Research outputs:

**Quantifying the power output and structural figure-of-merits of triboelectric nanogenerators in a charging system starting from the Maxwell's displacement current**

Conversion of mechanical energy into electricity using triboelectric nanogenerators (TENGs) is a rapidly expanding research area. Although the theoretical origin of TENGs has been proven using the Maxwell's displacement current ($I_D$), a profound quantitative understanding of its generation is not available. Moreover, a comprehensive analysis of the fundamental charging behavior of TENGs and building a standard to evaluate each TENG's unique charging characteristic are critical to ensure efficient use of them in practice. We present a thorough analysis of TENG's charging behavior through which a more complete evaluation of TENG charging is proposed by introducing the structural figure of merit (FOMCs) in a charging system (powering capacitors). The analysis is based on Maxwell's displacement current and results are verified experimentally. To achieve this, according to the distance-dependent electric field model, we provide a systematic discussion on the generation of $I_D$ in TENGs, along with the derived analytical formula and numerical calculations. This work suggests a new way to deeply understand the nature of the $I_D$ generated within the TENGs; and the modified FOMC can be used to predict the charging characteristics of TENGs in an energy storage system, allowing us to utilize the TENGs more efficiently towards different applications.
Symmetry of superconducting correlations in displaced bilayers of graphene
Using a Green’s function approach, we study phonon-mediated superconducting pairing symmetries that may arise in bilayer graphene where the monolayers are displaced in-plane with respect to each other. We consider a generic coupling potential between the displaced graphene monolayers, which is applicable to both shifted and commensurate twisted graphene layers; study intralayer and interlayer phonon-mediated BCS pairings; and investigate AA and AB (AC) stacking orders. Our findings demonstrate that at the charge neutrality point, the dominant pairings in both AA and AB stackings with intralayer and interlayer electron-electron couplings can have even-parity s-wave class and odd-parity p-wave class of symmetries with the possibility of invoking equal-pseudospin and odd-frequency pair correlations. At a finite doping, however, the AB (and equivalently AC) stacking can develop pseudospin-singlet and pseudospin-triplet d-wave symmetry, in addition to s-wave, p-wave, f-wave, and their combinations, while the AA stacking order, similar to the undoped case, is unable to host the d-wave symmetry. When we introduce a generic coupling potential, applicable to commensurate twisted and shifted bilayers of graphene, d-wave symmetry can also appear at the charge neutrality point. Inspired by a recent experiment where two phonon modes were observed in a twisted bilayer graphene, we also discuss the possibility of the existence of two-gap superconductivity, where the intralayer and interlayer phonon-mediated BCS picture is responsible for superconductivity. These analyses may provide a useful tool in determining the superconducting pairing symmetries and mechanism in bilayer graphene systems.

General information
Publication status: Published
Organisations: Rector’s office, Department of Photonics Engineering, Department of Physics, Center for Nanostructured Graphene, K.N. Toosi University of Technology
Corresponding author: Alidoust, M.
Contributors: Alidoust, M., Willatzen, M., Jauho, A.
Number of pages: 15
Publication date: 12 Apr 2019
Peer-reviewed: Yes

Control of superconducting pairing symmetries in monolayer black phosphorus
Motivated by recent experimental progress, we study the effect of mechanical deformations on the superconducting pairing symmetries in monolayer black phosphorus (MBP). Starting with phonon-mediated intervalley spin-singlet electron-electron pairing and making use of realistic band parameters obtained through first-principles calculations, we show that the application of weak mechanical strain in the plane of MBP can change the effective s-wave and p-wave symmetry of the superconducting correlations into effective d-wave and f-wave symmetries, respectively. This prediction of a change in the pairing symmetries might be experimentally confirmed through angular dependence high-resolution tunneling spectroscopy, the Meissner effect, and critical temperature experiments. The idea of manipulating the superconducting symmetry class by applying planar mechanical strain can be extended to other anisotropic materials as well and may help in providing important information of the symmetries of the order parameter, perhaps even in some high-Tc superconductors.

General information
Publication status: Published
Organisations: Department of Photonics Engineering, Department of Physics, Center for Nanostructured Graphene, K.N. Toosi University of Technology
Contributors: Alidoust, M., Willatzen, M., Jauho, A. P.
Number of pages: 10
Publication date: 2019
Peer-reviewed: Yes
High fidelity optical quantum gates based on type II double quantum dots in a nanowire

We propose an optical gating scheme for quantum computing based on crystal-phase type II double quantum dots in an InP nanowire. The qubit is encoded on the electron spin and the gate operations are performed using stimulated Raman adiabatic passage (STIRAP), using the orbital degree of freedom in double quantum dots to form an auxiliary ground state. Successful STIRAP gating processes require an efficient coupling of both qubit ground states of the double quantum dot to the gating auxiliary ground state, and we demonstrate that this can be achieved using a charged exciton state. Crucially, by using type II dots, the hole is localized between the two spatially separated electrons in the charged exciton complex, thereby efficiently coupling the electron ground state orbitals. By taking advantage of the high fidelity state transfer by means of STIRAP in type II double quantum dots, we propose a protocol for coherently manipulating the spin-orbital quantum state of confined electrons in a quantum dot chain of an InP nanowire. We subsequently exploit the protocol to realize single- and two-qubit gates with fidelity above 0.99.

General information
Publication status: Accepted/In press
Organisations: Quantum and Laser Photonics, Department of Photonics Engineering, Rector’s office, Technical University of Denmark, RAS - Pn Lebedev Physics Institute
Contributors: Taherkhani, M., Willatzen, M., Denning, E. V., Protsenko, I. E., Gregersen, N.
Number of pages: 12
Publication date: 2019
Peer-reviewed: Yes
The Four-Band Spin-Less Kane Model in Curvilinear Coordinates

The possibility to fabricate complicated nanostructure geometries with novel topological effects so as to tailor physical properties makes it adamant to develop advanced analytical and numerical methods. The first multiband k · p model in general curvilinear coordinates based on Kane's four-band spin-less model for the upper conduction and valence band states is developed. The model captures the combined effects of electron and light-hole bandstructure coupling and curvature effects. The formulation in curvilinear coordinates allows to obtain a simple set of equations, displaying directly the influence of the local curvature, and the explicit equation sets in the cases of a torus and a helix-shaped nanowire structure with a square cross section are given. The presented derivation can be generalized to other types of k · p multiband models.

Fraunhofer response and supercurrent spin switching in black phosphorus with strain and disorder

We develop theory models for both ballistic and disordered superconducting monolayer black phosphorus devices in the presence of magnetic exchange field and stress. The ballistic case is studied through a microscopic Bogoliubov-de Gennes formalism, while for the disordered case we formulate a quasiclassical model. Utilizing the two models, we theoretically study the response of supercurrent to an externally applied magnetic field in two-dimensional black phosphorus Josephson junctions. Our results demonstrate that the response of the supercurrent to a perpendicular
magnetic field in ballistic samples can deviate from the standard Fraunhofer interference pattern when the Fermi level and mechanical stress are varied. This finding suggests the combination of chemical potential and strain is an efficient external knob to control the current response in highly sensitive strain-effect transistors and superconducting quantum interference devices. We also study the supercurrent in a superconductor-ferromagnet-ferromagnet-superconductor junction where the magnetizations of the two adjacent magnetized regions are uniform with misaligned orientations. We show that the magnetization misalignment can control the excitation of harmonics higher than the first harmonic \sin \phi (in which \phi is the phase difference between the superconductors) in supercurrent and constitutes a full-spin-switching current element. Finally, we discuss possible experimental implementations of our findings. We foresee our models and discussions could provide guidelines to experimentalists in designing devices and future investigations.

General information
Publication status: Published
Organisations: Department of Photonics Engineering, Center for Nanostructured Graphene, Department of Micro- and Nanotechnology, Theoretical Nanotechnology, K.N. Toosi University of Technology
Contributors: Alidoust, M., Willatzen, M., Jauho, A. P.
Number of pages: 10
Publication date: 9 Nov 2018
Peer-reviewed: Yes

Publication information
Journal: Physical Review B
Volume: 98
Issue number: 18
Article number: 184505
ISSN (Print): 2469-9950
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
Original language: English
Electronic versions:
PhysRevB.98.184505.pdf
DOIs:
10.1103/PhysRevB.98.184505
Source: Scopus
Source-ID: 85056359126
Research output: Contribution to journal › Journal article – Annual report year: 2018 › Research › peer-review

Data-driven electronic structure calculations in semiconductor nanostructures — beyond the eight-band k · p formalism
In this work, we present a scheme to extract electronic structure parameters for multi-band k · p models beyond the well-established eight-band approach using up-to-date ab initio band structures. Our scheme allows us to identify parameters for k · p models with Hamiltonian matrices of arbitrary complexity and level of sophistication. The computational effort of our approach is very small and increases only slightly with the number of parameters that need to be fitted. We can furthermore apply priorities to specific bands or high-symmetry points of the Brillouin zone and can incorporate routines that help to increase the numerical stability of electronic structure simulations of semiconductor nanostructures using the obtained parameter sets.

General information
Publication status: Published
Organisations: Department of Photonics Engineering, Weierstraß-Institut fur Angewandte Analysis und Stochastik, Aalto University
Contributors: Marquardt, O., Mathe, P., Koprucki, T., Caro, M. A., Willatzen, M.
Pages: 55 - 56
Publication date: 2018

Host publication information
Title of host publication: Proceedings of 2018 International Conference on Numerical Simulation of Optoelectronic Devices
Publisher: IEEE
ISBN (Print): 9781538655993
Keywords: Computational modeling, Semiconductor nanostructures, Scattering, Crystals, Eigenvalues and eigenfunctions, Gallium arsenide, Couplings
DOIs:
10.1109/NUSOD.2018.8570274
Source: FindIt
Source-ID: 2442541837
On the Geometry of Nanowires and the Role of Torsion

A detailed analysis of the Schrödinger equation in curved coordinates, exact to all orders in the cross sectional dimension is presented, and we discuss the implications of the frame rotation for energies of both open and closed structures. For a circular cross-section, the energy spectrum is independent of the frame orientation for an open structure. For a closed curve, the energies depend on the holonomy angle of a minimal rotating frame (MR) which is equal to the area enclosed by the tangent image on the unit sphere. In the case of a curve with a well-defined torsion at all points this is up to a multiple of 2π equal to the total torsion, a result first found in 1992 by Takagi and Tanzawa. In both cases we find that the effect on the eigenstates is a phase shift. We validate our findings by accurate numerical solution of both the exact 3D equations and the approximate 1D equations for a helix structure and find that the error is proportional to the square of the diameter of the cross section. We discuss Dirichlet versus Neumann boundary conditions and show that care has to be taken in the latter case.

General information
Publication status: Published
Organisations: Department of Applied Mathematics and Computer Science, Mathematics, Department of Photonics Engineering
Contributors: Gravesen, J., Willatzen, M.
Number of pages: 11
Publication date: 2018
Peer-reviewed: Yes

Publication information
Journal: PHYSICA STATUS SOLIDI (RRL) - RAPID RESEARCH LETTERS
Article number: 1800357
ISSN (Print): 1862-6254
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
Original language: English
Keywords: Acoustics, Frame orientation, Quantum mechanics, Torsion
DOI:
10.1002/pssr.201800357
Source: FindIt
Source-ID: 2439991214
Research output: Contribution to journal > Journal article – Annual report year: 2018 > Research > peer-review

Pseudocanalizing propagation with hyperbolic surface waves

Negative magnetic permeability allows for reversed phase propagation in HMMs. However, magnetic properties are difficult to realize in the visible wavelengths. We propose a similar effect for surface waves without requiring magnetic properties.

General information
Publication status: Published
Organisations: Department of Photonics Engineering, Metamaterials
Contributors: Repán, T., Novitsky, A., Willatzen, M., Lavrinenko, A.
Number of pages: 2
Publication date: 2018

Host publication information
Title of host publication: Novel Optical Materials and Applications 2018
Publisher: Optical Society of America (OSA)
Article number: NoW4J.5
ISBN (Print): 978-1-943580-43-9
Electronic versions:
NOMA_2018_NoW4J.5.pdf
DOI:
10.1364/NOMA.2018.NoW4J.5

Bibliographical note
From the session: Polaritonics (NoW4J)
Pseudocanalization regime for surface waves
Magnetic properties can be used to reverse phase advancing in the pseudocanalization regime of hyperbolic metamaterials. However, practical implementations of required μ-negative media are challenging. Here we reveal analogous effect for the electromagnetic surface waves in non-magnetic materials.

General information
Publication status: Published
Organisations: Department of Photonics Engineering, Metamaterials, Technical University of Denmark
Contributors: Repan, T., Novitsky, A., Willatzen, M., Lavrinenko, A.
Number of pages: 2
Pages: 1-2
Publication date: 2018

Host publication information
Title of host publication: Proceedings of 2018 Conference on Lasers and Electro-Optics
Publisher: Optical Society of America (OSA)
Keywords: Optical surface waves, Surface waves, Metamaterials, Magnetic materials, Dielectrics, Hidden Markov models, Dispersion
DOIs: 10.1364/CLEO_AT.2018.JW2A.108
Source: FindIt
Source-ID: 2438377727
Research output: Chapter in Book/Report/Conference proceeding – Article in proceedings – Annual report year: 2018
Research: peer-review

Reversed phase propagation for hyperbolic surface waves
Magnetic properties can be used to control phase propagation in hyperbolic metamaterials. However, in the visible spectrum magnetic properties are difficult to obtain. We discuss hyperbolic surface waves allowing for a similar control over phase, achieved without magnetic properties.

General information
Publication status: Published
Organisations: Department of Photonics Engineering, Metamaterials
Contributors: Repän, T., Novitsky, A., Willatzen, M., Lavrinenko, A.
Pages: 56-56
Publication date: 2018

Host publication information
Title of host publication: Proceedings of XXVI International Workshop on Optical Wave & Waveguide Theory and Numerical Modelling.
Publisher: TU Dortmund University
ISBN (Print): 978-3-921823-98-9
Electronic versions: procOWTNM2018.pdf
Research output: Chapter in Book/Report/Conference proceeding – Article in proceedings – Annual report year: 2018
Research: peer-review

Strain-engineered Majorana zero energy modes and $\varphi_0$ Josephson state in black phosphorus
We develop a theory for strain control of Majorana zero energy modes and Josephson effect in black phosphorus (BP) devices proximity coupled to a superconductor. Employing realistic values for the band parameters subject to strain, we show that the strain closes the intrinsic band gap of BP, however the proximity effect from the superconductor reopens it and creates Dirac and Weyl nodes. Our results illustrate that Majorana zero energy flat bands connect the nodes within the band-inverted regime in which their associated density of states is localized at the edges of the device. In a ferromagnetically mediated Josephson configuration, the exchange field induces super-harmonics into the supercurrent phase relation in addition to a $\varphi_0$ phase shift, corresponding to a spontaneous supercurrent, and strain offers an efficient tool to control these phenomena. We analyze the experimental implications of our findings, and show that they can pave the way for creating a rich platform for studying two-dimensional Dirac and Weyl superconductivity.

General information
Publication status: Published
Organisations: Department of Photonics Engineering, Center for Nanostructured Graphene, Department of Micro- and Nanotechnology, Theoretical Nanotechnology, K.N. Toosi University of Technology
Strain-enhanced optical absorbance of topological insulator films

Topological insulator films are promising materials for optoelectronics due to a strong optical absorption and a thickness-dependent band gap of the topological surface states. They are superior candidates for photodetector applications in the THz-infrared spectrum, with a potential performance higher than graphene. Using a first-principles $k\cdot\pi$ Hamiltonian, incorporating all symmetry-allowed terms to second order in the wave vector $k$, first order in the strain $c$, and of order $ck$, we demonstrate a significantly improved optoelectronic performance due to strain. For Bi$_2$Se$_3$ films of variable thickness, the surface-state band gap, and thereby the optical absorption, can be effectively tuned by the application of uniaxial strain $\epsilon_{zz}$, leading to a divergent band-edge absorbance for $\epsilon_{zz} \geq 6\%$. Shear strain breaks the crystal symmetry and leads to an absorbance varying significantly with polarization direction. Remarkably, the directional average of the absorbance always increases with strain, independent of material parameters.

General information
Publication status: Published
Organisations: Department of Photonics Engineering, University of Copenhagen
Contributors: Brems, M. R., Paaske, J., Lunde, A. M., Willatzen, M.
Number of pages: 5
Publication date: 2018
Peer-reviewed: Yes

Publication information
Journal: Physical Review B
Volume: 97
Issue number: 8
Article number: 081402
ISSN (Print): 1098-0121
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
Original language: English
Keywords: Electronic, Optical and Magnetic Materials, Condensed Matter Physics, Microwave, radiofrequency and terahertz wave interactions with condensed matter, Optical constants and parameters (condensed matter), Infrared and Raman spectra in inorganic crystals, Optical properties of other inorganic semiconductors and insulators (thin films, low-dimensional and nanoscale structures)

Electronic versions:
DOIs:
10.1103/PhysRevB.97.081402
Source: FindIt
Source-ID: 2396470711
Research output: Contribution to journal › Journal article – Annual report year: 2018 › Research › peer-review
Symmetry analysis of strain, electric and magnetic fields in the Bi2Se3-class of topological insulators: Paper

Based on group theoretical arguments we derive the most general Hamiltonian for the Bi2Se3-class of materials including terms to third order in the wave vector, first order in electric and magnetic fields, first order in strain and first order in both strain and wave vector. We determine analytically the effects of strain on the electronic structure of Bi2Se3. For the most experimentally relevant surface termination we analytically derive the surface state (SS) spectrum, revealing an anisotropic Dirac cone with elliptical constant energy contours giving rise to a direction-dependent group velocity. The spin-momentum locking of strained Bi2Se3 is shown to be modified. Hence, strain control can be used to manipulate the spin degree of freedom via the spin–orbit coupling. We show that for a thin film of Bi2Se3 the SS band gap induced by coupling between the opposite surfaces changes opposite to the bulk band gap under strain. Tuning the SS band gap by strain, gives new possibilities for the experimental investigation of the thickness dependent gap and optimization of optical properties relevant for, e.g., photodetector and energy harvesting applications. We finally derive analytical expressions for the effective mass tensor of the Bi2Se3 class of materials as a function of strain and electric field.

General information
Publication status: Published
Organisations: Department of Photonics Engineering, Quantum and Laser Photonics, University of Copenhagen
Contributors: Brems, M. R., Paaske, J., Lunde, A. M., Willatzen, M.
Number of pages: 16
Publication date: 2018
Peer-reviewed: Yes

Publication information
Journal: New Journal of Physics
Volume: 20
Issue number: 5
Article number: 053041
ISSN (Print): 1367-2630
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
Original language: English
Keywords: Topological insulators, Electronic band structure, Group theory, Strain, Electric field
Electronic versions:
DOIs:
10.1088/1367-2630/aabcfc
Source: FindIt
Source-ID: 2409464213
Research output: Contribution to journal › Journal article – Annual report year: 2018 › Research › peer-review

Strain tuning of optical properties in Bi2Se3

Based on symmetry principles we determine the most general Hamiltonian for the low energy physics of Bi2Se3, including contributions due to a static electric field and strain. The full three-dimensional model is projected into the surface states at k= 0, giving an effective two-dimensional Hamiltonian for the surface states. Contributions from the strain tensor breaks the anisotropy of the surface state spectrum, giving an elliptical Dirac cone. Within this model we calculate the absorption spectrum for an ultra-thin film. We show that the fundamental absorption edge can be effectively tuned by application of uniaxial strain.

