagonal patterns. The upper row is the fundamental, and the lower row is the second harmonic field. Near and far field pictures are shown in the left and right columns, respectively.

An exciting prospect will be to study correlations in the patterns obtained in quadratic nonlinear processes. Theoretical work has proposed the existence of quantum correlations in the spatial structure of the generated fields.\(^1\) Two points in a pattern can be correlated better than the limit set by classical statistics (shot-noise level). In this sense the “quantum patterns” can be understood as the spatial analogue of squeezed light, which is temporal correlations below shot-noise level.
The possibility of using spatial solitary waves for implementation of optical logic and switching has led to a number of experimental and theoretical investigations of the interactions between spatial solitons. Initial experimental work in this area centred on Kerr or saturable Kerr type nonlinearities where phase dependent attraction and repulsion of one-dimensional, planar soliton beams was observed in media with a self-focusing nonlinearity.

During the last few years several groups have reported steady-state self-focusing and formation of spatial solitons in photorefractive media. Interest in photorefractives in the context of spatial switching stems in part from the possibility of soliton propagation at relatively low levels of the optical power. Self-focusing effects, and convergence to solitary profiles, have been observed for beams at μW power levels, which is significantly lower than that required in traditional Kerr type media. Interactions of both mutually coherent and mutually incoherent solitons have been studied. Mutually coherent beams exhibit attractive or repulsive forces depending on their relative phase.

In this work we have investigated the interaction of mutually coherent two-transverse dimensional [(2+1)D] bright spatial solitons in a photorefractive crystal. We show that switching the relative phase of the two input beams leads to a well resolved spatial shift of the beams at the output of the crystal. The interaction thus implements a phase dependent optical switch. When the input beams are in phase, and have a sufficiently small crossing angle, the output beams are observed to fuse. An example of our results is shown in Figure 58.

Figure 58. Integrated experimental output intensity distributions for in-phase (solid line) and out-of-phase (dashed line) input beams.

4.4.4 Anomalous interaction of spatial solitons in photorefractive media

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The nature of the forces between mutually coherent interacting solitons has been discussed in the literature for temporal as well as spatial solitons. It has been established that in the case of homogeneous self-focusing media the interaction force depends on the relative phase of the solitons. In particular, two in-phase solitons attract while out-of-phase solitons repel. Practical utilisation of coherent interaction effects for spatial switching is, however, troublesome. Phase control of a large number of beams in a switching fabric may be difficult to achieve. Furthermore, efficient coherent interaction requires that the relative phase between solitons is maintained under propagation.

To overcome these limitations one may consider the use of mutually incoherent solitons, whose interaction is independent of their relative phase. Incoherent solitons provide, however, a restricted range of spatial interactions since in typical isotropic self-focusing media mutually incoherent solitons always attract each other.

Figure 59. Numerical results showing attraction for beams separated by a small amount along the crystalline c-axis (a), repulsion for larger initial separation (b), attraction for orthogonal orientation (c) and spiralling for intermediate separation angle (d). Top row shows input beams, and bottom row shows output beams.

In this work¹ we demonstrate, theoretically and experimentally, that the restriction to attractive interactions is not fundamental, and that it is possible to achieve both attractive and repulsive forces between mutually incoherent solitons. This opens the possibility of accessing a significantly wider range of soliton logic operations with incoherent beams. This
anomalous situation occurs in photorefractive media where the particular anisotropic and nonlocal structure of the nonlinearity results in both attraction and repulsion of parallel beams depending on their relative spatial separation, as shown in Figure 59.


4.4.5 Bound dipole solitary solutions in anisotropic nonlocal self-focusing media

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The possibility of creating (2+1)D (two-transverse-dimensional) soliton-type structures of light in nonlinear media is of considerable interest due to potential applications in optical information processing systems. Dynamics of nonlinear propagation equations resulting in the formation of such structures can be very complex and may result in the generation of higher-order and multisoliton solutions. These solutions have been investigated extensively in the (1+1)D (one-transverse-dimensional) case. In two-transverse dimensions the majority of nonlinear equations of interest are not integrable, and the corresponding initial or boundary-value problems are usually analysed numerically. Existence and properties of higher-order and multisoliton solutions in the (2+1)D case have therefore been investigated much less than in the (1+1)D case.