General information
Publication status: Published
Organisations: Department of Photonics Engineering, Quantum and Laser Photonics
Corresponding author: Jensen, M. R.
Contributors: Jensen, M. R., Mørk, J., Willatzen, M.
Number of pages: 2
Pages: 85-86
Publication date: 11 Aug 2017

Host publication information
Title of host publication: 17th International Conference on Numerical Simulation of Optoelectronic Devices, NUSOD 2017
Publisher: IEEE Computer Society Press
Article number: 8010003
ISBN (Electronic): 9781509053230
DOIs:
3D continuum phonon model for group-IV 2D materials

A general three-dimensional continuum model of phonons in two-dimensional materials is developed. Our first-principles derivation includes full consideration of the lattice anisotropy and flexural modes perpendicular to the layers and can thus be applied to any two-dimensional material. In this paper, we use the model to not only compare the phonon spectra among the group-IV materials but also to study whether these phonons differ from those of a compound material such as molybdenum disulfide. The origin of quadratic modes is clarified. Mode coupling for both graphene and silicene is obtained, contrary to previous works. Our model allows us to predict the existence of confined optical phonon modes for the group-IV materials but not for molybdenum disulfide. A comparison of the long-wavelength modes to density-functional results is included.

Acousto-optical phonon excitation in cubic piezoelectric slabs and crystal growth orientation effects

In this paper we investigate theoretically the influence of piezoelectric coupling on phonon dispersion relations. Specifically we solve dispersion relations for a fully coupled zinc-blende freestanding quantum well for different orientations of the crystal unit cell. It is shown that the phonon mode density in GaAs can change by a factor of approximately 2–3 at qx a = 1 for different crystal-growth directions relative to the slab thickness direction. In particular, it is found that optical and acoustic phonon modes are always piezoelectrically coupled, independent of the crystal-growth direction, and will be jointly excited by electrical stimulus. We demonstrate this for an electrically excited freestanding slab for two cases of high-symmetry crystal-growth directions and finally show the impact of the Drude model for permittivity on the phonon dispersion. In particular, it is verified that the piezoelectric effect leads to a drastically enhanced coupling of acoustic and optical phonon modes and increase in the local phonon density of states near the plasma frequency where the permittivity approaches zero.
Acousto-optical phonon excitation in piezoelectric wurtzite slabs and crystal growth orientation effects

This paper presents a theoretical investigation of phonon dispersion in piezoelectric slabs of hexagonal crystal symmetry (wurtzite). Specifically, we solve the fully coupled dispersion relations in a GaN free standing quantum well by varying the crystal growth direction from the [001] axis to the [010] axis. Accounting for the Drude model in solving the fully-coupled dispersion relations, phonon modes will generate an additional phonon band, with a high local density of phonon states, close to the plasma frequency. As opposed to cubic crystals with isotropic permittivity, the location of this band varies with crystal orientation. We also find that the phonon mode dependence on the crystal orientation is more pronounced for small in-plane wavenumbers.

General information
Publication status: Published
Organisations: Department of Photonics Engineering, University of Southern Denmark
Contributors: Duggen, L., Willatzen, M.
Number of pages: 8
Publication date: 2017
Peer-reviewed: Yes

A valence force field-Monte Carlo algorithm for quantum dot growth modeling

We present a novel kinetic Monte Carlo version for the atomistic valence force fields algorithm in order to model a self-assembled quantum dot growth process. We show our atomistic model is both computationally favorable and capture
more details compared to traditional kinetic Monte Carlo models based on continuum elastic models. We anticipate the model will be useful to experimentalists in understanding better the growth dynamics of quantum dot systems.

**General information**
Publication status: Published
Organisations: Department of Photonics Engineering, Center for Electron Nanoscopy, Nanophotonic Devices, University of Rome Tor Vergata, Italian National Research Council
Number of pages: 2
Pages: 117-118
Publication date: 2017

**Host publication information**
Title of host publication: 2017 International Conference on Numerical Simulation of Optoelectronic Devices (NUSOD)
Publisher: IEEE
ISBN (Electronic): 978-1-5090-5323-0
DOIs: 10.1109/NUSOD.2017.8010019
Source: Findit
Source-ID: 2373491803
Research output: Chapter in Book/Report/Conference proceeding – Article in proceedings – Annual report year: 2017 – Research – peer-review

**Compensation of loss-induced beam broadening in HMMs by a μ-negative HMM**
Losses play a crucial role when realistic hyperbolic metamaterials are considered. Importantly, losses lead to a broadening of beams propagating through a hyperbolic medium. Here we show that a part of the loss-induced broadening can be attributed to phase accumulation of plane-wave components. This phase accumulation can be canceled out by utilizing hyperbolic media with a negative permeability.

**General information**
Publication status: Published
Organisations: Department of Photonics Engineering, Metamaterials
Contributors: Repan, T., Novitsky, A., Willatzen, M., Lavrinenko, A.
Number of pages: 3
Pages: 286-288
Publication date: 2017

**Host publication information**
Title of host publication: Proceedings of 2017 11th International Congress on Engineered Materials Platforms for Novel Wave Phenomena
Publisher: IEEE
ISBN (Print): 9781538637685
Keywords: Slabs, Hidden Markov models, Media, Metamaterials, Interference, Attenuation, Tensile stress
DOIs: 10.1109/MetaMaterials.2017.8107921
Source: Findit
Source-ID: 2393340471
Research output: Chapter in Book/Report/Conference proceeding – Article in proceedings – Annual report year: 2017 – Research – peer-review

**Efficient Modeling of Excitons in Type-II Nanowire Quantum Dots - Presented at: CLEO®/Europe-EQEC 2017, Munich**

**General information**
Publication status: Published
Organisations: Department of Photonics Engineering, Quantum and Laser Photonics
Contributors: Taherkhani, M., Gregersen, N., Mørk, J., Willatzen, M.
Number of pages: 1
Publication date: 2017
Peer-reviewed: Yes
Event:
Electronic versions:
CLEO2_NG.pdf
Source: PublicationPreSubmission
**Fundamentals of Silicene, Authors: Guzmán-Verri Gian G., Lok C. Lew Yan Voon and Willatzen Morten**

Silicene is a single atomic layer of silicon (Si) much like graphene, the first example of an elemental twodimensional (2D) nanomaterial whose study led to the 2010 Nobel Prize in Physics. Until 2010 or so, the only known crystalline form of elemental silicon was the one with the so-called diamond structure (a threedimensional cubic structure with sp3-bonded Si atoms). That silicon could potentially form a 2D structure was first postulated by Takeda and Shiraishi. This early work and others, both theoretical and experimental, went mostly unnoticed until the prediction that silicene could have similar exotic properties as graphene by Guzmán-Verri and Lew Yan Voon in 2007, and silicene nanoribbons were reported to have been fabricated on a silver substrate by Kara et al. in 2009. Since then, the study of silicene has exploded, mainly theoretically but also experimentally. The interest in silicene is exactly the same as that for graphene: in being two-dimensional and possessing a linear band structure, the so-called Dirac cone. One advantage relies on its possible application in electronics, whereby its natural compatibility with the current Si technology might make fabrication much more of an industrial reality. We will concentrate this tutorial on the properties of a single freestanding silicene sheet. Freestanding means that the silicene sheet is not chemically or physically bonded to any other material. The feat with graphene was the ability to peel off a single layer of graphene from a piece of graphite, a process known as mechanical exfoliation. Such a layered precursor is missing for silicene. A close analogue, though, is calcium disilicide, indeed a layered material and the related process of chemical exfoliation has been tried, with only partial success as the resulting product was mostly multilayers and functionalized. Not surprisingly, a number of review articles have already appeared that includes extensive discussions of silicone. The current review is more tutorial in nature.

**Numerical simulations of nanostructured gold films**

We present an approach to analyse near-field effects on nanostructured gold films by finite element simulations. The studied samples are formed by fabricating gold films near the percolation threshold and then applying laser damage. Resulting samples have complicated structures, which then was captured using scanning transmission electron microscopy (STEM) and the obtained dark field images are used to set up COMSOL simulations corresponding to actual structures.
**Piezoelectric and deformation potential effects of strain-dependent luminescence in semiconductor quantum well structures**

The mechanism of strain-dependent luminescence is important for the rational design of pressure-sensing devices. The interband momentum-matrix element is the key quantity for understanding luminescent phenomena. We analytically solved an infinite quantum well (IQW) model with strain, in the framework of the $6 \times 6 \mathbf{k} \cdot \mathbf{p}$ Hamiltonian for the valence states, to directly assess the interplay between the spin-orbit coupling and the strain-induced deformation potential for the interband momentum-matrix element. We numerically addressed problems of both the infinite and IQWs with piezoelectric fields to elucidate the effects of the piezoelectric potential and the deformation potential on the strain-dependent luminescence. The experimentally measured photoluminescence variation as a function of pressure can be qualitatively explained by the theoretical results.

**General information**

Publication status: Published
Organisations: Department of Photonics Engineering, Chinese Academy of Sciences
Number of pages: 11
Publication date: 2017
Peer-reviewed: Yes

**Publication information**

Journal: Nano Research
Volume: 10
Issue number: 1
Article number: 134–144
ISSN (Print): 1998-0124
Ratings:
- BFI (2017): BFI-level 2
- Scopus rating (2017): CiteScore 7.8 SJR 3.064 SNIP 1.394
- Web of Science (2017): Impact factor 7.994
Web of Science (2017): Indexed yes
Original language: English
Keywords: Piezoelectric potential, Deformation potential, Luminescence, Quantum well
DOI:
10.1007/s12274-016-1272-x

**Plasmon Modes of Vertically Aligned Superlattices**

By using the Finite Element Method we visualize the modes of vertically aligned superlattice composed of gold and dielectric nanocylinders and investigate the emitter-plasmon interaction in approximation of weak coupling. We find that truncated vertically aligned superlattice can function as plasmonic nanoresonator with capabilities of spectral control over the Purcell effect and Q-factor. Our second goal is related to an important issue of Finite Element Method convergence when applied to finite-length plasmonic arrays. Analysis of the layered nanostructures with finite extension in all three dimensions is complicated because of the large difference in element size across the modeling domain. In order to be sure that plasmonic modes are properly captured and the Purcell effect is accurately estimated, we perform mesh refinement study using three meshes.

**General information**

Publication status: Published
Organisations: Department of Photonics Engineering, University of Southern Denmark
Contributors: Filonenko, K., Duggen, L., Willatzen, M.
Pages: 2852-2857
Publication date: 2017

**Host publication information**

Title of host publication: Proceedings of the 2017 Progress In Electromagnetics Research Symposium - Spring (PIERS)
Pseudocanalization regime for magnetic dark-field hyperlenses

Hyperbolic metamaterials (HMMs) are the cornerstone of the hyperlens, which brings the superresolution effect from the near-field to the far-field zone. For effective application of the hyperlens it should operate in the so-called canalization regime, where the phase advancement of the propagating fields is maximally suppressed and thus field broadening is minimized. For conventional hyperlenses it is relatively straightforward to achieve canalization by tuning the anisotropic permittivity tensor. However, for a dark-field hyperlens designed to image weak scatterers by filtering out background radiation (dark-field regime) this approach is not viable because design requirements for such filtering and elimination of phase advancement i.e., canalization, are mutually exclusive. Here we propose the use of magnetic ($\mu$-positive and -negative) HMMs to achieve phase cancellation at the output equivalent to the performance of a HMM in the canalized regime. The proposed structure offers additional flexibility over simple HMMs in tuning light propagation. We show that in this “pseudocanalizing” configuration the quality of an image is comparable to a conventional hyperlens, while the desired filtering of the incident illumination associated with the dark-field hyperlens is preserved.

Type-II quantum-dot-in-nanowire structures with large oscillator strength for optical quantum gate applications

We present a numerical investigation of the exciton energy and oscillator strength in type-II nanowire quantum dots. For a single quantum dot, the poor overlap of the electron part and the weakly confined hole part of the excitonic wave function leads to a low oscillator strength compared to type-I systems. To increase the oscillator strength, we propose a double quantum dot structure featuring a strongly localized exciton wave function and a corresponding fourfold relative enhancement of the oscillator strength, paving the way towards efficient optically controlled quantum gate applications in
the type-II nanowire system. The simulations are performed using a computationally efficient configuration-interaction method suitable for handling the relatively large nanowire structures.

General information
Publication status: Published
Organisations: Department of Photonics Engineering, Quantum and Laser Photonics, University of Bristol
Contributors: Taherkhani, M., Willatzen, M., Mørk, J., Gregersen, N., McCutcheon, D. P. S.
Number of pages: 9
Publication date: 2017
Peer-reviewed: Yes

Publication Information
Journal: Physical Review B
Volume: 96
Issue number: 12
Article number: 125408
ISSN (Print): 2469-9950
Ratings:
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 3.34 SJR 1.604 SNIP 1.04
Web of Science (2017): Impact factor 3.813
Web of Science (2017): Indexed yes
Original language: English
Electronic versions:
PhysRevB.96.125408.pdf
DOIs: 10.1103/PhysRevB.96.125408
Source: FindIt
Source-ID: 2374290121
Research output: Contribution to journal › Journal article – Annual report year: 2017 › Research › peer-review

Type-II Quantum Dot Nanowire Structures with Large Oscillator Strengths for Optical Quantum Gating Applications
The exciton oscillator strength (OS) in type-II quantum dot (QD) nanowires is calculated by using a fast and efficient method. We propose a new structure in Double-Well QD (DWQD) nanowire that considerably increases OS of type-II QDs which is a key parameter in optical quantum gating in the stimulated Raman adiabatic passage (STIRAP) process [1] for implementing quantum gates.

General information
Publication status: Published
Organisations: Department of Photonics Engineering, Quantum and Laser Photonics
Contributors: Taherkhani, M., Gregersen, N., Willatzen, M., Mørk, J.
Pages: 7-8
Publication date: 2017

Host publication information
Title of host publication: Proceedings of NUSOD 2017
Publisher: IEEE
ISBN (Print): 978-1-5090-5323-0
Source: PublicationPreSubmission
Source-ID: 134229538
Research output: Chapter in Book/Report/Conference proceeding › Article in proceedings – Annual report year: 2017 › Research › peer-review

A theory of generalized Bloch oscillations
Bloch oscillations of electrons are shown to occur for cases when the energy spectrum does not consist of the traditional evenly-spaced ladders and the potential gradient does not result from an external electric field. A theory of such generalized Bloch oscillations is presented and an exact calculation is given to confirm this phenomenon. Our results allow for a greater freedom of design for experimentally observing Bloch oscillations. For strongly coupled oscillator systems displaying Bloch oscillations, it is further demonstrated that reordering of oscillators leads to destruction of Bloch oscillations. We stipulate that the presented theory of generalized Bloch oscillations can be extended to other systems such as acoustics and photonics.

General information
Publication status: Published
Dark-field hyperlens for high-contrast sub-wavelength imaging

By now superresolution imaging using hyperbolic metamaterial (HMM) structures – hyperlenses – has been demonstrated both theoretically and experimentally. The hyperlens operation relies on the fact that HMM allows propagation of waves with very large transverse wavevectors, which would be evanescent in common isotropic media (thus giving rise to the diffraction limit). However, nearly all hyperlenses proposed so far have been suitable only for very strong scatterers – such as holes in a metal film. When weaker scatterers, dielectric objects for example, are imaged then incident light forms a very strong background, and weak scatterers are not visible due to a poor contrast. We propose a so-called dark-field hyperlens, which would be suitable for imaging of weakly scattering objects. By designing parameters of the HMM, we managed to obtain its response in such way that the hyperlens structure exhibits a cut-off for waves with small transverse wavevectors (low-k waves). This allows the structure to filter out the background illumination, which is contained in low-k waves. We numerically demonstrate that our device achieves superresolution imaging while providing the strong contrast for weak dielectric scatterers. These findings hold a great promise for dark-field superresolution, which could be important in real-time dynamic nanoscopy of label-free biological objects for example. © (2016) COPYRIGHT Society of Photo-Optical Instrumentation Engineers (SPIE). Downloading of the abstract is permitted for personal use only.
Efficient Modeling of Coulomb Interaction Effect on Exciton in Crystal-Phase Nanowire Quantum Dot

The binding energy and oscillation strength of the ground-state exciton in type-II quantum dot (QD) is calculated by using a post Hartree-Fock method known as the configuration interaction (CI) method which is significantly more efficient than conventional methods like ab initio method. We show that the Coulomb interaction between electron and holes in these structures considerably affects the transition dipole moment which is the key parameter of optical quantum gating in STIRAP (stimulated Raman adiabatic passage) process for implementing quantum gates [1], [2].

General information
Publication status: Published
Organisations: Department of Photonics Engineering, Quantum and Laser Photonics, University of Bristol
Contributors: Taherkhani, M., Gregersen, N., Mørk, J., McCutcheon, D., Willatzen, M.
Number of pages: 2
Publication date: 2016

Parity-Time Synthetic Phononic Media

Classical systems containing cleverly devised combinations of loss and gain elements constitute extremely rich building units that can mimic non-Hermitian properties, which conventionally are attainable in quantum mechanics only. Parity-time (PT) symmetric media, also referred to as synthetic media, have been devised in many optical systems with the groundbreaking potential to create nonreciprocal structures and one-way cloaks of invisibility. Here we demonstrate a feasible approach for the case of sound where the most important ingredients within synthetic materials, loss and gain, are achieved through electrically biased piezoelectric semiconductors. We study first how wave attenuation and amplification can be tuned, and when combined, can give rise to a phononic PT synthetic media with unidirectional suppressed reflectance, a feature directly applicable to evading sonar detection.

General information
Publication status: Published
Organisations: Department of Photonics Engineering, Structured Electromagnetic Materials, Complutense University, Nanjing University
Contributors: Christensen, J., Willatzen, M., Velasco, V. R., Lu, M.
Number of pages: 5
Publication date: 2016
Peer-reviewed: Yes

Publication information
Journal: Physical Review Letters
Volume: 116
Article number: 207601
ISSN (Print): 0031-9007
Ratings:
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 6.33 SJR 4.196 SNIP 2.61
Web of Science (2016): Impact factor 8.462
Web of Science (2016): Indexed yes
Original language: English
Electronic versions:
PhysRevLett.116.207601_JC_MW.pdf
DOIs:
Theoretical study of the electromechanical efficiency of a loaded tubular dielectric elastomer actuator

The electromechanical efficiency of a loaded tubular dielectric elastomer actuator (DEA) is investigated theoretically. In previous studies, the external system, on which the DEA performs mechanical work, is implemented implicitly by prescribing the stroke of the DEA in a closed operation cycle. Here, a more generic approach, modelling the external system by a frequency-dependent mechanical impedance which exerts a certain force on the DEA depending on its deformation, is chosen. It admits studying the dependence of the electromechanical efficiency of the DEA on the external system. A closed operation cycle is realized by exciting the DEA electrically by a sinusoidal voltage around a bias voltage. A detailed parametric study shows that the electromechanical efficiency is highly dependent on the frequency, amplitude, and bias of the excitation voltage and the mechanical impedance of the external system as well. Efficiencies of up to 93% can be observed for the Danfoss PolyPower tubular DEA if the mechanical impedance of the external system is adjusted to the mechanical impedance of the DEA or vice versa. The study shows that a tubular DEA can be dimensioned and operated such that it performs most efficiently for a given application.

General information
Publication status: Published
Organisations: Department of Photonics Engineering, University of Southern Denmark
Contributors: Rechenbach, B., Willatzen, M., Lassen, B.
Number of pages: 15
Pages: 1232–1246
Publication date: 2016
Peer-reviewed: Yes

Publication information
Journal: Applied Mathematical Modelling
Volume: 40
Issue number: 2
ISSN (Print): 0307-904X
Ratings:
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.03 SJR 1.139 SNIP 1.784
Web of Science (2016): Impact factor 2.35
Web of Science (2016): Indexed yes
Original language: English
Keywords: Dielectric elastomer, Efficiency, Electromechanical coupling, Energy conversion, Tubular dielectric, Elastomer actuator
DOIs:
10.1016/j.apm.2015.06.029

A flow meter for ultrasonically measuring the flow velocity of fluids.
The invention regards a flow meter for ultrasonically measuring the flow velocity of fluids comprising a duct having a flow channel with an internal cross section comprising variation configured to generate at least one acoustic resonance within the flow channel for a specific ultrasonic frequency, and at least two transducers for generating and sensing ultrasonic pulses, configured to transmit ultrasonic pulses at least at said specific ultrasonic frequency into the flow channel such that the ultrasonic pulses propagate through a fluid flowing in the flow channel, wherein the flow meter is configured to determine the flow velocity of the fluid flowing in the flow channel based on a change in transit time, phase and/or pulse such as amplitude and/or form, of the ultrasonic pulses.

General information
Publication status: Published
Organisations: Department of Photonics Engineering, Department of Applied Mathematics and Computer Science , Mathematics
Contributors: Willatzen, M., Gravesen, J., Nørtoft, P.
Publication date: 7 May 2015

Publication information
Band parameters of phosphorene

Phosphorene is a two-dimensional nanomaterial with a direct band-gap at the Brillouin zone center. In this paper, we present a recently derived effective-mass theory of the band structure in the presence of strain and electric field, based upon group theory. Band parameters for this theory are computed using a first-principles theory based upon the generalized-gradient approximation to the density-functional theory. These parameters and Hamiltonian will be useful for modeling physical properties of phosphorene.

Effective Hamiltonians for phosphorene and silicene

We derived the effective Hamiltonians for silicene and phosphorene with strain, electric field and magnetic field using the method of invariants. Our paper extends the work of Geissler et al 2013 (NewJ. Phys. 15 085030) on silicene, and Li and Appelbaum 2014 (Phys. Rev. B 90, 115439) on phosphorene. Our Hamiltonians are compared to an equivalent one for graphene. For silicene, the expression for band warping is obtained analytically and found to be of different order than for graphene. Weprove that a uniaxial strain does not open a gap, resolving contradictory numerical results in the literature. For phosphorene, it is shown that the bands near the Brillouin zone center only have terms in even powers of the wave vector. We predict that the energies change quadratically in the presence of a perpendicular external electric field but linearly in a perpendicular magnetic field, as opposed to those for silicene which vary linearly in both cases. Preliminary ab
initio calculations for the intrinsic bandstructures have been carried out in order to evaluate some of the $k \cdot p$ parameters.

**General information**
Publication status: Published
Organisations: Department of Photonics Engineering, The Citadel - The Military College of South Carolina, Argonne National Laboratory, University of North Carolina
Number of pages: 10
Publication date: 2015
Peer-reviewed: Yes

**Publication information**
Journal: New Journal of Physics
Volume: 17
Article number: 025004
ISSN (Print): 1367-2630
Ratings:
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 2.8 SJR 1.902 SNIP 0.967
Web of Science (2015): Impact factor 3.57
Web of Science (2015): Indexed yes
Original language: English
Keywords: Silicene, Phosphorene, Two-dimensional material, k.p , Method of invariant, Group theory, Band structure
Electronic versions:
New_J_Phys_Willatzen_2015_1_.pdf
DOIs:
10.1088/1367-2630/17/2/025004

**Bibliographical note**
Content from this work may be used under the terms of the Creative Commons Attribution 3.0 licence.
Source: PublicationPreSubmission
Source-ID: 105415881
Research output: Contribution to journal › Journal article – Annual report year: 2015 › Research › peer-review

**Isogeometric analysis of sound propagation through laminar flow in 2-dimensional ducts**
We consider the propagation of sound through a slowly moving fluid in a 2-dimensional duct. A detailed description of a flow-acoustic model of the problem using B-spline based isogeometric analysis is given. The model couples the nonlinear, steady-state, incompressible Navier-Stokes equation in the laminar regime for the flow field, to a linear, time-harmonic acoustic equation in the low Mach number regime for the sound signal. B-splines are used both to represent the duct geometry and to approximate the flow and sound fields. This facilitates an exact representation of complex duct geometries, as well as high continuity approximations of state variables. Acoustic boundary conditions on artificial truncation boundaries are treated using a mode matching formulation. We validate the model against known acoustic modes for a uniform flow through a straight duct. Improved error convergence rates are found when the acoustic pressure is approximated by higher order polynomials. Based on the model, we examine how the acoustic signal varies with sound frequency, flow speed and duct geometry. A combination of duct geometry and sound frequency is identified for which the acoustic signal is particularly sensitive to the flow speed.

**General information**
Publication status: Published
Organisations: Department of Applied Mathematics and Computer Science , Mathematics , Department of Photonics Engineering
Contributors: Nørtoft, P., Gravesen, J., Willatzen, M.
Pages: 1098-1119
Publication date: 2015
Peer-reviewed: Yes

**Publication information**
Journal: Computer Methods in Applied Mechanics and Engineering
Volume: 284
ISSN (Print): 0045-7825
Ratings:
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 3.91 SJR 2.952 SNIP 2.023
Mechanical Properties of Laminate Materials: From Surface Waves to Bloch Oscillations

We propose hitherto unexplored and fully analytical insights into laminate elastic materials in a true condensed-matter-physics spirit. Pure mechanical surface waves that decay as evanescent waves from the interface are discussed, and we demonstrate how these designer Scholte waves are controlled by the geometry as opposed to the material alone. The linear surface wave dispersion is modulated by the crystal filling fraction such that the degree of confinement can be engineered without relying on narrow-band resonances but on effective stiffness moduli. In the same context, we provide a theoretical recipe for designing Bloch oscillations in classical plate structures and show how mechanical Bloch oscillations can be generated in arrays of solid plates when the modal wavelength is gradually reduced. The design recipe describes how Bloch oscillations in classical structures of arbitrary dimensions can be generated, and we demonstrate this numerically for structures with millimeter and centimeter dimensions in the kilohertz to megahertz range. Analytical predictions agree entirely with full wave simulations showing how elastodynamics can mimic quantum-mechanical condensed-matter phenomena.

General information
Publication status: Published
Organisations: Department of Photonics Engineering, Structured Electromagnetic Materials, Shenzhen University
Contributors: Liang, Z., Willatzen, M., Christensen, J.
Number of pages: 8
Publication date: 2015
Peer-reviewed: Yes

Publication information
Journal: Physical Review Applied
Volume: 4
Issue number: 4
Article number: 044012
ISSN (Print): 2331-7019
Ratings:
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 3.31 SJR 2.345 SNIP 1.214
Web of Science (2015): Impact factor 4.061
DOIs:
10.1103/PhysRevApplied.4.044012
Source: PublicationPreSubmission
Source-ID: 117296267
Research output: Contribution to journal › Journal article – Annual report year: 2015 › Research › peer-review

On the $\kappa^2$-dependence of $\{\varepsilon_r\}$ and/or $\{\mu_r\}$ for optimum absorption efficiency of electrically small homogeneous spheres with $\{\varepsilon_r\}$ and/or $\{\mu_r\} = -2$

The absorption efficiency of a homogenous sphere illuminated by a plane electromagnetic wave can be found exactly using Lorenz-Mie theory and the Optical Theorem. The solution is expressed in terms of an infinite sum of spherical modes (see e.g. C. F. Bohren and D. Huffman, Absorption and scattering of light by small particles, Wiley, 1983, Chap. 4).

General information
Publication status: Published
Organisations: Department of Electrical Engineering, Electromagnetic Systems, Department of Photonics Engineering
Purcell effect of asymmetric dipole source distributions in nanowire resonators
Metal nanowire resonators allow subwavelength mode confinement and thereby the strong Purcell effect. Recent progress in fabrication of plasmonic nanowire lasers requires reliable approaches in studying resonators, where metal nanowire is an essential constitutive element. A semi-analytic study, capable of treating finite-length axially-symmetric nanowire configurations, was reported in. In some nanolaser configurations, however, one needs to treat asymmetric source distributions, e.g. the single quantum dot placed at some distance from the nanowire axis. We investigate the Purcell effect of the asymmetric source distributions in proximity to the metal nanowire in two configurations: a metal cylinder truncated by the PEC plates and finite metal cylinder in free-space. In order to evaluate Purcell factor the mode eigenvalues are precalculated using Comsol Multiphysics radio frequency module. We compare the eigenfrequency and Purcell factor values calculated in PEC-truncated model against an analytic theory, which accounts for the fundamental surface plasmon - polariton mode in the form of a standing wave between two PEC planes.

Tunable Broadband Acoustic Gain in Piezoelectric Semiconductors at ε-Near-Zero Response
Piezoelectric semiconductors have emerged as materials capable to amplify sound waves when electrons are set to drift at supersonic speeds. Several experiments have demonstrated this behaviour at moderate amplification levels for some intrinsic semiconductors and carrier concentrations. On a theoretical basis we show that amplification of sound can be significantly enhanced when the materials are operated close to the plasma frequency. If the drifting carriers collectively oscillate with the plasma the electromechanical coupling is enhanced since the permittivity is related inversely proportional to the mechanical stress and vanishes near the bulk plasma frequency. By optically or electrically doping GaAs and InSb as exemplified in this work, we predict that amplification of sound can be achieved effectively for a bandwidth exceeding several decades making this active system very attractive for loss-compensation in metamaterials and applicable for sensing such as nonlinear devices. The paper contains a detailed derivation and discussion of transmission and reflection coefficients for pressure pulses impinging on a semiconductor slab and the acoustic gain enhancement that can be achieved by dynamic switching of the electric field as well as tuning flexibility through dynamic control of the carrier density.
Unified treatment of coupled optical and acoustic phonons in piezoelectric cubic materials

A unified treatment of coupled optical and acoustic phonons in piezoelectric cubic materials is presented whereby the lattice displacement vector and the internal ionic displacement vector are found simultaneously. It is shown that phonon couplings exist in pairs only; either between the electric potential and the lattice displacement coordinate perpendicular to the phonon wave vector or between the two other lattice displacement components. The former leads to coupled acousto-optical phonons by virtue of the piezoelectric effect. We then establish three new conjectures that entirely stem from piezoelectricity in a cubic structured material slab. First, it is shown that isolated optical phonon modes generally cannot exist in piezoelectric cubic slabs. Second, we prove that confined acousto-optical phonon modes only exist for a discrete set of in-plane wave numbers in piezoelectric cubic slabs. Third, it is shown that coupled acousto-optical phonons do not exist at the longitudinal-optical (LO) phonon frequency where the dielectric constant vanishes.

Acoustic gain in piezoelectric semiconductors at $\varepsilon$-near-zero response

We demonstrate strong acoustic gain in electric-field biased piezoelectric semiconductors at frequencies near the plasmon frequency in the terahertz range. When the electron drift velocity produced by an external electric field is higher than the speed of sound, Cherenkov radiation of phonons generates amplification of sound. It is demonstrated that this effect is particularly effective at $\varepsilon$-near-zero response, leading to giant levels of acoustic gain. Operating at conditions with strong acoustic amplification, we predict unprecedented enhancement of the scattered sound field radiated from an electrically controlled piezoelectric slab waveguide. This extreme sound field enhancement in an active piezo material shows potential for acoustic sensing and loss compensation in metamaterials and nonlinear devices.
Acoustic wave propagation and stochastic effects in metamaterial absorbers
We show how stochastic variations of the effective parameters of anisotropic structured metamaterials can lead to increased absorption of sound. For this, we derive an analytical model based on the Bourret approximation and illustrate the immediate connection between material disorder and attenuation of the averaged field. We demonstrate numerically that broadband absorption persists at oblique irradiation and that the influence of red noise comprising short spatial correlation lengths increases the absorption beyond what can be archived with a structured but ordered system.

An Adaptable Robot Vision System Performing Manipulation Actions With Flexible Objects
This paper describes an adaptable system which is able to perform manipulation operations (such as Peg-in-Hole or Laying-Down actions) with flexible objects. As such objects easily change their shape significantly during the execution of an action, traditional strategies, e. g., for solve path-planning problems, are often not applicable. It is therefore required to integrate visual tracking and shape reconstruction with a physical modeling of the materials and their deformations as well as action learning techniques. All these different submodules have been integrated into a demonstration platform, operating in real-time. Simulations have been used to bootstrap the learning of optimal actions, which are subsequently improved through real-world executions. To achieve reproducible results, we demonstrate this for casted silicone test objects of regular shape. Note to Practitioners-The aim of this work was to facilitate the setup of robot-based automation of delicate handling of flexible objects consisting of a uniform material. As examples, we have considered how to optimally maneuver flexible objects through a hole without colliding and how to place flexible objects on a flat surface with minimal introduction of internal stresses in the object. Given the material properties of the object, we have demonstrated in these
two applications how the system can be programmed with minimal requirements of human intervention. Rather than being an integrated system with the drawbacks in terms of lacking flexibility, our system should be viewed as a library of new technologies that have been proven to work in close to industrial conditions. As a rather basic, but necessary part, we provide a technology for determining the shape of the object when passing on, e. g., a conveyor belt prior to being handled. The main technologies applicable for the manipulated objects are: A method for realtime tracking of the flexible objects during manipulation, a method for model-based offline prediction of the static deformation of grasped, flexible objects and, finally, a method for optimizing specific tasks based on both simulated and real-world executions.

General information
Publication status: Published
Organisations: Department of Photonics Engineering, University of Southern Denmark, Danish Technological Institute, Kiel University
Pages: 749-765
Publication date: 2014
Peer-reviewed: Yes

Publication information
Journal: IEEE Transactions on Automation Science and Engineering
Volume: 11
Issue number: 3
ISSN (Print): 1545-5955
Ratings:
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 3.49 SJR 1.731 SNIP 2.451
Web of Science (2014): Impact factor 2.428
Web of Science (2014): Indexed yes
Original language: English
Keywords: AUTOMATION, DEFORMABLE OBJECTS, MODEL, GENERATION, TRACKING, Action learning, deformation modeling, flexible objects, shape tracking, 3D-modeling, control engineering computing, deformation, flexible manipulators, image reconstruction, learning (artificial intelligence), object tracking, robot vision, shape recognition, Robotics and Control Systems, action execution, action learning techniques, adaptable robot vision system, bootstrap learning, casted silicone test objects, Deformable models, demonstration platform, flexible object handling, flexible object maneuver, internal stresses, laying-down actions, manipulation actions, manipulation operations, material properties, Mathematical model, model-based offline prediction, object shape, optimal actions, peg-in-hole actions, physical modeling, real-time tracking, real-world executions, robot-based automation, Robots, Shape, shape reconstruction, Splines (mathematics), static deformation, Surface reconstruction, Surface topography, visual tracking, ROBOT vision
DOIs: 10.1109/TASE.2014.2320157
Source: Findit
Source-ID: 267908144
Research output: Contribution to journal › Journal article – Annual report year: 2014 › Research › peer-review

Differential Geometry Applied to Rings and Möbius Nanostructures
Nanostructure shape effects have become a topic of increasing interest due to advancements in fabrication technology. In order to pursue novel physics and better devices by tailoring the shape and size of nanostructures, effective analytical and computational tools are indispensable. In this chapter, we present analytical and computational differential geometry methods to examine particle quantum eigenstates and eigenenergies in curved and strained nanostructures. Example studies are carried out for a set of ring structures with different radii and it is shown that eigenstate and eigenenergy changes due to curvature are most significant for the groundstate eventually leading to qualitative and quantitative changes in physical properties. In particular, the groundstate in-plane symmetry characteristics are broken by curvature effects, however, curvature contributions can be discarded at bending radii above 50 nm. In the second part of the chapter, a more complicated topological structure, the Möbius nanostructure, is analyzed and geometry effects for eigenstate properties are discussed including dependencies on the Möbius nanostructure width, length, thickness, and strain.

General information
Publication status: Published
Organisations: Department of Photonics Engineering, Department of Applied Mathematics and Computer Science, Mathematics, University of Southern Denmark
Contributors: Lassen, B., Willatzen, M., Gravesen, J.
Pages: 409-435
Publication date: 2014
Epitaxial growth of quantum dots on InP for device applications operating at the 1.55 μm wavelength range

The development of epitaxial technology for the fabrication of quantum dot (QD) gain material operating in the 1.55 μm wavelength range is a key requirement for the evolution of telecommunication. High performance QD material demonstrated on GaAs only covers the wavelength region 1-1.35 μm. In order to extract the QD benefits for the longer telecommunication wavelength range the technology of QD fabrication should be developed for InP based materials. In our work, we take advantage of both QD fabrication methods Stranski-Krastanow (SK) and selective area growth (SAG) employing block copolymer lithography. Due to the lower lattice mismatch of InAs/InP compared to InAs/GaAs, InP based QDs have a larger diameter and are shallower compared to GaAs based dots. This shape causes low carrier localization and small energy level separation which leads to a high threshold current, high temperature dependence, and low laser quantum efficiency. Here, we demonstrate that with tailored growth conditions, which suppress surface migration of adatoms during the SK QD formation, much smaller base diameter (13.6nm versus 23nm) and an improved aspect ratio are achieved. In order to gain advantage of non-strain dependent QD formation, we have developed SAG, for which the growth occurs only in the nano-openings of a mask covering the wafer surface. In this case, a wide range of QD composition can be chosen. This method yields high purity material and provides significant freedom for reducing the aspect ratio of QDs with the possibility to approach an ideal QD shape.

Exergy costing for energy saving in combined heating and cooling applications

The aim of this study is to provide a price model that motivates energy saving for a combined district heating and cooling system. A novel analysis using two thermoeconomic methods for apportioning the costs to heating and cooling provided simultaneously by an ammonia heat pump is demonstrated. In the first method, referred to as energy costing, a conventional thermoeconomic analysis is used. Here the ammonia heat pump is subject to a thermodynamic analysis with mass and energy balance equations. In the second method referred to as exergy costing, an exergy based economic analysis is used, where exergy balance equations are used in conjunction with mass and energy balance equations. In both costing methods the thermodynamic analysis is followed by an economic analysis which includes investment and operating costs. For both methods the unit costs of heating and cooling are found and compared. The analysis shows that the two methods yield significantly different results. Rather surprisingly, it is demonstrated that the exergy costing method...
results in about three times higher unit cost for heating than for cooling as opposed to equal unit costs when using the energy method. Further the exergy-based cost for heating changes considerably with the heating temperature while that of cooling is much less affected.