In this work, for the first time to our knowledge, we find and investigate (2+1)D dipole solitary solutions for a light beam in a self-focusing nonlocal anisotropic optical medium. This solution is a bound pair consisting of two elliptical beams spaced some distance apart which are in anti-phase to each other (have a \(\pi\) relative phase shift). The above dipole solution is unique to the (2+1)D case and has no analogues in the (1+1)D case for neither anisotropic nor Kerr-type isotropic nonlinear media.

We demonstrate experimentally the importance of the relative phase of the two lobes of the dipole in determining the subsequent spatial evolution. The particulars of our analysis pertain to a photorefractive nonlinear response, but general conclusions should be qualitatively applicable to other media.

4.4.6 Solitary attractors and low-order filamentation in anisotropic self-focusing media

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We have performed a detailed theoretical analysis of optical self-focusing in media with anisotropic nonlocal photorefractive material response. These media support single solitons, as well as higher order bound dipole pair solutions. The single solitons are elliptical beams, whereas the dipole pairs are formed by a pair of displaced elliptical beams with a $\pi$ phase shift between their fields. The theory predicts convergence of Gaussian beams to the solitary states within a certain basin of attraction. Experimental observation of these solitons has been presented previously.\textsuperscript{1,2} When the initial conditions lie outside the basin of attraction of the solitary solutions, more complex spatial dynamics are observed. These include low-order, asymmetric filamentation into several beamlets followed, in some cases, by fusion of the beamlets, as shown in Figure 60. Such effects have been studied numerically and experimentally,\textsuperscript{3} for a range of physical parameters.

![Figure 60. Experimentally observed output intensity distributions versus saturation parameter. For low saturation (middle pictures in top row) there is convergence to an elliptical solitary profile. For higher saturation there is splitting into filaments, followed by rejoining.](image)

4.4.7 Time dependent evolution of an optical vortex in photorefractive media

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Three-dimensional solitary vortex solutions of the nonlinear Schrödinger equation were first considered in the context of superfluidity and are an active topic in nonlinear optics. It has been demonstrated experimentally that Kerr-type optical media with a cubic, isotropic and local nonlinearity support stable (2+1)D vortex solitons that have radial symmetry. Photorefractive materials offer the opportunity of studying soliton and vortex dynamics in nonlinear media with a response that is significantly different from that found in Kerr media. Anisotropy leads to characteristic features of localised solitary solutions. In the case of a self-focusing nonlinearity the lowest order solitary solutions are always elliptically shaped, with a transverse width that is narrowest along the anisotropy axis (direction of applied field). These solutions are intuitively reasonable generalisations of the radially symmetric solitary solutions found in isotropic Kerr-type media.

In the self-defocusing case studied here the situation is dramatically different. The radially symmetric vortex solutions observed in Kerr media have no direct counterpart in photorefractives. By comparison with the self-focusing case one might naively expect to observe an elliptically shaped solitary vortex, with a fixed alignment relative to the anisotropy axis. However, the phase structure of the vortex implies that an elliptically shaped vortex core rotates as it propagates so that it is impossible to maintain correct alignment. The result is that in the steady state, and when the light intensity is comparable with the saturation intensity in the medium, excitation of the medium with a circular vortex leads to charge dependent rotation, stretching and eventual decay of the localised structure.

In this work we analyse the transient nonlinear evolution of vortex beams in photorefractive media. Our results show that transient evolution of the vortex results in its decay. This decay is characterised by charge dependent rotation, and stretching of the vortex along the direction of the photogalvanic or externally applied field (the charge is the accumulated phase in multiples of $2\pi$ acquired in going around the vortex). Figure 61 gives an example of observations in a LiNbO$_3$ crystal showing the time dependent decay of a vortex.
Figure 61. Evolution of a charge-one vortex in LiNbO$_3$ at times of 0, 77, 192 and 339 sec. The final frame is for an oppositely charged vortex at 120 sec. The insets show interferograms demonstrating the sign of the input vortex. The pictures are negative images with low intensities represented by white regions, and the c-axis is horizontal.