**General information**
Publication status: Published
Organisations: Department of Photonics Engineering, University of Southern Denmark, Fjernvarme Fyn A/S
Contributors: Nguyen, C., Veje, C. T., Willatzen, M., Andersen, P.
Pages: 349-355
Publication date: 2014
Peer-reviewed: Yes

**Publication information**
Journal: Energy Conversion and Management
Volume: 86
ISSN (Print): 0196-8904
Ratings:
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 5.35 SJR 1.985 SNIP 2.827
Web of Science (2014): Indexed yes
Original language: English
Keywords: Energy, Exergy, Costing methods, Co-generation, District energy
DOI: 10.1016/j.enconman.2014.05.040
Source: FindIt
Source-ID: 267956778
Research output: Contribution to journal ⇒ Journal article – Annual report year: 2014 ⇒ Research ⇒ peer-review

**Extraordinary absorption of sound in porous lamella-crystals**
We present the design of a structured material supporting complete absorption of sound with a broadband response and functional for any direction of incident radiation. The structure which is fabricated out of porous lamellas is arranged into a low-density crystal and backed by a reflecting support. Experimental measurements show that strong all-angle sound absorption with almost zero reflectance takes place for a frequency range exceeding two octaves. We demonstrate that lowering the crystal filling fraction increases the wave interaction time and is responsible for the enhancement of intrinsic material dissipation, making the system more absorptive with less material.

**General information**
Publication status: Published
Organisations: Department of Photonics Engineering, Structured Electromagnetic Materials, Polytechnic University of Valencia, Institut de Ciències Fotòniques, University of Southern Denmark
Contributors: Christensen, J., Romero-García, V., Picó, R., Cebrecos, A., de Abajo, F. J. G., Mortensen, N. A., Willatzen, M., Sánchez-Morcillo, V. J.
Number of pages: 5
Publication date: 2014
Peer-reviewed: Yes

**Publication information**
Journal: Scientific Reports
Volume: 4
Article number: 4674
ISSN (Print): 2045-2322
Ratings:
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 4.75 SJR 2.037 SNIP 1.478
Web of Science (2014): Indexed yes
Original language: English
Electronic versions:
SREP_14_01833_Revised_PDF_5.pdf
DOI: 10.1038/srep04674
Source: FindIt
Geometry optimization of tubular dielectric elastomer actuators with anisotropic metallic electrodes

This paper presents an experimentally verified static three-dimensional model for core free tubular dielectric elastomer actuators with anisotropic compliant metal electrodes. Due to the anisotropy of the electrodes, the performance (force versus voltage, force versus stroke, and stroke versus voltage) of the actuators depends strongly on their geometry. Based on the three-dimensional model, the performance of the actuators is optimized by means of the length of the axes of their inner elliptical cross section and their wall thickness.

General information
Publication status: Published
Organizations: Department of Photonics Engineering, University of Southern Denmark, Danfoss AS
Contributors: Rechenbach, B., Willatzen, M., Sarban, R., Liang, C., Lassen, B.
Number of pages: 13
Publication date: 2014
Peer-reviewed: Yes

Publication information
Journal: Proceedings of SPIE, the International Society for Optical Engineering
Volume: 9056
Article number: 905606
ISSN (Print): 0277-786X
Ratings:
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 0.3 SJR 0.188 SNIP 0.176
Original language: English
DOIs:
10.1117/12.2046276
Source: RIS
Source-ID: urn:B11E019F90E79125843A4BE552F47DD3
Research output: Contribution to journal › Conference article – Annual report year: 2014 › Research › peer-review

Maximum absorption by homogeneous magneto-dielectric sphere

In order to obtain a benchmark for electromagnetic energy harvesting, we investigate the maximum absorption efficiency by a magneto-dielectric homogeneous sphere illuminated by a plane wave, and we arrive at several novel results. For electrically small spheres we show that the optimal relative permeability and permeability of materials where \(\gamma, \mu r > 1\) is \((1+i3)\) independent of sphere size, while that of metamaterials is \((-2+i\delta)\), where the imaginary part \(\delta\) decreases strongly with decreasing sphere size. For larger spheres we show that while maximum absorption efficiency occurs at the resonances of the spherical modes, there exists a wide plateau of high absorption efficiency when material intrinsic impedance is constant; in the case of free-space intrinsic impedance and electrical radius \(\kappa=1\), the absorption efficiency becomes 2.8. The investigation is analytic/numerical and based on the Lorenz–Mie theory combined with the optical theorem.

General information
Publication status: Published
Organizations: Department of Electrical Engineering, Electromagnetic Systems, Department of Photonics Engineering
Contributors: Palvig, M. F., Breinbjerg, O., Willatzen, M.
Pages: 1912-1918
Publication date: 2014
Peer-reviewed: Yes

Publication information
Journal: Journal of the Optical Society of America A
Volume: 31
Issue number: 9
ISSN (Print): 0740-3232
Ratings:
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 1.72
Web of Science (2014): Impact factor 1.558
Web of Science (2014): Indexed yes
Original language: English
Minimal model for spoof acoustoelastic surface states

Similar to textured perfect electric conductors for electromagnetic waves sustaining artificial or spoof surface plasmons we present an equivalent phenomena for the case of sound. Aided by a minimal model that is able to capture the complex wave interaction of elastic cavity modes and airborne sound radiation in perfect rigid panels, we construct designer acoustoelastic surface waves that are entirely controlled by the geometrical environment. Comparisons to results obtained by full-wave simulations confirm the feasibility of the model and we demonstrate illustrative examples such as resonant transmissions and waveguiding to show a few examples of many where spoof elastic surface waves are useful.

Modelling the acoustical response of lossy lamella-crystals.

The sound propagation properties of lossy lamella-crystals are analysed theoretically utilizing a rigorous wave expansion formalism and an effective medium approach. We investigate both supported and free-standing crystal slab structures and predict high absorption for a broad range of frequencies. A detailed derivation of the formalism is presented, and we show how the results obtained in the subwavelength and superwavelength regimes qualitatively can be reproduced by homogenizing the lamella-crystals. We come to the conclusion that treating this structure within the metamaterial limit only makes sense if the crystal filling fraction is sufficiently large to satisfy an effective medium approach.
Purcell effect for finite-length metal-coated and metal nanowires

We investigate the modification (enhancement and suppression) of the spontaneous emission rate of a dipole emitter in two configurations: inside a finite-length semiconductor nanowire surrounded by bulk metal and in the vicinity of a finite metal nanowire. Our analysis is based on a first-principle approach, which is reduced to a seminumeric one in the limit of large nanowire aspect ratios. The numerical calculations are carried out for an emitter in a GaAs nanowire embedded in Ag or Au and for that nearby an Ag or Au nanowire in vacuum or dielectric. We consider in detail the Purcell and β factors as functions of the cylinder radius, the emitter position, and the transition frequency for both configurations. We contrast the results for finite-length nanowires with those obtained in the infinite-length approximation and find considerable differences in the Purcell factor magnitude.

An Electromechanical Model for a Dielectric ElectroActive Polymer Generator

Smart electroactive materials have attracted much of the scientific interest over the past few years, as they reflect a quite promising alternative to conservative approaches used nowadays in various transducer applications. Especially Dielectric ElectroActive Polymers (DEAPs), which are constantly gaining momentum due to their superior low-speed performance, light-weighted nature and higher energy density when compared with competing technologies. In this paper an electromechanical model for a DEAP generator is presented, accounting for both the visco-hyperelastic characteristics of the polymer material, as well as the later one's experimentally determined stretch-capacitance dependence. Apart from the visco-hyperelastic model validation via purely mechanical experiments, the model's electromechanical coupling is verified as well, via experiments conducted under all three distinct energy harvesting cycles; namely the Constant Charge (CC), Constant Voltage (CV) and Constant E-field (CE) cycles.
Design optimization of a linear actuator

The mechanical contacting of a dielectric elastomer actuator is investigated. The actuator is constructed by coiling the dielectric elastomer around two parallel metal rods, similar to a rubber band stretched by two index fingers. The goal of this paper is to design the geometry and the mechanical properties of a polymeric interlayer between the elastomer and the rods, gluing all materials together, so as to optimize the mechanical durability of the system. Finite element analysis is employed for the theoretical study which is linked up to experimental results performed by Danfoss PolyPower A/S.

Metadevices for the confinement of sound and broadband double-negativity behavior

We show that the acoustic response of perforated and elastically filled rigid screens can give rise to a broad landscape of tunable devices. We begin presenting deep-subwavelength transmission properties of a structured plate and demonstrate the immediate relationship to truly bound surface modes. We extend our theoretical model to analyze structured metal-fluid-metal wave guides for the confinement of sound and present exact expressions for the dispersion relations which describe the hybridization of resonances. We discuss the validity of our analytical model by direct comparison to full-wave simulations and use this technique in the search for broadband response in composite structures where the effective mass density and bulk modulus are simultaneously negative and exhibiting weak influences by viscous losses.
Near infrared photoacoustic detection of heptane in synthetic air

Trace contaminations of n-heptane in synthetic air is measured in the parts-per-billion (ppb) range using near infrared photoacoustic detection. We describe the fundamental theory used in the design of the photoacoustic cell for trace gas analysis and determine the detection limit of the cell. On the basis of a modified procedure from the American Clinical and Laboratory Standards Institute for the case that it is practically impossible to produce perfectly blank samples, a residual detection limit of 3 ppm n-heptane is confirmed. We investigate theoretically the impact of changing the buffer diameter on the window generated signal and find good correlation with previously reported experimental results.

Spontaneous Emission Enhancement at Finite-length Metal

We study spontaneous emission enhancement of a two-level atomic emitter placed in a dielectric medium near a finite-length cylindrical metal nanowire. We calculate the dependence of the Purcell factor and the normalized decay rate to a continuous spectrum on the nanowire radius for several emitter transition wavelengths and different orientations of the transition dipole moment. For a particular transition wavelength we calculate the dependence of these quantities as well as the β-factor on the emitter distance from the nanowire and the nanowire radius. The obtained results demonstrate that the spontaneous emission characteristics exhibit significant differences as compared to the case of an infinite wire.
Computational Methods for Electromechanical Fields in Self-Assembled Quantum Dots

A detailed comparison of continuum and valence force field strain calculations in quantum-dot structures is presented with particular emphasis to boundary conditions, their implementation in the finite-element method, and associated implications for electronic states. The first part of this work provides the equation framework for the elastic continuum model including piezoelectric effects in crystal structures as well as detailing the Keating model equations used in the atomistic valence force field calculations. Given the variety of possible structure shapes, a choice of pyramidal, spherical and cubic-dot shapes is made having in mind their pronounced shape differences and practical relevance. In this part boundary conditions are also considered; in particular the relevance of imposing different types of boundary conditions is highlighted and discussed. In the final part, quantum dots with inhomogeneous indium concentration profiles are studied in order to highlight the importance of taking into account the exact In concentration profile for real quantum dots. The influence of strain, electric-field distributions, and material inhomogeneity of spherical quantum dots on electronic wavefunctions is briefly discussed.

Dynamic Electromechanical Modeling of Dielectric Elastomer Actuators With Metallic Electrodes

In this paper, a nonlinear electromechanical model for a PolyPower dielectric elastomer actuator is proposed based on an electric circuit model coupled with a viscoelastic mechanical model. The parameters of the model are found by fitting to an electrical step impulse for the mechanical part and by standard methods for the electric circuit. The resulting model is compared with experiments for a range of sinusoidal stimuli. The comparison shows good agreement between
Dynamic Modeling of Phase Crossings in Two-Phase Flow

Two-phase flow and heat transfer, such as boiling and condensing flows, are complicated physical phenomena that generally prohibit an exact solution and even pose severe challenges for numerical approaches. If numerical solution time is also an issue the challenge increases even further. We present here a numerical implementation and novel study of a fully distributed dynamic one-dimensional model of two-phase flow in a tube, including pressure drop, heat transfer, and variations in tube cross-section. The model is based on a homogeneous formulation of the governing equations, discretized by a high resolution finite difference scheme due to Kurganov and Tadmore. The homogeneous formulation requires a set of thermodynamic relations to cover the entire range from liquid to gas state. This leads a number of numerical challenges since these relations introduce discontinuities in the derivative of the variables and are usually very slow to evaluate. To overcome these challenges, we use an interpolation scheme with local refinement. The simulations show that the method handles crossing of the saturation lines for both liquid to two-phase and two-phase to gas regions. Furthermore, a novel result obtained in this work, the method is stable towards dynamic transitions of the inlet/outlet boundaries across the saturation lines. Results for these cases are presented along with a numerical demonstration of conservation of mass under dynamically varying boundary conditions. Finally we present results for the stability of the code in a case of a tube with a narrow section.
Flow-induced resonance shift in sonic slit array metamaterials
A modal analysis of flow-acoustic wave propagation through slit array metamaterials is presented. It is demonstrated that the transmission-coefficient change versus flow speed is a sensitive function of frequency. Our results further confirm that transmission resonance positions and resonance widths change significantly with the flow speed. As a reverse application, the present metamaterial slit structures allow for flow tuning of slit cavity modes, design of surface bound states such as superlens applications where a broad frequency operation interval is sought. Finally, it is shown rather surprisingly that the flow-acoustic coupling is almost independent of the angle of incidence.

Gap-plasmon nanoantennas and bowtie resonators
Plasmonic bowtie resonators involving gap surface plasmons (GSPs) in metal-insulator-metal (MIM) structures, in which only the top metal layer is structured, are investigated using numerical simulations. We demonstrate that the considered configuration features two efficiently excitable GSP resonances associated with distinct charge distributions with the domination of the dipole and quadrupole moments resulting in low- and high-Q resonances, respectively. The typical Q factors for the high-Q resonances are shown to achieve ~25 in the near-infrared, thus potentially exceeding the quasistatic limit. Detailed physical interpretations of the obtained results and consistent dependencies of the resonance characteristics on the geometrical structural parameters are presented. Excellent resonant characteristics, the simplicity of fabrication, and tuning of the resonance wavelength by adjusting the size of the bowtie arms, separation between them, and/or thickness of the insulator (SiO2) layer in the MIM structure appear attractive for a wide variety of applications, ranging from surface sensing to photovoltaics.
Laplace boundary-value problem in paraboloidal coordinates

This paper illustrates both a problem in mathematical physics, whereby the method of separation of variables, while applicable, leads to three ordinary differential equations that remain fully coupled via two separation constants and a five-term recurrence relation for series solutions, and an exactly solvable problem in electrostatics, as a boundary-value problem on a paraboloidal surface. In spite of the complex nature of the former, it is shown that the latter solution can be quite simple. Results are provided for the equipotential surfaces and electric field lines are given near a paraboloidal conductor.

General information
Publication status: Published
Organisations: Wright State University, University of Southern Denmark
Contributors: Duggen, L., Willatzen, M., Voon, L. C. L. Y.
Pages: 689-696
Publication date: 2012
Peer-reviewed: Yes

Publication information
Journal: European Journal of Physics
Volume: 33
Issue number: 3
ISSN (Print): 0143-0807
Ratings:
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 0.63 SJR 0.45 SNIP 0.837
Web of Science (2012): Impact factor 0.644
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
Original language: English
DOIs:
10.1088/0143-0807/33/3/689
Source: dtu
Source-ID: n::oai:DTIC-ART:iop/363625935::30597
Research output: Contribution to journal › Journal article – Annual report year: 2012 › Research › peer-review

Learning peg-in-hole actions with flexible objects

This paper presents a method for learning Peg-In-Hole actions with flexible objects. To learn the actions we parametrize the entire trajectory by a single point and use Kernel Density Estimation to reflect the different variations of the action and the object characteristics. The object is characterized by its elastic behaviour rather than geometric properties. Thereby an action learned for one object can be transferred to a new object that behaves similarly although it might have different elastic properties, dimensions and geometries. To bootstrap the learning mechanism, the system performs simulated actions and utilizes the detailed information obtained from the simulation environment. Subsequently Peg-In-Hole actions are tested successfully on the real life setup.

General information
Publication status: Published
Organisations: University of Southern Denmark
Modeling Frequency Response of Photoacoustic Cells using FEM for Determination of N-heptane Contamination in Air: Experimental Validation

We briefly present the basic principle of the photoacoustic effect in gases. We present the equations and boundary conditions governing the acoustic field generated by the absorption of a modulated laser beam. We solve these equations using Finite Element Methods and compare the results with experiment. We find that apparently there are effects not taken into account in the classic acoustic theory as we find a larger damping than theory predicts. However, we see that these effects have significant negative influence on the quality factor of the cell and thereby the performance limit.

Modeling Heterostructures with Schrödinger–Poisson–Navier Iterative Schemes, Effect of Carrier Charge, and Influence of Electromechanical Coupling

This paper presents a detailed investigation of the effects of piezoelectricity, spontaneous polarization and charge density on the electronic states and the quasi-Fermi level energy in wurtzite-type semiconductor heterojunctions. This has required a full solution to the coupled Schrödinger-Poisson-Navier model, as a generalization of earlier work on the Schrödinger-Poisson problem. Finite-element-based simulations have been performed on a AlN/GaN quantum well by using both one-step calculation as well as the self-consistent iterative scheme. Results have been provided for field distributions corresponding to cases with zero-displacement boundary conditions and also stress-free boundary conditions. It has been further demonstrated by using four case study examples that a complete self-consistent coupling of electromechanical fields is essential to accurately capture the electromechanical fields and electronic wavefunctions. We have demonstrated that electronic energies can change up to approximately 0.5 eV when comparing partial and complete coupling of electromechanical fields. Similarly, wavefunctions are significantly altered when following a self-consistent procedure as opposed to the partial-coupling case usually considered in literature. Hence, a complete self-consistent procedure is necessary when addressing problems requiring more accurate results on optoelectronic properties of low-dimensional nanostructures compared to those obtainable with conventional methodologies.
Modelling of the Heating Process in a Thermal Screw
The procedure of separating efficiently dry-stuff (proteins), fat, and water is an important process in the handling of waste products from industrial and commercial meat manufactures. One of the sub-processes in a separation facility is a thermal screw where the raw material (after proper mincing) is heated in order to melt fat, coagulate protein, and free water. This process is very energy consuming and the efficiency of the product is highly dependent on accurate temperature control of the process. A key quality parameter is the time that the product is maintained at temperatures within a certain threshold. A detailed mathematical model for the heating process in the thermal screw is developed and analysed. The model is formulated as a set of partial differential equations including the latent heat for the melting process of the fat and the boiling of water, respectively. The product is modelled by three components; water, fat and dry-stuff (bones and proteins). The melting of the fat component is captured as a plateau in the product temperature. The model effectively captures the product outlet temperature and the energy consumed. Depending on raw material composition, "soft" or "dry", the model outlines the heat injection and screw speeds necessary to obtain optimal output quality.

Multilayer piezoelectric transducer models combined with Field II
One-dimensional and three-dimensional axisymmetric transducer model have been compared to determine their feasibility to predict the volt-to-surface impulse response of a circular Pz27 piezoceramic disc. The ceramic is assumed mounted
with silver electrodes, bounded at the outer circular boundary with a polymer ring, and submerged into water. The transducer models are developed to account for any external electrical loading impedance in the driving circuit. The models are adapted to calculate the surface acceleration needed by the Field II software in predicting pressure pulses at any location in front of the transducer. Results show that both models predict the longitudinal resonances with consistency. The one-dimensional model is found to exhibit approximately 2.9 dB peak overshoot at the lowest longitudinal resonance frequencies prediction. These values are decreasing for higher longitudinal modes. If the three-dimensional model is restricted in its radial movement at the circular boundary both models exhibit identical results. The Field II predicted pressure pulses are found to have oscillating consistency with a 2.0 dB overshoot on the maximum amplitude using the one-dimensional compared to the three-dimensional model. This is with no electronic loading. With a 50 Ω loading an amplitude overshoot is found to be 1.5 dB.

**Simulation of flexible objects in robotics**

In this paper, we present what appears to be the first simulation model for grasping of flexible bodies based on the three-dimensional elastic constitutive relations and Newton's Second Law for solids known as the Navier-Cauchy equations. We give an overview of the most important equations for strain, stress, and elasticity tensors based on which we outline the format of the Navier-Cauchy equations of motion in the general anisotropic case. We then specifically study the equations for homogeneous isotropic bodies. We formulate a numerical scheme based on finite differences for solving the equations. Finally, we present preliminary experimental work and outline future directions.
Simultaneous estimation of material properties and pose for deformable objects from depth and color images

In this paper we consider the problem of estimating 6D pose, material properties and deformation of an object grasped by a robot gripper. To estimate the parameters we minimize an error function incorporating visual and physical correctness. Through simulated and real-world experiments we demonstrate that we are able to find realistic 6D poses and elasticity parameters like Young's modulus. This makes it possible to perform subsequent manipulation tasks, where accurate modelling of the elastic behaviour is important.

Spatial impulse response of a rectangular double curved transducer

Calculation of the pressure field from transducers having both a convex and a concave surface geometry is a complicated assignment that often is accomplished by subdividing the transducer surface into smaller flat elements of which the spatial impulse response is known. This method is often seen applied to curved transducers because an analytical solution is unknown. In this work a semi-analytical algorithm for the exact solution to a first order in diffraction effect of the spatial impulse response of rectangular shaped double curved transducers is presented. The algorithm and an approximation of it are investigated. The approximation reformulates the algorithm to an analytically integrable expression which is computationally efficient to solve. Simulation results are compared with the simulation software Field II. Calculating the response from 200 different points yields a mean error for the different approximations ranging from 0.03 % to 0.8 % relative to a numerical solution for the spatial impulse response. It is shown that the presented algorithm gives consistent results with Field II for a linear flat, a linear focused, and a convex non-focused element. Best solution was found to be 0.01 % with a three-point Taylor expansion.
**Strain in Inhomogeneous InAs/GaAs quantum dot structures**

Most non-destructive experimental approaches for the determination of indium concentration profiles give information about average indium concentration profiles only. Due to this, there is a need to extrapolate the indium concentration profiles in a way that takes into account the geometry of the quantum dots. We here present two extrapolation approaches. In the first approach we assume that the indium concentration profile is constant in the direction perpendicular to the measurement plane, while in the second approach we take into account the symmetry of the structure. Both approaches are compared to a profile with a constant indium concentration inside the dot.

**Strong curvature effects in Neumann wave problems**

Waveguide phenomena play a major role in basic sciences and engineering. The Helmholtz equation is the governing equation for the electric field in electromagnetic wave propagation and the acoustic pressure in the study of pressure dynamics. The Schrödinger equation simplifies to the Helmholtz equation for a quantum-mechanical particle confined by infinite barriers relevant in semiconductor physics. With this in mind and the interest to tailor waveguides towards a desired spectrum and modal pattern structure in classical structures and nanostructures, it becomes increasingly important to understand the influence of curvature effects in waveguides. In this work, we demonstrate analytically strong curvature effects for the eigenvalue spectrum of the Helmholtz equation with Neumann boundary conditions in cases where the waveguide cross section is a circular sector. It is found that the linear-in-curvature contribution originates from parity symmetry breaking of eigenstates in circular-sector tori and hence vanishes in a torus with a complete circular cross section. The same strong curvature effect is not present in waveguides subject to Dirichlet boundary conditions where curvature contributions contribute to second-order in the curvature only. We demonstrate this finding by considering wave propagation in a circular-sector torus corresponding to Neumann and Dirichlet boundary conditions, respectively. Results for relative eigenfrequency shifts and modes are determined and compared with three-dimensional finite element method results. Good agreement is found between the present analytical method using a combination of differential geometry with perturbation theory and finite element results for a large range of curvature ratios.
Tunable acoustic double negativity metamaterial

Man-made composite materials called “metamaterials” allow for the creation of unusual wave propagation behavior. Acoustic and elastic metamaterials in particular, can pave the way for the full control of sound in realizing cloaks of invisibility, perfect lenses and much more. In this work we design acousto-elastic surface modes that are similar to surface plasmons in metals and on highly conducting surfaces perforated by holes. We combine a structure hosting these modes together with a gap material supporting negative modulus and collectively producing negative dispersion. By analytical techniques and full-wave simulations we attribute the observed behavior to the mass density and bulk modulus being simultaneously negative.

General information
Publication status: Published
Organisations: University of Southern Denmark, CSIC
Contributors: Liang, Z., Willatzen, M., Li, J., Christensen, J.
Number of pages: 5
Publication date: 2012
Peer-reviewed: Yes

Publication information
Journal: Scientific Reports
Volume: 2
Article number: 859
ISSN (Print): 2045-2322
Ratings:
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 2.44 SJR 1.443 SNIP 0.886
Web of Science (2012): Impact factor 2.927
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
Original language: English
DOIs:
An outline for an intelligent system performing peg-in-hole actions with flexible objects

We describe the outline of an adaptable system which is able to perform grasping and peg-in-hole actions with flexible objects. The system makes use of visual tracking and shape reconstruction, physical modeling of flexible material and learning based on a kernel density approach. We show results for the different sub-modules in simulation as well as real world data. © 2011 Springer-Verlag.

Bending-induced strain and curvature effects on semiconductor nanowire electronic eigenstates

The combined influence of strain and geometry bending is analyzed quasi-analytically for nanostructures using differential geometry arguments. Appropriate general coordinates u1, u2, u3 are chosen with u1 along the nanowire centerline and u2, u3 locally spanning the nanowire cross section. This choice allows us to assume, for large aspect-ratio nanostructures, that terms proportional to u2, u3 or higher powers including combinations of u2, u3 are negligible. This assumption has been justified for nanostructures where the nanostructure radius is up to 10% of the local radius-of-curvature according to previous works. We show that the influence of bending-induced strains may lead to substantial electronic eigenstate and associated energy eigenvalue changes in the case of circular-bent nanowires (© 2011 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim)
Comparison of Atomistic and Continuum Quantum-Dot Elastic Models and Implications for Optoelectronic Properties

A comparison between continuum and atomistic valence force field (VFF) strain models is presented for zincblende InGaAs/GaAs spherical quantum dots (QD), showing differences in the off-diagonal components of the strain tensor, relevant for optoelectronic properties. We also present a comparison with the continuum model between different homogeneous compositions and concentration profiles. It is shown that the biaxial strain component is different from zero inside the QD in the linear concentration case which is known to have an effect on the valence band electrons.

Comparison of continuum and atomistic methods for the analysis of InAs/GaAs quantum dots

We present a comparison of continuum $k \cdot p$ and atomistic empirical Tight Binding methods for the analysis of the optoelectronic properties of InAs/GaAs quantum dots.

Control of the input efficiency of photons into solar cells with plasmonic nanoparticles

We study numerically the photon input efficiency of silicon solar cells due to gold plasmonic nanoparticles deposited on the cells. At low densities, when collective effects in light scattering by the nanoparticle ensemble are negligible, the absorption dependence increases linearly for a significant range of the solar spectrum. Collective effects lead to the input efficiency saturates, reaches its maximum and then decreases with nanoparticle density. The maximal input efficiency depends on the photon wavelength, nanoparticle shape and size, their distance to the cell, and the cell thickness, and can
reach ~95% in thick solar cells. Finally, we show that aluminum nanoparticles improve the input efficiency in comparison with gold nanoparticles.

**General information**
Publication status: Published
Organisations: University of Southern Denmark, P. N. Lebedev Physical Institute
Contributors: Pors, A., Uskov, A. V., Willatzen, M., Protosenko, I. E.
Pages: 2226-2229
Publication date: 2011
Peer-reviewed: Yes

**Publication information**
Journal: Optics Communications
Volume: 284
Issue number: 8
ISSN (Print): 0030-4018
Ratings:
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 1.62 SJR 0.868 SNIP 1.231
Web of Science (2011): Impact factor 1.486
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
Original language: English
Keywords: Nanoplasmonics, Solar cell, Nanoparticles, Photovoltaics
DOIs:
10.1016/j.optcom.2010.12.067
Source: dtu
Source-ID: n::oai:DTIC-ART:elsevier/285920844::30691
Research output: Contribution to journal › Journal article – Annual report year: 2011 › Research › peer-review

Detuned electrical dipoles metamaterial with bianisotropic response

The optical properties of a pair of gold nanorods with slightly different plasmon resonance frequencies, i.e., detuned electrical dipoles (DED), are studied in the near-infrared. Using a multipole expansion of the induced polarization current, we argue that the transmission enhancement (transparency) at the intermediate frequency is due to the suppression of the electric dipole moment in favor of a (weakly radiating) magnetic one. This suppression is found to be robust with respect to variations in geometrical parameters, but may depend on the direction of light incidence. Metamaterials consisting of DED unit cells are examined by making use of a new homogenization method based on the numerical calculation of dispersion curves of Bloch modes, an approach that we propose and exploit for retrieving the effective material parameters. We demonstrate that DED-based metamaterials feature magnetic and bianisotropic responses, implying the important property of optical activity without chirality and opening thereby a way to new promising applications.

**General information**
Publication status: Published
Organisations: University of Southern Denmark
Contributors: Pors, A., Willatzen, M., Albrektsen, O., Bozhevolnyi, S. I.
Number of pages: 8
Pages: 245409
Publication date: 2011
Peer-reviewed: Yes

**Publication information**
Journal: Physical Review B
Volume: 83
Issue number: 24
ISSN (Print): 0163-1829
Ratings:
Scopus rating (2011): CiteScore 3.61 SJR 3.382 SNIP 1.438
Web of Science (2011): Impact factor 3.691
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
Original language: English
Keywords: Physics, Electromagnetically induced transparancy, Optical metamaterials, Negative index, Resonators, Homogenization, Refraction, Analog
**Effect of strain on optical properties of bent nanowires**

In this work we study the deformation of ZnO nanowires under the influence of an applied force at the top of the wire. We show that the Euler-Bernoulli beam equation can be used even for relatively high forces although a full non linear theory does show quantitative differences, however, not qualitative differences. We furthermore show that strain induces a confinement of the electrons which results in a significant increase in the conduction band energy spacing. It is known that piezoelectric effects are important in ZnO nanowire, however, these are disregarded in this work in order to wholly focus on the effect of strain.

**General information**

Publication status: Published
Organisations: University of Southern Denmark
Contributors: Lassen, B., Willatzen, M.
Pages: 495-496
Publication date: 2011

**Host publication information**

Title of host publication: Physics of Semiconductors : 30th International Conference on the Physics of Semiconductors
Keywords: Nanowires, Elasticity, Euler-Bernoulli beam equation, Non linear strain, Electronic band structure
DOIs: 10.1063/1.3666470
Source: dtu
Source-ID: n::oai:DTIC-ART:isi/363206667::30706

**Effects of hydrostatic strain on eigenstates of Möbius strips**

In this paper we theoretically investigate the allowed energies and associate wave-functions for Möbius strips with varying thicknesses. We show that the induced strain in fabricating these Möbius strips will have a pronounced impact on the energies and wave-functions for thick strips, while for thin strips the impact of strain is negligible. We furthermore, show that a simpler strain free approximate theory based on differential geometry is in excellent agreement with detailed finite element calculations. © 2011 IEEE.

**General information**

Publication status: Published
Organisations: Department of Informatics and Mathematical Modeling, University of Southern Denmark
Contributors: Lassen, B., Willatzen, M., Gravesen, J.
Pages: 3-4
Publication date: 2011

**Host publication information**

Title of host publication: Proceedings of the 2011 11th International Conference on Numerical Simulation of Optoelectronic Devices (NUSOD)
Publisher: IEEE Computer Society Press
ISBN (Print): 978-1-61284-876-1
Keywords: Computer simulation, Electrooptical devices, Wave functions, Optoelectronic devices
DOIs: 10.1109/NUSOD.2011.6041125
Source: dtu
Source-ID: n::oai:DTIC-ART:compendex/313560778::30716

**Electromechanical phenomena in semiconductor nanostructures**

Electromechanical phenomena in semiconductors are still poorly studied from a fundamental and an applied science perspective, even though significant strides have been made in the last decade or so. Indeed, most current
Electromechanical devices are based on ferroelectric oxides. Yet, the importance of the effect in certain semiconductors is being increasingly recognized. For instance, the magnitude of the electric field in an AlN/GaN nanostructure can reach 1-10 MV/cm. In fact, the basic functioning of an (0001) AlGaN/GaN high electron mobility transistor is due to the two-dimensional electron gas formed at the material interface by the polarization fields. The goal of this review is to inform the reader of some of the recent developments in the field for nanostructures and to point out still open questions. Examples of recent work that involves the piezoelectric and pyroelectric effects in semiconductors include: the study of the optoelectronic properties of III-nitrides quantum wells and dots, the current controversy regarding the importance of the nonlinear piezoelectric effect, energy harvesting using ZnO nanowires as a piezoelectric nanogenerator, the use of piezoelectric materials in surface acoustic wave devices, and the appropriateness of various models for analyzing electromechanical effects. Piezoelectric materials such as GaN and ZnO are gaining more and more importance for energy-related applications; examples include high-brightness light-emitting diodes for white lighting, high-electron mobility transistors, and nanogenerators. Indeed, it remains to be demonstrated whether these materials could be the ideal multifunctional materials. The solutions to these and other related problems will not only lead to a better understanding of the basic physics of these materials, but will validate new characterization tools, and advance the development of new and better devices. We will restrict ourselves to nanostructures in the current article even though the measurements and calculations of the bulk electromechanical coefficients remain challenging. Much of the literature has focused on InGaN/GaN, AlGaN/GaN, ZnMgO/ZnO, and ZnCdO/ZnO quantum wells, and InAs/GaAs and AlGaN/AlN quantum dots for their optoelectronic properties; and work on the bending of nanowires have been mostly for GaN and ZnO nanowires. We hope the present review article will stimulate further research into the field of electromechanical phenomena and help in the development of applications. (C) 2011 American Institute of Physics. [doi:10.1063/1.3533402]

General information
Publication status: Published
Organisations: Wright State University, University of Southern Denmark
Contributors: Voon, L. C. L. Y., Willatzen, M.
Number of pages: 24
Pages: 031101
Publication date: 2011
Peer-reviewed: Yes

Publication information
Journal: Journal of Applied Physics
Volume: 109
Issue number: 3
ISSN (Print): 0021-8979
Ratings:
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 2.24 SJR 1.39 SNIP 1.32
Web of Science (2011): Impact factor 2.168
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
Original language: English
Keywords: Physics, Field-effect transistors, Surface acoustic-waves, Piezoresponse force microscopy, Strained-layer superlattices, Quantum-confined stark, Single ZNO nanowire, III-V nitrides, Piezoelectric fields, Spontaneous polarization, Electronic-structure
DOIs:
10.1063/1.3533402
Source: dtu
Source-ID: n:oai:DTIC-ART:isi/301753521::30696
Research output: Contribution to journal › Review – Annual report year: 2011 › Research › peer-review

Experimental determination of the refractive index of metamaterials
We present a simple experimental technique based on diffraction for determining the complex refractive index of metamaterials, and demonstrate it with metamaterials that consist of detuned electrical dipoles (DEDs), mimicking the dressed-state picture of electromagnetically induced transparency (EIT). The metamaterials are realized by fabricating lithographically defined gold nanorods on a silica substrate, covered with a similar to 15 mu m thick polymer layer, and feature EIT-like transmission spectra with transparency windows centered at wavelengths near similar to 800 nm. The refractive indices are determined for wavelengths where the DED metamaterials exhibit enhanced transmission. Thereby, we experimentally demonstrate normal dispersion in the transmission window and estimate the group refractive index to similar to 3.6. Furthermore, finite-element simulations are conducted on a monolayer of DED unit cells, which similarly exhibit the EIT-like behavior in terms of enhanced transmission revealed in the transmission spectra. Simulated transmission and reflection spectra are utilized for calculations of the real and imaginary parts of the metamaterial refractive index, showing consistent trends with those obtained experimentally.
Finite Element Simulation of Photoacoustic Pressure in a Resonant Photoacoustic Cell Using Lossy Boundary Conditions

The finite-element method (FEM) is used to simulate the photoacoustic signal in a cylindrical resonant photoacoustic cell. Simulations include loss effects near the cell walls that appear in the boundary conditions for the inhomogeneous Helmholtz equation governing the acoustic pressure. Reasonably good agreement is obtained between theoretical results and experimental data. However, it was anticipated that loss mechanisms other than viscous and thermal boundary losses occur and should be included. Nevertheless, the feasibility to use FEM together with the derived boundary conditions to simulate the photoacoustic signal was demonstrated and good agreement with experiments for the actual resonance frequency and the quality factor of the cell was obtained despite its complicated geometry.
Möbius semiconductor nanostructures and deformation potential strain effects

A discussion of Möbius nanostructures is presented with focus on (1) the accuracy of the approximate differential-geometry formalism by Gravesen and Willatzen and (2) to assess the influence of bending-induced strain on Schrödinger equation eigenstates in semiconductor Möbius structures. The differential-geometry model assumed complete confinement of a quantum-mechanical particle to a zero-thickness Möbius structure where the shape was computed based on minimization of elastic bending energy only and imposing the relevant boundary conditions. In the latter work, while bending was accounted for in finding the shape of the Möbius structure it was, for simplicity, neglected altogether in determining the direct strain influence on electronic eigenstates. However, as is well-known, deformation-potential strain effects in many semiconductor materials can lead to important changes in not only the energy levels but, perhaps more so, the symmetry of the associated eigenstates and, henceforth, optical and electronic properties. In this work, we investigate finite-thickness effects of different-sized Möbius structures as well as deformation-potential hydrostatic strain implications using the Finite Element Model commercial software COMSOL. The paper contains a detailed comparison of general Finite Element Model results with the differential-geometry method. Copyright © 2011 American Scientific Publishers All rights reserved.

Optical transparency by detuned electrical dipoles

We demonstrate that optical transparency can be realized with plasmonic metamaterials using unit cells consisting of detuned electrical dipoles (DED), thereby mimicking the dressed-state picture of the electromagnetically induced transparency (EIT) in atomic physics. Theoretically analyzing the DED cells with two and three different silver ellipsoids, we show the possibility of reaching a ≥10 times decrease in group velocity and a propagation loss of ≤1 dB per cell within the optical wavelength range of 625–640 nm. Similar configurations are realized with lithographically fabricated gold nanorods placed on a glass substrate and subsequently covered with a ~15-μm-thick polymer layer, featuring EIT-like transmission spectra with transparency windows at wavelengths of ~850 nm.
Plasmonic metamaterial wave retarders in reflection by orthogonally oriented detuned electrical dipoles

We demonstrate that a pair of perpendicular electrical dipolar scatterers resonating at different frequencies can be used as a metamaterial unit cell to construct a nanometer-thin retarder in reflection, designing nanocross and nanobrick plasmonic configurations to function as reflecting quarter-wave plates at ~1520 and 770nm, respectively. The design is corroborated experimentally with a monolayer of gold nanobricks, transforming linearly polarized incident radiation into circularly polarized radiation at ~780nm.

© 2011 Optical Society of America.