4.4.8 Evolution of wave beams in media with anisotropic dispersion

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The three-dimensional cubic Schrödinger equation (CSE) models a slowly varying amplitude field of electromagnetic waves in media where the refractive index depends linearly on the field intensity, i.e. Kerr-type media. The equation reads in normalised form:

\[ \frac{i}{t} \frac{\partial \psi}{\partial t} + \nabla^2 \psi + s \frac{\partial^2 \psi}{\partial z^2} + p |\psi|^2 \psi = 0 \]

where \( \psi \) is the complex envelope field and \( z \) is the direction of propagation. The second term models the diffraction in the transverse plane; the third term models the dispersion along the axis of propagation (\( s > 0 \) yields anomalous dispersion, \( s < 0 \) yields normal dispersion). The last term on the left-hand side models the Kerr effect, where \( p > 0 \) corresponds to focusing, and \( p < 0 \) corresponds to defocusing. Here we only considered \( p > 0 \), and the investigations were mainly concerned with the propagation of wave beams in media with anisotropic dispersion (\( s < 0 \)). The cubic Schrödinger equation was solved numerically on a three-dimensional triple periodic domain.

We have investigated the internal dynamics of light beams (light bullets) and found that in anisotropic media with \( s < 0 \) a splitting takes place before the field can collapse (a spherical Gaussian light bullet), as predicted theoretically.\(^1\) Furthermore, the number of resulting cells was below the maximum number predicted.

We also considered stationary beam solutions to the CSE in the form of radially-symmetric waveguides that are perturbed in the \( z \)-direction. It is known that for such perturbed beams, bunching-type (sausage-like) perturbations can modulate and break up the waveguide solution periodically in both cases, viz. \( s > 0 \) and \( s < 0 \).\(^1\) Moreover, snake-like perturbations with angular dependency promote the bending of the waveguide solution in the case \( s < 0 \).\(^2\) We have investigated both kinds of perturbations by numerically solving the CSE. The evolution is in accordance with the stability analysis: bunches emerge from a perturbed cylindrically-symmetric waveguide both for \( s > 0 \) and \( s < 0 \), while initially-bent waveguides are stable for \( s > 0 \) and unstable for \( s < 0 \).

As snake-like instability can grow for \( s < 0 \), we exploit the idea of initially bending two co-propagating beams in such a way that they may interact in their regions of closest approach. We observe amplification of the bending of the two waveguides and that they merge at their point of closest approach, around which strong self-focusing develops transversally. Ultimately, the lobe resulting from this process splits up into two new pulses that were not observed to collapse but, instead, spread out in time.

4.4.9 Interaction of light beams in Kerr-type media

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Self-trapping and self-focusing of intense optical beams that propagate in nonlinear, dispersive media have been widely investigated during the last three decades. In particular, self-trapped beams evolving in two spatial dimensions are well-known to self-focus until they collapse at a finite propagation distance, when their power exceeds a certain threshold so that the nonlinear effects dominate over the diffraction of the wave. These results apply to individual light beams. Often a number of light filaments are formed as a result of the modulational instability of a broad light beam. The filaments are observed to interact, but up to now only a few quantitative investigations of this interaction dynamics have been performed.

We have extended our previous work on the interaction of light beams in a self-focusing Kerr medium,\textsuperscript{1} where we in particular considered the interaction of two identical beams. The main result was: beams with a power above \( N_c/4 \), where \( N_c \) is the critical self-focusing threshold for a single beam, will fuse into a single central lobe that may self-focus until collapse, if their initial separation distance is below a critical distance depending on the power. Here we consider beams that have different initial power. Still a critical separation distance can be identified below which the beams will merge and ultimately collapse at the position of their “centre of mass”. The critical separation distance seems to be determined by the smallest power. We also “measured” the power transfer during the merging and collapse which indicated a transfer of power from the weak to the strong beam. In contrast to the case of equal beams, two unequal beams with initial opposite phases may also merge and collapse if their separation is below a critical value, since their phases develop differently and, thus, their phase difference will change.


4.4.10 Interaction of two-dimensional spatial solitons in saturable media

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Spatial solitons consist of self-trapped beams of electromagnetic waves in a nonlinear medium, where the diffractive spreading is balanced by the nonlinearity whereby an intensity dependent refractive index is introduced. For the case of so-called Kerr media with cubic nonlinearity, two-dimensional solitons are known to be unstable leading to unlimited self-focusing. In media with saturation of the nonlinear refractive index,
on the other hand, two-dimensional spatial solitons will be stable. Stable spatial solitons are thought to have potential as building blocks for all-optical devices. They may, e.g., be used for guiding a signal beam of low power.