Scattering suppression and field enhancement of the fundamental plasmonic mode in bent nanorods

We study the absorption and scattering cross sections of three-dimensional retardation-based plasmonic resonators as straight gold nanorod antennas are transformed gradually to split-ring resonators. Using a multipole expansion of the scattered field, we show by bending the nanoantennas that it is possible at the fundamental resonance to suppress the scattering due to a decrease in the electric dipole response in favor of a magnetic dipole response. The decrease in scattering strength is accompanied by an increase in the Q-factor which in the split-ring resonator limit is improved by a factor of ~1.9 (equivalent to ~1.2 times larger than the quasi-static value). Additionally, the split-ring resonator shows promising prospects in surface enhanced sensing applications with local field enhancement of ≥50 in the split-ring gap.

Copyright © 2011 American Scientific Publishers.
Strain and piezoelectric effects in quantum-dot structures
A discussion of computational methods for calculating strain and piezoelectric fields in nanostructures is presented. Emphasis is on a comparison of continuum and valence force field atomistic models and the validity of the former in predicting, accurately, strain fields for nanostructures with dimensions down to a few nm. This is done on the experimentally relevant InAs/InGaAs quantum-dot wetting layer structures and on spherical quantum dot structures. We next address the influence of boundary conditions imposed at the computational domain for strain fields near and inside the quantum dot; a point largely missing in literature. Boundary conditions discussed include fixed, free, fixed-free, and periodic, and it is shown that the particular choice of boundary conditions is unimportant for the strain results; a conclusion that allows to choose the computationally most effective one being the fixed-free boundary conditions as it requires the smallest computational domain for obtaining convergent results. While this result is fortunate, it is not obvious from a mathematical point of view. A further important, and a priori not obvious conclusion, is that a continuum model captures well atomistic strain results; a fact that allows us to use a continuum formulation even in cases where structure dimensions are down to only a few lattice constants. In realistically grown structures, inhomogeneous concentration profiling exists. We present investigations for strain and piezoelectric results in the case where a spherical quantum dot region is gradually profiled from GaAs to InAs assuming the concentration is a function of the distance to the quantum dot sphere center. It is shown that quantum dot concentration profiling affects strain fields and biaxial strains in particular, electronic states and hence optical properties. We finally present some effective quasi-analytical studies of electronic states and strain fields in curved quantum dots based on applications of differential geometry and perturbation theory.
Analysis of optical properties of strained semiconductor quantum dots for electromagnetically induced transparency

Using multiband \( k\p \) theory we study the size and geometry dependence on the slow light properties of conical semiconductor quantum dots. We find the V-type scheme for electromagnetically induced transparency (EIT) to be most favorable, and identify an optimal height and size for efficient EIT operation. In case of the ladder scheme, the existence of additional dipole allowed intraband transitions along with an almost equidistant energy level spacing adds additional decay pathways, which significantly impairs the EIT effect. We further study the influence of strain and band mixing comparing four different \( k\p \) band structure models. In addition to the separation of the heavy and light holes due to the biaxial strain component, we observe a general reduction in the transition strengths due to energy crossings in the valence bands caused by strain and band mixing effects. We furthermore find a non-trivial quantum dot size dependence of the dipole moments directly related to the biaxial strain component. Due to the separation of the heavy and light holes the optical transition strengths between the lower conduction and upper most valence-band states computed using one-band model and eight-band model show general qualitative agreement, with exceptions relevant for EIT operation.

General information
Publication status: Published
Organisations: Department of Micro- and Nanotechnology, Nanophotonics, Department of Photonics Engineering, Quantum and Laser Photonics, Theoretical Nanotechnology, University of Southern Denmark
Number of pages: 22
Publication date: 2010
Peer-reviewed: Yes

Publication information
Journal: ArXiv Astrophysics e-prints
Issue number: arXiv:1002.2102
Original language: English
URLs:
http://arxiv.org/abs/1002.2102
Source: dtu
Source-ID: n:oai:DTIC-ART:arxiv/372450170::30770
Research output: Contribution to journal › Journal article – Annual report year: 2010 › Research › peer-review

Analytic theory of curvature effects for wave problems with general boundary conditions

A formalism based on a combination of differential geometry and perturbation theory is used to obtain analytic expressions for confined eigenmode changes due to general curvature effects. In cases of circular-shaped and helix-shaped structures, where alternative analytic solutions can be found, the perturbative solution is shown to yield the same result. The present technique allows the generalization of earlier results to arbitrary boundary conditions. The power of the method is illustrated using examples based on Maxwell's and Schrödinger’s equations for applications in photonics and nanoelectronics.

General information
Publication status: Published
Organisations: Geometry, Department of Mathematics, Wright State University
Contributors: Willatzen, M., Gravesen, J., Voon, L. C. L. Y.
Pages: 060102
Publication date: 2010
Peer-reviewed: Yes

Publication information
Journal: Physical Review A
Volume: 81
Issue number: 6
ISSN (Print): 2469-9926
Ratings:
Scopus rating (2010): SJR 2.474 SNIP 1.225
Web of Science (2010): Indexed yes
Original language: English
Electronic versions:
Gravesen.pdf
DOIs:
10.1103/PhysRevA.81.060102
URLs:
Band-mixing and strain effects in InAs/GaAs quantum rings

We analyze for the first time the coupled influence of band mixing, strain, and piezoelectricity on electronic structure, eigenstates, and optical transition strengths for InAs/GaAs quantum-ring structures. It is shown that band mixing and strain alter the level energies and optical absorption coefficients significantly.

Calibration of Field II using a Convex Ultrasound Transducer

Field II is an ultrasound simulation program capable of simulating the pressure scattering from inhomogeneous tissue. The simulations are based on a convolution between spatial impulse responses from the field in front of the transducer and the volt-to-surface acceleration impulse response of the transducer. For such simulations to reflect actual measured intensities and pressure levels, the transducer impulse response is to be known. This work presents the results of combining a modified form of a 1D linear transducer model originally suggested by Willatzen with the Field II program to calibrate the pressure simulations of a 128 element convex medical transducer with elevation focus at 70 mm. The simulations are compared to pressure measurements from an automatic water bath needle hydrophone setup. The transducer was driven at 4.0 MHz using a research scanner with a commercial transducer amplifier from BK-Medical (Herlev, Denmark). As input waveform for the Field model we measured the output voltage of the research amplifier, which peak voltage was limited to 31 V to avoid too high non linear effects. We measured the hydrophone output from three transducer front elements by averaging 40 shoot sequences on each element using a remotely controlled Agilent MSO6014A oscilloscope. The pressure along the elevation line in 32 mm, 70 mm (elevation focus) and 112 mm for each element are measured.
Comparison of wurtzite atomistic and piezoelectric continuum strain models: Implications for the electronic band structure

We compare continuum and atomistic models for the electromechanical fields in wurtzite GaN/AlN quantum dots and their relative impact on the electronic band structure. Qualitative agreement between atomistic strain calculations and continuum elastic models for a wurtzite hexagonal quantum-dot structure is demonstrated; however, significant quantitative discrepancies of up to 100 meV are observed. A smaller difference of approximately 15 meV is found between fully coupled and semi-coupled continuum models.

Crystal orientation effects on wurtzite quantum well electromechanical fields

A one-dimensional continuum model for calculating strain and electric field in wurtzite semiconductor heterostructures with arbitrary crystal orientation is presented and applied to GaN/AlGaN and ZnO/MgZnO heterostructure combinations. The model is self-consistent involving feedback couplings of spontaneous polarization, strain, and electric field. Significant differences between fully coupled and semicoupled models are found for the longitudinal and shear-strain components as a function of the crystal-growth direction. In particular, we find that the semicoupled model, typically used in the literature for semiconductors, is inaccurate for ZnO/MgZnO heterostructures where shear-strain components play an important role. An interesting observation is that a growth direction apart from [1¯21¯0] exists for which the electric field in the quantum well region becomes zero. This is important for, e.g., optimization of light-emitting-diode quantum efficiency.
Cylindrical symmetry and spurious solutions in eight band k·p theory
Spurious solutions in eight band k·p theory for low-dimensional semiconductor heterostructures is a well-known problem. In this paper we study two approaches for the removal of spurious solutions, the plane wave cutoff approach [1] and the approach suggested by Foreman [2] where the Kane parameter is changed. We show that in order to use the plane wave cutoff approach for a cylindrical symmetric system Bessel functions has to be used as the expansion basis in the radial direction. Furthermore we compare the two approaches for a InAs/GaAs conical quantum dot.

Detuned Electrical Dipoles for Plasmonic Sensing
We demonstrate that a pair of electrical dipolar scatterers resonating at different frequencies, i.e., detuned electrical dipoles, can be advantageously employed for plasmonic sensing of the environment, both as an individual subwavelength-sized sensor and as a unit cell of a periodic array. It is shown that the usage of the ratio between the powers of light scattered into opposite directions (or into different diffraction orders), which peaks at the intermediate frequency, allows one to reach a sensitivity of ≈400 nm/RIU with record high levels of figure of merit exceeding 200. Qualitative considerations are supported with detailed simulations and proof-of-principle experiments using lithographically fabricated gold nanorods with resonances at ∼800 nm.
Dynamic Electro-Mechanical Modelling of Dielectric EAP

In this paper a nonlinear electromechanical model for a dielectric electro-active polymer (DEAP) actuator is proposed based on an electric-circuit model coupled with a viscoelastic mechanical model. The parameters of the model are found by fitting to a creep test for the mechanical part and by standard methods for the electric circuit. The resulting model is compared with experiments for a sinusoidal and a sweep stimulus. The comparison shows a good agreement between experiments and model results.

Electron conductance in curved quantum structures

A differential-geometry analysis is employed to investigate the transmission of electrons through a curved quantum-wire structure. Although the problem is a three-dimensional spatial problem, the Schrodinger equation can be separated into three general coordinates. Hence, the proposed method is computationally fast and provides direct (geometrical) parameter insight as regards the determination of the electron transmission coefficient. We present, as a case study, calculations of the electron conductivity of a helically shaped quantum-wire structure and discuss the influence of the quantum-wire centerline radius of curvature and pitch length for the conductivity versus the chemical potential.
**Electrostriction Coefficients of GaN, AlN, MgO and ZnO in the Wurtzite Structure from First-Principles**

First-principles calculations have been performed on wurtzite AlN, GaN, MgO and ZnO, with a view to obtaining electrostriction coefficients.

**Extension of the Landau theory for hysteretic electric dynamics in ferroelectric ceramics**

In this paper, a macroscopic differential model for the nonlinear dynamics of the electric field in ferroelectric ceramics is developed on the basis of polarization switching theory. In a one-dimensional description, dynamics with hysteresis caused by polarization switching is modelled by using the Landau theory of phase transitions for single-crystal cases. For ferroelectric ceramics, the orientation of the principal axis of grains is assumed to have a certain distribution. The overall dynamics is determined by making a weighted combination of the dynamics of each grain. The weight function for the combination is taken phenomenologically based on experimental observations. It is shown that experimental hysteresis can be reproduced by the macroscopic differential model precisely.

**FEM analysis of cylindrical resonant photoacoustic cells**

Using a mathematical model on photoacoustics that includes both temperature and pressure effects explicitly, we analyze the behaviour of resonances of a cylindrical photoacoustic cell consisting of two buffer volumes and a resonator. We excite the cell at a certain frequency and find the ratio of resonator versus buffer diameter needed to obtain resonance. The results show that the resonance ratio depends on the absolute cell size. Also the amplitude of the acoustic signal measured in the middle of the resonator does not necessarily decrease when the total cell volume is increased. If the
resonator diameter is sufficiently small, decreasing its diameter will increase the acoustic signal, although the total cell volume has to be increased to obtain resonance. This gives the advantage of being able to obtain a comparably large signal and at the same time use large buffer diameters to suppress window absorption signals. Finally we also compare the quality of the above-mentioned model and the lossy Helmholtz equation. We find that there is a shift in resonance ratio and the signal damping differs slightly. Albeit these differences are not large, and in many cases negligible, the model can be easily coupled with a solid absorption model in order to investigate the importance of thermal and pressure coupling between two acoustic media subject to heat absorption.

General information
Publication status: Published
Organisations: University of Southern Denmark
Contributors: Duggen, L., Frese, R., Willatzen, M.
Number of pages: 5
Pages: 012036
Publication date: 2010
Peer-reviewed: Yes

Publication information
Journal: Journal of Physics: Conference Series (Print)
Volume: 214
ISSN (Print): 1742-6588
Ratings:
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.288 SNIP 0.351
Web of Science (2010): Indexed yes
Original language: English
DOIs:
10.1088/1742-6596/214/1/012036
Source: dtu
Source-ID: n:oai:DTIC-ART:isi/302189374::30752
Research output: Contribution to journal › Conference article – Annual report year: 2010 › Research › peer-review

From plasmonic nanoantennas to split-ring resonators: Tuning scattering strength
Evolution of the absorption and scattering cross sections, quality-factor (Q-factor), and field enhancement of three-dimensional retardation-based plasmonic resonators being transformed from straight gold nanorod antennas to split-ring resonators by bending is considered. The optical resonances are confirmed to be of plasmonic origin and are specifically shown to be related to the formation of standing waves of short-range surface plasmon polaritons supported by straight and bent nanorods. We verify that by bending nanoantennas it is possible to reduce and ultimately, in the split-ring resonator limit, practically eliminate their scattering at the fundamental resonance, resulting in a substantial increase in the corresponding Q-factors. The decrease in scattering by bending is connected with the attenuation of the electric-dipole response in favor of a magnetic-dipole one, leading to Q-factors exceeding the quasi-static limit by a factor of ~1.7. Simultaneously, the structures exhibit local field enhancements of >50.

General information
Publication status: Published
Organisations: University of Southern Denmark
Contributors: Pors, A., Willatzen, M., Albrektsen, O., Bozhevolnyi, S. I.
Pages: 1680-1687
Publication date: 2010
Peer-reviewed: Yes

Publication information
Journal: Journal of the Optical Society of America B (Optical Physics)
Volume: 27
Issue number: 8
ISSN (Print): 0740-3224
Ratings:
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.568 SNIP 1.382
Web of Science (2010): Impact factor 2.097
Web of Science (2010): Indexed yes
Original language: English
DOIs:
10.1364/JOSAB.27.001680
Investigating the effect of magnetic pipes connected to electromagnetic flowmeters using experimentally validated finite element models

This paper describes a finite element model for computing the magnetic field distribution in commercial electromagnetic flowmeter designs. The model is validated through an experimental setup, measuring the magnetic flux density in the radial direction at the inner perimeter of the flowmeter wall. The predicted flux densities are in overall good agreement with experimental obtained data. The model is used to evaluate the effect of having magnetic pipes connected to flowmeters of two different designs. Using analytic models, the flowmeter sensitivity is computed both with magnetic and non-magnetic pipes connected.

General information
Publication status: Published
Organisations: University of Southern Denmark, Siemens
Contributors: Christensen, T. A., Willatzen, M.
Pages: 62-69
Publication date: 2010
Peer-reviewed: Yes

Publication information
Journal: Flow Measurement and Instrumentation
Volume: 21
Issue number: 1
ISSN (Print): 0955-5986
Ratings:
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.649 SNIP 1.41
Web of Science (2010): Impact factor 0.808
Web of Science (2010): Indexed yes
Original language: English
Keywords: Electromagnetic flowmeter, Sensitivity, Finite element, Magnetic field measurement
DOI: 10.1016/j.flowmeasinst.2009.11.006

Investigations of scattering and field enhancement effects in retardation-based plasmonic nanoantennas

Modifications in scattering strength of and local field enhancement by retardation-based plasmonic nanoantennas when being transformed from straight nanorods to split-rings are investigated. The scattering properties are monitored by linear reflection and extinction spectroscopy whereas local field enhancement is estimated from measurements on individual nanoantennas by nonlinear scanning optical microscopy in which two-photon-excited photoluminescence (TPL) is detected. The linear and nonlinear optical characterizations reveal, that the optical response of nanoantennas is dominated by constructively interfering short-range surface plasmon polaritons (SR-SPP) and that the transformation of straight nanorods into split-rings by bending significantly influences the scattering strength. Importantly, strong suppression of scattering for the fundamental SR-SPP mode is observed when the bend radius is decreased, a feature that we attribute to the decrease in the nanoantenna electric-dipole response in tact with its bending. The experimental observations are corroborated with numerical simulations using the finite-element method.

General information
Publication status: Published
Organisations: Nanophotonics, Department of Photonics Engineering, University of Southern Denmark
Contributors: Nielsen, M. G., Pors, A., Nielsen, R. B., Boltasseva, A., Albrektsen, O., Willatzen, M., Bozhevolnyi, S. I.
Number of pages: 11
Pages: 77573O
Publication date: 2010

Host publication information
Title of host publication: Plasmonics: Metallic Nanostructures and Their Optical Properties VIII
(Proceedings of S P I E - International Society for Optical Engineering, Vol. 7757),
Keywords: Surface plasmons, Metal optics, Resonators, Scattering, Nonlinear optics, Nanostructure fabrication
Modeling transducer impulse responses for predicting calibrated pressure pulses with the ultrasound simulation program Field II

FIELD II is a simulation software capable of predicting the field pressure in front of transducers having any complicated geometry. A calibrated prediction with this program is, however, dependent on an exact voltage-to-surface acceleration impulse response of the transducer. Such impulse response is not calculated by FIELD II. This work investigates the usability of combining a one-dimensional multilayer transducer modeling principle with the FIELD II software. Multilayer here refers to a transducer composed of several material layers. Measurements of pressure and current from Pz27 piezoceramic disks as well as pressure and intensity measurements in front of a 128 element commercial convex medical transducer are compared to the simulations. Results show that the models can predict the pressure from the piezoceramic disks with a root mean square (rms) error of 11.2% to 36.2% with a 2 dB amplitude decrease. The current through the external driving circuits are predicted within 8.6% to 36% rms error. Prediction errors of 30% and in the range of 5.8%-19.9% for the pressure and the intensity, respectively, are found when simulating the commercial transducer. It is concluded that the multilayer transducer model and the FIELD II software in combination give good agreement with measurements.

General information
Publication status: Published
Organisations: Biomedical Engineering, Department of Electrical Engineering, Center for Fast Ultrasound Imaging
Contributors: Bæk, D., Jensen, J. A., Willatzen, M.
Pages: 2825-2835
Publication date: 2010
Peer-reviewed: Yes

Publication information
Volume: 127
Issue number: 5
ISSN (Print): 0001-4966
Ratings:
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 0.796 SNIP 1.523
Web of Science (2010): Impact factor 1.644
Web of Science (2010): Indexed yes
Original language: English
Electronic versions:
Bæk.pdf
DOIs:
10.1121/1.3365317

Bibliographical note
Copyright (2010) Acoustical Society of America. This article may be downloaded for personal use only. Any other use requires prior permission of the author and the Acoustical Society of America.

Photoacoustics in a Cylindrical Resonator Containing a Flowing Gas
A detailed study of photoacoustics in circular resonators and waveguides in the presence of a gas flow is presented based on the Green's function method. In the first part of the paper, a wave equation is derived describing sound propagation in a flowing (perfect) gas due to a localized heating source. Analytical results are obtained for the acoustic pressure in the case of a constant gas flow subject to different boundary conditions. In the second part of the paper, the derived wave equation is solved for a parabolic flow profile using the finite-element method and results are compared with the constant-flow case. It is demonstrated that the gas-flow profile does not change the pattern of acoustic resonance frequencies significantly. In particular it is noted that the presence of flow gives rise to new peaks and we show that non-linearities with respect to the mean flow velocity appear already at 1% of the speed of sound at certain frequencies.
Simulating Capacitive Micromachined Ultrasonic Transducers (CMUTs) using Field II

Field II has been a recognized simulation tool for piezoceramic medical transducer arrays for more than a decade. The program has its strength in doing fast computations of the spatial impulse response (SIR) from array elements by dividing the elements into smaller mathematical elements (ME)s from which it calculates the SIR responses. The program features predefined models for classical transducer geometries, but currently none for the fast advancing CMUTs. This work addresses the assumptions required for modeling CMUTs with Field II. It is shown that rectangular array elements, populated with cells, can be well approximated by neglecting the cells. Further, it is demonstrated that scaling of the SIR translates into better computational efficiency.

Testing of a spatial impulse response algorithm for double curved transducers

The spatial impulse response (SIR) method for solving the Rayleigh integral is a well known method for fast time response simulation of acoustic waves. Several analytical expressions have been found for simple transducer geometries such as rectangles and discs. However, no analytical solution is known for double curved transducers (DCT), i.e. transducers with...
both concave and convex radius. To calculate the SIR from such transducers Field II uses a far-field approximation by dividing the surface into smaller flat elements and then performs a summation of the response from all the elements using Huygen’s principle. This calculation method involves several summations, and it relies on an exact phase calculation to avoid numerical noise in the response. A stable analytical expression for the SIR would thus be beneficial to the Field II software as an alternative solver. A semi-analytic algorithm (SAA) has been developed, and it is the objective of this work to validate an analytical approximation of the algorithm as an alternative solver for Field II. Two approximations of a SAA that efficiently finds the SIR for DCT have been implemented into a MATLAB and a C-code environment. The root mean square (RMS) error of calculating the SIR using Field II and the C-implemented approximation was calculated relative to a high resolution solution obtained with MATLAB on a DCT, a linear concave, and a flat transducer. The computation time for solving apoint 400 times is also found. Calculations are performed at sampling frequencies ranging from 100 MHz to 15 GHz in steps of 100 MHz. The transducer width is 250 μm and the height is 10 mm. The C-implementation exhibits errors ranging from 4.9.10-4 % to 0.91 % and Field II 0.0117 % to 0.94 %. A slight trade-off between accuracy and computation time is found. Field II outperforms the SAA in computation time if high accuracy is not needed. However, if a higher accuracy is required, the SAA is the best model choice. © 2010 IEEE.

Curved nanowire structures and exciton binding energies

Growth of quantum-confined semiconductor structures is a complicated process that may lead to imperfect and complex shapes as well as geometrical nonuniformities when comparing a large number of intended identical structures. On the other hand, the possibility of tuning the shape and size of nanostructures allows for extra optimization degrees when considering electronic and optical properties in various applications. This calls for a better understanding of size and shape effects. In the present work, we express the one-band Schrödinger equation in curved coordinates convenient for determining eigenstates of curved quantum-wire and quantum-dash structures with large aspect ratios. Firstly, we use this formulation to solve the problem of single-electron and single-hole states in curved nanowires. Secondly, exciton states for the curved quantum-wire Hamiltonian problem are found by expanding exciton eigenstates on a product of single-particle eigenstates. A simple result is found for the Coulomb matrix elements of an arbitrarily curved structure as long as the radius-of-curvature is much larger than the cross-sectional dimensions. We use this general result to compute the groundstate exciton binding energy of a bent nanowire as a function of the bending radius-of-curvature. It is demonstrated that the groundstate exciton binding energy increases by 40 meV as the radius-of-curvature changes from 20 to 2 nm while keeping the total length (and volume) of the nanowire constant.
Effective computation of complex-shaped quantum-dot structures
The possibility of growing complex-shaped nanodot structures of various material composition allows optimization of
certain physical parameters. In the present work, we present effective analytical methods for computing conduction-band
eigenstates in quantum-dot structures of complex shape. Comparison with detailed finite-element computations is made.
The electronic bandstructure model used is a one-band $\vec{k}\cdot\vec{p}$ model assuming infinite barriers. Results
based on two semi-analytical models are presented. The first model employs geometrical perturbation theory to obtain the
quantitative effect of quantum-dot surface perturbations on electron energy levels. Furthermore, the method output
includes the level of degeneracy and variations with geometry to be assessed. The second model allows both energy
levels and eigenstates to be easily determined for three-dimensional axisymmetrical GaAs structures of varying radius
embedded in an AlGaAs matrix by extending a method originally due to Stevenson on electromagnetic waveguide
structures (Stevenson in J. Appl. Phys. 22:1447, 1951) to account for electron states. The latter model simplifies the
description of a three-dimensional partial-differential equation problem into a small set of ordinary differential equations.
For structures with a large aspect ratio, the small set reduces to a single ordinary differential equation yet maintaining high
accuracy. A case study is presented to exemplify the models shown.

Electromagnetic-wave propagation along curved surfaces
We show that Maxwell's equations for a nonmagnetic, isotropic, but electrically inhomogeneous medium in the absence of
charges or current sources lead to a wave equation governing surface electromagnetic wave propagation along a general
curved, smooth surface which, when recasted using an appropriate choice of curvilinear coordinates $u_1,u_2,u_3$, can be fully
separated in the spatial dimensions. It is shown that surface electromagnetic wave solutions decay exponentially away
from the surface (along the $u_3$ coordinate) with the same decay rate independent of the shape of the surface.
Transmission and reflection coefficients governing scattering of electromagnetic waves on a varying surface shape are
derived. Two test cases of a Gaussian-shaped and a sinusoidal-shaped surface are solved in details and discussed
numerically in terms of transmission and reflection coefficients including dependencies on surface-shape parameters in
the wavelength range 250-750 nm. The present method for determining surface electromagnetic wave propagation along
complex-shaped metal-dielectric surfaces allows better insight into the importance of surface geometry as well as
considerably faster computational speeds than those provided by standard numerical methods.
Exciton states in three-dimensional ring structures: A differential-geometric analysis

An effective method for computing excitonic shifts in curved quantum-wire geometries is presented. As a case example, we consider a GaAs quantum ring with infinite barriers along the cross-sectional dimensions assumed to be of square shape albeit this assumption can be easily avoided. A simple analytic expression for excitonic shifts is found using first-order perturbation theory.

Modelling of nonlinear dynamics for reciprocal multi-layer piezoceramic transducer systems

The dynamics of multi-layer transducer systems are modelled and simulated by use of a multi-domain spectral method. The model accounts for a nonlinear constitutive relation between the electric displacement and the electric field. Simulation of resonance and wave propagation in the transducer is implemented using a domain-decomposition method and governing equations in each layer are discretized using a Chebyshev collocation method. The model is applied to a reciprocal transducer system, as used in many engineering applications including ultrasonic flowmeter applications and blood-velocity measurement setups, where the transducer consists of a PZT5 piezoceramic layer and a matching layer.
Optical properties and optimization of electromagnetically induced transparency in strained InAs/GaAs quantum dot structures

Using multiband k center dot p theory we study the size and geometry dependence on the slow light properties of conical semiconductor quantum dots. We find the V-type scheme for electromagnetically induced transparency (EIT) to be most favorable and identify an optimal height and size for efficient EIT operation. In case of the ladder scheme, the existence of additional dipole allowed intraband transitions along with an almost equidistant energy-level spacing adds additional decay pathways, which significantly impairs the EIT effect. We further study the influence of strain and band mixing comparing four different k center dot p band-structure models. In addition to the separation of the heavy and light holes due to the biaxial-strain component, we observe a general reduction in the transition strengths due to energy crossings in the valence bands caused by strain and band-mixing effects. We furthermore find a nontrivial quantum dot size dependence of the dipole moments directly related to the biaxial-strain component. Due to the separation of the heavy and light holes the optical transition strengths between the lower conduction and upper most valence-band states computed using one-band model and eight-band model show general qualitative agreement, with exceptions relevant for EIT operation.
Parameter sensitivity study of a Field II multilayer transducer model on a convex transducer

A multilayer transducer model for predicting a transducer impulse response has in earlier works been developed and combined with the Field II software. This development was tested on current, voltage, and intensity measurements on piezoceramics discs (Bæk et al. IUS 2008) and a convex 128 element ultrasound imaging transducer (Bæk et al. ICU 2009). The model benefits from its 1D simplicity and has shown to give an amplitude error around 1.7-2 dB. However, any prediction of amplitude, phase, and attenuation of pulses relies on the accuracy of manufacturer supplied material characteristics, which may be inaccurate estimates. The previous test cases have assumed the simulation parameters to be exact as received from the manufacturer. In this paper the influence of a deviation in the accuracy of the different parameters is studied by comparing simulation and measurement. The long term objective is a quantitative calibrated model for a complete ultrasound system. This includes a sensitivity study as presented here.

Statement of Contribution/Methods
The study alters 35 different model parameters which describe a 128 element convex transducer from BK Medical Aps. The changes are within ±20 % of the values supplied by the manufacturer, which are considered the zero reference (ZR). Simulations of a system consisting of a transmit unit, a five material layer transducer, and the FIELD II predicted pressure are performed by altering in turn the value of a single parameter in steps of 2 %. The remaining simulation parameters are held fixed at the ZR. The influence of the parameter change is determined by calculating the pressure and the intensity at a distance of 112 mm on an element’s center axis and comparing it with hydrophone measurements. These are performed with a water bath hydrophone setup using an Agilent MSO6014A oscilloscope that is set to average consecutive pulses 48 times for noise reduction of the hydrophone output. A commercial transmitter unit is used to drive the transducer with a 10 cycle tone burst at a frequency of 4.0 MHz and a maximum excitation amplitude of 31 volt. Results

Predictions using the ZR give a pressure pulse error (PPE) and an intensity error (IE) of 32 % and 23 %, respectively, relative to the measured. Altering the piezoelectric permittivity +12 % from ZR decreases the PPE to 30 % and the IE to 2 % relative to the measured. Changing the stiffness constant of the lens -4 % from ZR increases the PPE and the IE with 6 % and 1 %, respectively. Performing the same with the ceramic stiffness the PPE is lowered 1.5 % and the IE is lowered 12 %. Discussion and Conclusions
PPEs are found mainly to be sensitive to lens properties and piezoceramic properties, but minor sensitive to changes in matching layers. IEs are mainly sensitive to the piezoceramic properties. The study shows that minor changes can improve predictions significantly.

General information
Publication status: Published
Organisations: Biomedical Engineering, Department of Electrical Engineering, Center for Fast Ultrasound Imaging
Contributors: Bæk, D., Jensen, J. A., Willatzen, M.
Number of pages: 4
Publication date: 2009

Host publication information
Title of host publication: 2009 IEEE International Ultrasonics Symposium (IUS)
Publisher: IEEE
ISBN (Electronic): 978-1-4244-4390-1
Keywords: Transducer modeling, Field II, Sensitivity study, piezo
Electronic versions:
Baek 2009.pdf
DOIs:
10.1109/ULTSYM.2009.5441669
URLs:
http://ewh.ieee.org/conf/ius_2009/

Bibliographical note
Copyright 2009 IEEE. Personal use of this material is permitted. However, permission to reprint/republish this material for advertising or promotional purposes or for creating new collective works for resale or redistribution to servers or lists, or to reuse any copyrighted component of this work in other works must be obtained from the IEEE.
Source: orbit
Source-ID: 247993

Research output: Chapter in Book/Report/Conference proceeding › Article in proceedings – Annual report year: 2009 › Research › peer-review

Spurious Solutions in the Multiband Effective Mass Theory Applied to Low Dimensional Nanostructures

In this paper we analyze a long standing problem of the appearance of spurious, non-physical solutions arising in the application of the effective mass theory to low dimensional nanostructures. The theory results in a system of coupled eigenvalue PDEs that is usually supplemented by interface boundary conditions that can be derived from a variational formulation of the problem. We analyze such a system for the envelope functions and show that a failure to restrict their Fourier expansion coefficients to small k components would lead to the appearance of non-physical solutions. We survey the existing methodologies to eliminate this difficulty and propose a simple and effective solution. This solution is
demonstrated on an example of a two-band model for both bulk materials and low-dimensional nanostructures. Finally, based on the above requirement of small \( k \), we derive a model for nanostructures with cylindrical symmetry and apply the developed model to the analysis of quantum dots using an eight-band model.

**General information**
Publication status: Published
Organisations: University of Southern Denmark, Wilfrid Laurier University
Contributors: Lassen, B., Melnik, R. V. N., Willatzen, M.
Pages: 699-729
Publication date: 2009
Peer-reviewed: Yes

**Publication information**
Journal: Communications in Computational Physics
Volume: 6
Issue number: 4
ISSN (Print): 1815-2406
Ratings:
Scopus rating (2009): SJR 1.388 SNIP 1.627
Web of Science (2009): Indexed yes
Original language: English
Keywords: Effective envelope theory, Quantum confinement, Abrupt interfaces, Multiband models, \( k \) space, Fourier coefficients, Highly oscillatory integrals, Variational formulation, Coupled systems of PDEs, Multiple scales, Continuum and atomistic models, Eigenvalue problem, Interface boundary conditions, Band gap, Spurious solutions, Low dimensional semiconductor nanostructures
DOIs:
Source: dtu
Source-ID: n:oai:DTIC-ART:isi/246331675::30787
Research output: Contribution to journal › Review – Annual report year: 2009 › Research › peer-review

Crystal orientation effects on the piezoelectric field of strained zinc-blende quantum-well structures
A three-layered zinc-blende quantum-well structure is analyzed subject to both static and dynamic conditions for different crystal growth directions taking into account piezoelectric effects and lattice mismatch. It is found that the strain component \( S_{zz} \) in the quantum-well region strongly depends on the crystal growth direction and that a piezoelectric strain contribution exists in zinc blende as in wurtzite, albeit smaller. It is also found in the absence of loss effects that resonance frequencies, giving large strains in the structure, depend strongly on the crystal growth direction. Due to the higher symmetry of the zinc-blende structure, we find in a one-dimensional model that piezoelectric effects do not affect strain values for zinc-blende structures grown along the [001] direction in contrast to the corresponding wurtzite result. However, zinc-blende structures grown along a general crystal direction show important changes in strain and the electric distribution due to piezoelectric effects. The findings indicate the quantitative importance of a fully coupled model even for zinc blende, in particular when discussing electronic band structure and optoelectronic properties.

**General information**
Publication status: Published
Organisations: University of Southern Denmark
Contributors: Duggen, L., Willatzen, M., Lassen, B.
Number of pages: 6
Pages: 205323
Publication date: 2008
Peer-reviewed: Yes

**Publication information**
Journal: Physical Review B Condensed Matter
Volume: 78
Issue number: 20
ISSN (Print): 0163-1829
Ratings:
Scopus rating (2008): SJR 2.982 SNIP 1.516
Web of Science (2008): Indexed yes
Original language: English
Keywords: Physcis, Effect transistors, Gan, Parameters, Wurtzite
DOIs:
10.1103/PhysRevB.78.205323
Electromechanical effects in electron structure for GaN/AlN quantum dots

We study the impact of using the fully coupled electromechanical equations including piezoelectric effect and spontaneous polarization as compared to the semi-coupled approach, where the strain is solved first without piezoelectric coupling and then inserted into the equation for the electric potential. We show that for circular GaN/AlN quantum dots the fully coupled approach is needed for dots with a radius comparable to or larger than the height, however, when the radius is smaller than the height the semi-coupled approach is sufficient. We highlight this by studying the effect on the electronic structure using an effective mass approximation.

Electromechanical fields in GaN/AlN wurtzite quantum dots

We show that the governing equations for the electromechanical fields of wurtzite structures are axisymmetric, hence all electric- and mechanical-field solutions are axisymmetric as well and the original three-dimensional problem can be solved as a two-dimensional mathematical-model problem [1]. We present results of the combined influence of lattice mismatch, piezoelectric effects, and spontaneous polarization for wurtzite (WZ) structures consisting of a GaN quantum dot embedded in a AlN matrix.
Electronic properties of nanowire superlattices in the presence of strain and magnetic-field effects

A calculation of the effective electron barrier potential in quantum-wire superlattices subject to magnetic-field and strain effects is presented. It is shown that, besides the lateral-confinement contributions to the barrier potential emphasized by the authors in earlier work (Lew Yan Voon and Willatzen 2003 J. Appl. Phys. 93 9997; Lew Yan Voon et al 2004 J. Appl. Phys. 96 4660), strong contributions from strain (lattice mismatch) may be present as well. This is due to the fact that strain values can be several percent in heterostructures while electron deformation potentials are of the order of 10 eV. It is also shown that Landau and Landé magnetic-field contributions become important at magnetic fields of 10 T or higher. The driving force behind the lateral-confinement and the Landau magnetic-field contributions is the same, namely, the electron effective-mass difference in the two material constituents forming the superlattice structure; however, the dependences of the two contributions on lateral dimensions are inverse squared and squared, respectively. Similarly, the driving force behind the Landé magnetic-field contribution, being independent of lateral dimensions, is the difference in electron g factors between the two material constituents. We note that, for InAs/GaAs nanowire superlattices, it is possible to tune the effective barrier potential around 0 for cross-sectional dimensions of 5–6 nm by use of a magnetic field. Further, since the effective barrier potential is different for spin-up and spin-down polarized electrons, magnetic-field tuning can be used to separate spin-up and spin-down electrons in quantum-wire superlattices.

Electronic Properties of Semiconductor Nanowires

This paper provides a review of the state-of-the-art electronic-structure calculations of semiconductor nanowires. Results obtained using empirical k . ρ, empirical tight-binding, semi-empirical pseudopotential, and with ab initio, methods are compared. For conciseness, we will restrict our detailed discussions to free-standing plain and modulated nanowires. Connections to relevant experimental data, particularly band gaps and polarization anisotropy, will be made since these results depend crucially on the electronic properties. For completeness, a brief review on the synthesis of nanowires is included.
**Electron states in curved quantum structures with varying radius**

The influence of size and shape is investigated for quantum-dot electronic states and intra-band oscillator strengths adapting a method originally due to Stevenson. The present work solves the one-band envelope-function problem for conduction-band eigenstates in the framework of k·p theory using general curved coordinates. The eigenstates found are subsequently employed to express intra-band oscillator strengths and emphasis is given to the dependence of oscillator strengths on quantum-dot size and shape. We finally provide four simple examples.

**General information**

Publication status: Published
Organisations: Geometry, Department of Mathematics
Contributors: Gravesen, J., Willatzen, M.
Pages: 441-444
Publication date: 2008
Peer-reviewed: Yes

**Publication information**

Journal: Journal of Nanoscience and Nanotechnology
Volume: 8
Issue number: 1
ISSN (Print): 1533-4880
Ratings:
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.836 SNIP 0.653
Web of Science (2008): Indexed yes
Original language: English
Keywords: Semiconductor nanowires, Electronic properties, Optical properties, Theoretical methods
DOIs:
10.1166/jnn.2008.N03
Source: dtu
Source-ID: n:oai:DTIC-ART:swets/85439276::30806
Research output: Contribution to journal › Review – Annual report year: 2008 › Research › peer-review

**Electrostriction in GaN/AlN heterostructures**

A one-dimensional model accounting for electrostriction, lattice mismatch, piezoelectricity, and strain is presented with special emphasis on GaN/AlN heterostructures recently examined extensively in the literature. It is shown that electrostriction, being a second-order effect in the strain–electric field relation, plays a significant, sometimes dominant contribution subject to DC voltage conditions and externally imposed hydrostatic pressure. Model results are based on experimentally reported values for electrostriction coefficients in GaN.