We have investigated the interaction of such spatial solitons in a saturable medium. The investigations are based on the saturable nonlinear Schrödinger equation in the normalised form for the propagation of the slowly varying wave beam envelope:

\[
\frac{\partial \psi}{\partial t} + \nabla^2 \psi + f(|\psi|^2)\psi = 0, \quad \text{where} \quad f(|\psi|^2)\psi = \frac{|\psi|^2}{1+|\psi|^2}.
\]

We have solved the equation numerically and the results are supported by analytical investigations based on the variational approach. In general, it is found that two solitons of the same phases will attract each other. Their interaction may take various different forms depending on the initial separation and the initial velocities of the solitons: they may pass through each other; they may fuse and form a new soliton after radiating away excess energy. On the other hand, two solitons of opposite phases will expel each other. In particular, we have investigated the case of two identical solitons that spiral around each other for an initial configuration of the two solitons that possesses a finite angular momentum. This is found to be possible for a specific initial velocity of the solitons. For initial velocities below this critical velocity the two solitons are seen to merge, while they separate for initial velocities above the critical velocity.

4.4.11 Fusion and collapse of coupled waves in cubic media

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The non-resonant - or incoherent - interaction of two light beams that propagate in a nonlinear Kerr medium is described by two nonlinear Schrödinger (NLS) equations that are coupled through the nonlinear terms that account for cross-phase modulations. We have studied the interaction of two such beams analytically and numerically. By means of virial arguments we show that collapse cannot occur in one (spatial) dimension and predict the power threshold for collapse in two and three dimensions. The results are supported by direct numerical solutions of the coupled NLS equations. Above the collapse threshold, wave beams that are initially separated from each other may either collapse individually or attract each other, merge and collapse as a single beam depending on their separation distance. We have predicted the dependence of the critical separation below which the beams merge before collapsing as a single beam. The phase difference between the beams has no influence on the interaction dynamics which is in contrast to the case of coherent interaction of beams (see 4.4.9),\(^1\) where the evolution is governed by a single NLS.
Determination of the dynamic properties of physical systems with competition between discreteness, nonlinearity and dispersion has attracted growing interest because of the wide applicability of such models in various physical problems. Examples are coupled optical fibres, arrays of coupled Josephson junctions, nonlinear charge and excitation transport in biological systems, and elastic energy transfer in an-harmonic crystals. It has been shown that the balance between nonlinearity and dispersion in a weak nonlinearity (large dispersion) limit provides the existence of low-energy soliton-like excitations. These excitations are very robust objects that essentially propagate without energy loss, and their collisions are almost elastic. As a result of the interplay between discreteness, dispersion and nonlinear interaction, a new type of nonlinear excitations may appear: intrinsically localised oscillatory states, which are also termed discrete breathers.

Until recently the main attention was paid to systems with short-ranged dispersive interaction and a nearest-neighbour approximation was used. However, long-range interaction is often of importance in discrete nonlinear systems.

We have investigated the dynamics of discrete two-dimensional nonlinear Schrödinger models with long-range dispersive interaction. In particular, we focus on the cases where the dispersion arises from a dipole-dipole interaction, assuming that the dipole moments at each lattice site are aligned either in the lattice plane (anisotropic case) or perpendicular to the lattice plane (isotropic case). We investigate the nature of the linear dispersion relation for these two cases, and derive a criterion for the modulational instability of a plane wave with respect to long wavelength perturbations. Furthermore, we study the on-site localised stationary states of the system numerically and analytically using a variational approach. In general, the narrow, intrinsically localised states are found to be stable, while broad, 'continuum-like' excitations are unstable and may either collapse into intrinsically localised modes or disperse when a small perturbation is applied.
Diffractive optical elements (DOEs) have gained increasing interest in recent years. Among the possible applications are compact optical sensors where DOEs can be used for out-of-plane coupling of light from integrated optical waveguides.

Modelling of DOEs is in general a highly complex task, and analytic solutions only exist for periodic elements of infinite length. For non-periodic elements of finite length, numerical methods must be applied for accurate calculation of the DOE characteristics. One approach has been to employ the finite difference time-domain method (FDTD). However, in order accurately to resolve the optical wave, up to 40 points per wavelength are needed in the discrete finite difference grid. For DOEs, which may be several hundred wavelengths long, this leads to excessive computer resource requirements.

We have chosen to follow another approach, namely to employ spectral methods. Such methods have been used extensively within the field of fluid dynamics for many years and were recently also employed in electromagnetic scattering problems.¹

Spectral methods have a number of attractive features. First of all, using as few as 8-10 points per wavelength, the optical wave can be fully resolved. This clearly reduces the computer resource demand in comparison with FDTD, especially in three dimensions. Another advantage of spectral methods is the ease by which the computing domain can be decomposed into subdomains. Because of the hyperbolic nature of the time-domain Maxwell’s equations, these may be solved locally in each subdomain and, subsequently, the global solution is found by patching the local solutions through the use of characteristic variables. Domain decomposition makes spectral methods well-suited for complex geometries and facilitates the use of parallel computers.

As an example, Figure 62 shows the computing domain for an out-of-plane diffractive optical coupler and its division into subdomains. Physically, the DOE consists of a slab waveguide formed by sandwiching a layer of a refractive index $n_2$ between two cladding layers of refractive index $n_1$, where $n_2 > n_1$. The top cladding layer has a modulated surface and this modulation causes radiation of the optical field in directions determined by the modulation period. The layers are indicated by different colours in the figure.
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Figure 62. Calculation domain for out-of-plane coupling diffractive optical element divided into subdomains indicated by yellow lines. Different colours correspond to different refractive indices: Blue: cladding refractive index, $n_1$. Green: core refractive index, $n_2$. Grey: free space.

Figure 63 shows a snapshot of the $E_y$ component of a TE field propagating in the structure at some time $t = t_0$ which has been chosen to be sufficiently long so that steady-state has been reached.

Figure 63. Snapshot of the $E_y$-component of a TE mode propagating in an out-of-plane DOE. Boundaries between layers of different dielectric constants are indicated by white lines.

4.5 Biophysics

4.5.1 Microtubule dynamics: kinetics of self-assembly

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Inverse scattering theory describes the conditions that are necessary and sufficient to determine unknown potential from known scattering data. No similar theory exists for when and how one may deduce the kinetics of an unknown chemical reaction from quantitative information about its final state and its dependence on initial conditions - except that it is known to be impossible for equilibrium reactions. We have made a case study of a far-from-equilibrium reaction: it presents a systematic phenomenological analysis of experimental time series for the amount of final product, a bio-polymer, formed from various initial concentrations of monomers. Distinct mathematical properties of the kinetics of the unknown reaction pathway are found. These properties are shown to restrict the kinetics to a single model that generalises Oosawa's classical nucleation-polymerisation model. The methods used here to analyse the self-assembly of microtubules from tubulin are general, and many other reactions and processes may be studied as inverse problems with these methods when sufficient experimental data are available.


4.5.2 Modelling microtubule oscillations

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Synchronisation of molecular reactions in a macroscopic volume may cause the volume's physical properties to change dynamically and thus reveal much about the reactions. As an example, experimental time series for so-called microtubule oscillations are analysed in terms of a minimal model for this complex polymerisation-depolymerisation cycle. The model reproduces well the qualitatively different time series that result from different experimental conditions, and illuminates the role and importance of individual processes in the cycle. Simple experiments are suggested that can further test and define the model and the polymer's reaction cycle.

4.5.3 Prompt recognition of brain states by their EEG signals

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Brain states corresponding to the intention of movement of left and right index fingers and right foot are classified by a "committee" of artificial neural networks processing individual channels of 56-electrode electroencephalograms (EEGs). Correct recognition is achieved in 83% of cases not previously seen by the system on the basis of 1 sec long EEGs.

5. Combustion Facilities

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In the long term, pressurised combustion and gasification technologies are expected to have the largest potential as regards high efficiency and low environmental impact. During 1996 and the beginning of 1997 the combustion and gasification laboratory at Risø National Laboratory has investigated fuel reactivity under pressurised conditions – experimentally as well as theoretically. The experimental part covered pressures up to 10 bar and temperatures up to 1400 °C. Analyses of these data are in progress and have partly been reported.¹,²

A European project, which describes the state-of-art of biomass utilisation for heat and energy production in small systems, has been completed, where the Danish part has primarily been a description of the present status of gasification in Denmark and Norway.⁴

As a part of a European project concerning agglomeration of different sorts of biomass, Risø National Laboratory and Energi Center Nederland have performed an intensive study of agglomeration properties of different kinds of biomass. The Danish part of the work has in 1997 mainly been dealing with wheat straw and a mixture of wheat straw and sludge. This work has been carried out in cooperation with Energiteknisk Center in Piteå where a large number of experiments have been performed in a small 5 kW fluid bed. The analyses of the data also include high temperature microscopy in a scanning electron microscope and modelling using the CHEMSAGE programme.

Furthermore, work related to tar reduction in gasification in small biomass gasification power plants has been finished and published.³ A project between the Danish utilities ELSAM and ELKRAFT in cooperation with Ansaldo Volund R&D Centre, Technical University of Denmark, The FORCE Institute and Risø National Laboratory dealing with testing of superheater materials and superheaters in incineration power plants has been completed and reported in a Danish report.⁵

6. Publications and Educational Activities

6.1 Optical Materials

6.1.1 International Publications


6.1.2 Danish Publications


6.1.3 Conference Lectures


Johansen, P.M.; Pedersen, H.C., Response of photorefractive Bi$_{12}$SiO$_{20}$ to running gratings and AC electric field. In: Proceedings. 1997 Topical meeting on photorefractive materials, effects and devices. PR '97,


6.1.4 Publications for a Broader Readership


Petersen, P.M., En ny optikuddannelse i Danmark?. DOPS-Nyt (1997) v. 12 (no.1) p. 6.


Petersen, P.M.; Dam-Hansen, C.; Johansen, P.M., Optisk datalagring i ulineære materialer. DOPS-Nyt (1997) v. 12 (no.4) p. 4-7.

6.1.5 Unpublished Lectures


6.2 Optical Diagnostics and Information Processing

6.2.1 International Publications


6.2.2 Danish Publications


6.2.3 Conference Lectures


Imam, H.; Rose, B.; Hanson, S.G.; Lading, L., Laser time-of-flight velocimetry: Proposals for miniaturisation. In: Diffractive optics and optical microsystems. 20. Course of the international school of


6.2.4 Publications for a Broader Readership

Andersen, P.E., Ulineær vekselvirkning mellem gitre i fotorefraktive krystaller. DOPS-Nyt (1997) v. 12 (no.3) p. 13-17.
Petersen, P.M.; Dam-Hansen, C.; Johansen, P.M., Optisk datalagring i ulineære materialer. DOPS-Nyt (1997) v. 12 (no.4) p. 4-7.

6.2.5 Unpublished Lectures
Hanson, S.G.; Rose, B.; Yura, H.T., Speckle methods for analyzing linear and angular velocities and displacements. 22. Course: Optical sensors


6.2.6 Internal Reports


6.3 Plasma and Fluid Dynamics

6.3.1 International Publications


6.3.2 Danish Publications

6.3.3 Conference Lectures
Michelsen, P.K.; Sunn Pedersen, T.; Juul Rasmussen, J., Lyapunov exponents and particle dispersion in drift-wave turbulence. In:
6.3.4 Publications for a Broader Readership


6.3.5 Unpublished Lectures


Flyvbjerg, H., Modeling microtubule dynamics: Doing molecular biology with the tools of theoretical physics. Hong Kong University of Science and Technology, Physics Department Seminar, Hong Kong (CN), 6 Nov 1997. Unpublished.
Flyvbjerg, H., Error estimates on averages of correlated data. Hong Kong University of Science and Technology, Physics Department seminar, Hong Kong (CN), 25 Nov 1997. Unpublished.
Flyvbjerg, H., Stochastic dynamics of microtubules. Hong Kong University of Science and Technology, Physics Department seminar, Hong Kong (CN), 2 Dec 1997. Unpublished.
Konijnenberg, J.A. van de; Nielsen, A.H.; Nijs, R. de; Juul Rasmussen, J.; Stenum, B., Shear-flow instability in a parabolic vessel. IUTAM


Stenum, B., Drift velocities of forced monopoles in a rotating paraboloid.


7. Personnel

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Abstract (max. 2000 char.)

Research in the Optics and Fluid Dynamics Department has been performed within the following three programme areas: (1) optical materials, (2) optical diagnostics and information processing and (3) plasma and fluid dynamics. The work is concentrated on combinations of systems, structures and materials. The systems work is focused on sensors, information processing and storage; the structures work is concentrated on pattern formation and diffractive elements; the materials work is centred on the understanding and utilisation of nonlinear phenomena. Scientific computing is an integral part of the work. The activities are supported by several EU programmes, including EURATOM, by research councils and by industry. A summary of the activities in 1997 is presented.