**General information**

Publication status: Published
Organisations: University of Southern Denmark, Wright State University
Pages: 436-440
Publication date: 2008
Peer-reviewed: Yes

**Publication information**

Journal: Superlattices and Microstructures
Volume: 43
Issue number: 5-6
ISSN (Print): 0749-6036
Ratings:
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.937 SNIP 0.859
Web of Science (2008): Indexed yes
Original language: English
DOIs:
10.1016/j.spmi.2007.06.020
Source: orbit
Source-ID: 203104
Research output: Contribution to journal › Conference article – Annual report year: 2008 › Research › peer-review
Flow acoustics in solid-fluid structures.

The governing two-dimensional equations of a heterogeneous material composed of a fluid (allowed to flow in the absence of acoustic excitations) and a crystalline piezoelectric cubic solid stacked one-dimensionally (along the z direction) are derived and special emphasis is given to the discussion of acoustic group velocity for the structure as a function of the wavenumber component perpendicular to the stacking direction (being the x axis). Variations in physical parameters with y are neglected assuming infinite material homogeneity along the y direction and the flow velocity is assumed to be directed along the x direction. In the first part of the paper, the governing set of differential equations are derived as well as the imposed boundary conditions. Solutions are provided using Hamilton's equations for the wavenumber vs. frequency as a function of the number and thickness of solid layers and fluid layers in cases with and without flow (also the case of a position-dependent flow in the fluid layer is considered). In the first part of the paper, emphasis is given to the small-frequency case. Boundary conditions at the bottom and top parts of the full structure are left unspecified in the general solution but examples are provided for the case where these are subject to rigid-wall conditions (Neumann boundary conditions in the acoustic pressure). In the second part of the paper, emphasis is given to the general case of larger frequencies and wavenumber-frequency bandstructure formation. A wavenumber condition for an arbitrary set of consecutive solid and fluid layers, involving four propagating waves in each solid region, is obtained again using the monodromy matrix method. Case examples are finally discussed.

General information
Publication status: Published
Organisations: Department of Photonics Engineering
Contributors: Willatzen, M., Mads, M. V. D.
Pages: 15
Publication date: 2008
Peer-reviewed: Yes
Modelling nonlinear electro-mechanical effects in nano-heterostructures using domain-decomposition methods

In this work, a continuum-three-dimensional axi-symmetrical model for a nonlinear coupled multiphysics system is constructed accounting for self-consistency in electromechanical fields. A cylindrical GaN/AIN wurtzite nano-heterostructure is considered so as to simplify the mathematical problem to a two-dimensional model. To cope with the inherent discontinuity of the physical parameters and lattice mismatch across the interface, the domain-decomposition strategy is combined together with the Chebyshev spectral methods for the numerical analysis of the nonlinear problem. We report numerical results in the current presentation. We provide details on continuous mechanical and electric displacements and quantify jumps of discontinuities in the electric fields and strain distributions occurring across the interface between the two material. The importance of using a nonlinear model (with electrostriction) is investigated by comparison with a linear model (without electrostriction). We also point out significant differences qualitatively in the self-consistent electric fields and strains found using a two-dimensional and a one-dimensional model analysis. © 2008 Civil-Comp Press.

Nonlinearities in ultrasonic flow measurement

The governing equations of flow acoustics including nonlinearities are solved and analyzed in terms of ultrasonic flow-measurement properties. The effect of nonlinearities for sound propagation is expected to be most significant for gas-flow measurement applications as gas-sound speeds are much smaller while fluid flows generally are much higher in the corresponding case of liquid-flow measurement applications. The equation framework is applied to the case of a sinusoidal ultrasound transducer speed excitation at one location and detected by a receiver at another location. Flowmeter errors due to nonlinearities are highlighted in this work based on the well-known transit-time reciprocal transducer system setup. It is found that accounting for nonlinear effects leads to, for a given flowmeter configuration and in a large flow range, an almost constant error which can be calibrated out in applications.
Physics-Based Mathematical Models for Nanotechnology

PREFACE

In November 2007, some of the world’s best nanoscientists and nanoengineers met at the Banff Centre, where the Banff International Research Station hosted a workshop on recent developments in the mathematical study of the physics of nanomaterials and nanostructures. The Banff International Research Station for Mathematical Innovation and Discovery (BIRS) is a collaborative Canada–US–Mexico venture that provides an environment for creative interaction as well as the exchange of ideas, knowledge, and methods within the Mathematical Sciences, with related disciplines and with industry. The research station is located in a scenic part of Alberta, Canada and is supported by Canada’s Natural Science and Engineering Research Council (NSERC), the US National Science Foundation (NSF), Alberta’s Advanced Education and Technology, and Mexico’s Consejo Nacional de Ciencia y Tecnología (CONACYT). We would like to thank the BIRS and its sponsors for the given opportunity and the BIRS staff for their excellent support during the workshop. Nanotechnology is the study and application of phenomena at or below the dimensions of 100 nm and has received a lot of public attention following popular accounts such as in the bestselling book by Michael Crichton, Prey. It is an area where fundamental questions of applied mathematics and mathematical physics, design of computational methodologies, physical insight, engineering and experimental techniques are meeting together in a quest for an adequate description of nanomaterials and nanostructures which will profoundly influence our life in the 21st century and beyond. There are already hundreds of applications in daily life such as in cosmetics and the hard drives in MP3 players (the 2007 Nobel prize in physics was recently awarded for the science that allowed the miniaturization of the drives), delivering drugs, high-definition DVD players and stain-resistant clothing, but with thousands more anticipated. The focus of this interdisciplinary workshop was on determining what kind of new theoretical and computational tools will be needed to advance the science and engineering of nanomaterials and nanostructures. Thanks to the stimulating environment of the BIRS, participants of the workshop had plenty of opportunity to exchange new ideas on one of the main topics of this workshop—physics-based mathematical models for the description of low-dimensional semiconductor nanostructures (LDSNs) that are becoming increasingly important in technological innovations. The main objective of the workshop was to bring together some of the world leading experts in the field from each of the key research communities working on different aspects of LDSNs in order to (a) summarize the state-of-the-art models and computational techniques for modeling LDSNs, (b) identify critical problems of major importance that require solution and prioritize them, (c) analyze feasibility of existing mathematical and computational methodologies for the solution of some such problems, and (d) use some of the workshop working sessions to explore promising approaches in addressing identified challenges. The problems that were addressed at this meeting are of immense importance in determining such quantum-mechanical properties and the group of invited participants covered very well all the relevant disciplines in the cross-disciplinary research area: low-dimensional semiconductor nanostructures. Since the main properties of two-dimensional heterostructures (such as quantum wells) are now quite well understood, there has been a consistently growing interest in the mathematical physics community to further dimensionality reduction of semiconductor structures. Experimental achievements in realizing one-dimensional and quasi-zero-dimensional heterostructures have opened new opportunities for theory and applications of such low-dimensional semiconductor nanostructures. One of the most important implications of this process has been a critical re-examining of assumptions under which traditional quantum mechanical models have
been derived in this field. Indeed, the formation of LDSNs, in particular quantum dots, is a competition between the surface energy in the structure and strain energy. However, current models for bandstructure calculations use quite a simplified analysis of strain relaxation effects, although such effects are in the heart of nanostructure formation. By now, it has been understood that traditional models in this field may not be adequate for modeling realistic objects based on LDSNs due to neglecting many effects that may profoundly influence optoelectronic properties of the nanostructures. Among such effects are electromagnetic effects, including strain relaxation, piezoelectric effect, spontaneous polarization, and higher order nonlinear effects. Up to date, major efforts have been concentrated on the analysis of idealized, isolated quantum dots, while a typical self-assembled semiconductor quantum dot nanostructure is an array (or a molecule) of many individual quantum dots sitting on the same 'substrate' known as the wetting layer. Each such dot contains several hundred thousand atoms. In order to account for quantum effects accurately in a situation like that, attempts can be made to apply ab initio or atomistic methodologies, but then one would face a task of enormous computational complexity in solving a large-scale many-body problem. On the other hand, taking each quantum dot in isolation would lead to a manageable task for modern supercomputers, but accounting for the wetting layer even in the individual quantum dot model would increase the computational complexity of the problem in several times. As a result, the entire problem in its generality would be hardly feasible from a practical, routine-based simulation, point of view. Moreover, in calculating atomic positions the definitions of atomic forces that enter the Hamiltonian in such large scale atomic simulations are approximate by nature and a number of important coupled effects, such as piezoelectric, remain frequently outside the scope of the analysis. To attack the problem in hand, one needs to resort to some clever averaging over atomic scales. Such averaging can be achieved by empirical tight-binding, pseudopotential, and k.p approximations. These approximations are very important in further development of mathematical models for LDSNs due to the fact they are well suited for incorporating additional effects into the model, including strain, piezoelectric effects, spontaneous polarization, geometric and materials nonlinearities. These effects, despite their importance, have not been studied with vigor they deserve, in particular in the context of mathematical models for bandstructure calculations. There is a growing interest to such models as they should provide a key to better predicting optoelectromechanical properties of LDSNs. With anticipated new discoveries in theoretical and experimental analysis of LDSNs in the coming years, one of the main emphases of the workshop was on the models that would allow incorporating these effects consistently into the state-of-the-art models for LDSNs. From a mathematical point of view, many such models can be reduced to a large eigenvalue PDE problem (e.g., with the Hamiltonian accounting for the Burt-Foreman correction) coupled to strain and piezoelectric potential calculation. In its turn, in its general setting the problem of strain and piezoelectric potential calculation requires the solution of a nonlinear system of partial differential equation. A large experience in solving these two parts of the problem, independently of each other, has been already accumulated in the district communities of the researchers. This BIRS workshop effectively combined expertise of these research communities, summarized the state-of-the-art for modeling LDSNs and key challenges facing these communities, and explored ways to address those challenges in interdisciplinary team settings. The workshop brought together researchers working on different aspects of the analysis and modeling of LDSNs which require a concerted efforts of teams of researchers with close interactions between applied and pure mathematicians, physicists (theoreticians and experimentalists), computational scientists, and engineers. These scientific and engineering communities were represented in Banff by the researchers from Japan, Canada, the USA, Russia, France, Denmark, Germany, and the UK (further details can be found at http://www.m2netlab.wlu.ca/ldsn-banff/). We had four main plenary talks of one hour duration that gave state-of-the-art overviews of the subject from perspectives of applied mathematics (Professor Russel Caflisch of the University of California at Los Angeles), physics (Professor Antti-Pekka Jaaho of the Danish Technical University), and computational science and engineering communities (Professor Gerhard Klimeck of Purdue University), as well as from a point of view of experimentalists (Dr Gail Brown of the Materials Lab/Air Force Research Lab at Wright-Patterson AFB). These talks helped identify the areas where joint efforts needed to be directed to, and they set up the scene for further work during the workshop, including discussions at the workshop open problem sessions. All participants had time to present their research and a specific time was allocated for on-site demonstrations of software and explanations of tools applied in the LDSN analysis. This special issue provides a flavor of the problems discussed at the workshop. It contains 12 refereed papers. Additional information, including the abstracts of all presented talks, can be found at http://www.m2netlab.wlu.ca/ldsn-banff/. Using this opportunity, we would like to thank the referees of this volume for their time and efforts. Without their timely professional comments this volume would not have been made possible. In conclusion, we note that advances in mathematics, physics and computation of LDSNs, impact such seemingly distant applications as biotechnology and medicine, quantum information processing and optoelectronics. The research into LDSNs offered exciting new challenges that are intrinsically interdisciplinary in nature and should be addressed by a multidisciplinary team of applied mathematicians, theoretical and experimental physicists, engineers and computational scientists. We hope that we are able to pass this idea to the reader. Lok C Lew Yan Voon(Wright State University, OH, USA) Roderick Melnik(M2NeT Lab, Wilfrid Laurier University, ON, Canada) Morten Willatzen(MCI, University of Southern Denmark, Denmark)
Piezoelectric models for semiconductor quantum dots

The importance of fully coupled and semi-coupled piezoelectric models for quantum dots are compared. Differences in the strain of around 30% and in the electron energies of up to 30meV were found possible for GaN/AlN dots.

Plasmonic effects in dynamic tunable metal-dielectric composites

Sub-wavelength metal-dielectric-metal (MDM) composites support localized electromagnetic modes that are strongly confined in periodic structures. These modes can be controlled by tuning the shape of the composites as we demonstrated in previous works. Moreover, the Localized Surface Plasmon Resonance (LSPR) can be applied in new sensor applications. In this paper, we use the Finite-Difference Time-Domain (FDTD) method to study double-periodic metal-dielectric-metal composites and put emphasis to interactions with the dielectric cover layer. The numerical results demonstrate that variation of the refractive index (RI) of the cover layer as well as the layer thickness affect the LSPR response of the proposed MDM composite. The resonance-curve min/max groove period, the resonance-curve width, and the resonance-curve amplitudes from the MDM sensor output indicate that the proposed composite may find use as an effective sub-wavelength dielectric sensing optical component for photonic applications.
Testing of a one dimensional model for Field II calibration

Field II is a program for simulating ultrasound transducer fields. It is capable of calculating the emitted and pulse-echoed fields for both pulsed and continuous wave transducers. To make it fully calibrated a model of the transducer’s electro-mechanical impulse response must be included. We examine an adapted one dimensional transducer model originally proposed by Willatzen [9] to calibrate Field II. This model is modified to calculate the required impulse responses needed by Field II for a calibrated field pressure and external circuit current calculation. The testing has been performed with Pz27 piezoceramic discs from Ferroperm Piezoceramics A/S, Kvistgaard, Denmark. The transmitted acoustic pressures from two sets of each five disc samples with 10.08 mm diameters were measured in an automatic water bath needle hydrophone setup together with the current flow through the driving circuit. Resonance frequencies at 2.1 MHz and 4 MHz were applied. Two types of circuits were considered, one circuit with a simple resistance load of 47.5 Ohm and one with an example of a LR tuning circuit typically found in commercial transducers. The measurements were averaged 128 times and afterwards compared to the calibrated Field II program for 1, 4, and 10 cycle excitations. Two parameter sets were applied for modeling, one real valued Pz27 parameter set, manufacturer supplied, and one complex valued parameter set found in literature, Algueró et al. [11]. The latter implicitly accounts for attenuation. Results show that the combination of the model and Field II can calculate the pressure within −15 % to 5 % RMS error for long excitation bursts and 7 % to 23 % for short excitation bursts. Furthermore it is shown that current simulations can be done within 1 % to maximum 33 % RMS error, where best current simulations are found for 4 MHz long burst simulations and worst case is found for 2.1 MHz short bursts. Finally it is shown that maximum pressure deviation for the real parameter set and the complex parameter simulation is 3 % for pressure and 5.3 % for current.

General information
Publication status: Published
Organisations: Biomedical Engineering, Department of Electrical Engineering, Center for Fast Ultrasound Imaging
Contributors: Bæk, D., Jensen, J. A., Willatzen, M.
Pages: 1417-1420
Publication date: 2008

Nonlinear gain suppression in semiconductor lasers due to carrier heating

We present a simple model for carrier heating in semiconductor lasers from which the temperature dynamics of the electron and hole distributions can be calculated. Analytical expressions for two new contributions to the nonlinear gain coefficient epsilon are derived, which reflect carrier heating due to stimulated emission and free carrier absorption. In typical cases, carrier heating and spectral holeburning are found to give comparable contributions to nonlinear gain suppression. The results are in good agreement with recent measurements on InGaAsP laser diodes.

General information
Publication status: Published
Organisations: Teleteknisk Forskningslaboratorium, University of Copenhagen
Contributors: Willatzen, M., Uskov, A., Mørk, J., Olesen, H., Tromborg, B., Jauho, A.
Pages: 606-609
Publication date: 1991
Peer-reviewed: Yes
Projects:

**Photonic quantum technologies in structured environments**
Denning, E. V., PhD Student, Department of Photonics Engineering
Mørk, J., Main Supervisor
Iles-Smith, J., Supervisor
Willatzen, M., Supervisor
Grundforskningsfonden
01/02/2017 → 31/01/2020
Award relations: Photonic quantum technologies in structured environments
Project: PhD

**Ulineær Dynamik i Halvlederlasere**
Blaaberg, S., PhD Student, Department of Photonics Engineering
Rottwitt, K., Main Supervisor
Petersen, P. M., Supervisor
Tromborg, B., Supervisor
Mørk, J., Examiner
Willatzen, M., Examiner
Grisen, G., Examiner
Risø (Løn)
01/11/2002 → 30/01/2007
Award relations: Ulineær Dynamik i Halvlederlasere
Project: PhD

**Opto-elektroniske komponenter baseret på kvante-strukturer**
Berg, T. W., PhD Student, Department of Photonics Engineering
Mørk, J., Main Supervisor
Birkedal, D., Supervisor
Tromborg, B., Supervisor
Jauho, A., Examiner
Willatzen, M., Examiner
DTU-lønned stipendie
15/10/2000 → 06/09/2004
Award relations: Opto-elektroniske komponenter baseret på kvante-strukturer
Project: PhD

**k.p Theory of Two-Dimensional Materials**
Brems, M. R., PhD Student, Department of Photonics Engineering
Mørk, J., Supervisor
Willatzen, M., Main Supervisor
Grundforskningsfonden
01/07/2016 → 29/11/2019
Award relations: k.p Theory of Two-Dimensional Materials
Project: PhD

**Dark-field hyperlens: high-contrast subwavelength imaging in optics and acoustics**
Repän, T., PhD Student, Department of Photonics Engineering
Laurynenka, A., Main Supervisor
Arslanagic, S., Examiner
Volkov, V. S., Examiner
Busch, K., Examiner
Willatzen, M., Supervisor
Privatist
01/09/2015 → 03/04/2019
Award relations: Dark-field hyperlens: high-contrast subwavelength imaging in optics and acoustics
Project: PhD

Quantum Hall effects in nanostructured graphene
Jauho, A., Main Supervisor
Power, S., Supervisor
Willatzen, M., Examiner
Ferreira, M., Examiner
Harju, A., Examiner
Samfinansieret - Andet
01/04/2014 → 14/06/2017
Award relations: Quantum Hall effects in nanostructured graphene
Project: PhD

Non-linear ultrasound imaging
Du, Y., PhD Student, Department of Electrical Engineering
Jensen, J. A., Main Supervisor
Ferkinghoff-Borg, J., Examiner
Torp, H., Examiner
Willatzen, M., Examiner
Jensen, H., Supervisor
ErhvervsPhD-ordningen VTU
01/06/2008 → 28/09/2011
Award relations: Non-linear ultrasound imaging
Project: PhD

Slow light enhancement and limitations in periodic media
Grgic, J., PhD Student, Department of Photonics Engineering
Mortensen, N. A., Main Supervisor
Jauho, A., Supervisor
Mark, J., Supervisor
Lauryinenka, A., Examiner
De Rossi, A., Examiner
Willatzen, M., Examiner
Eksternt finansieret virksomhed
01/01/2009 → 19/04/2012
Award relations: Slow light enhancement and limitations in periodic media
Project: PhD

Negative Index Materials and Plasmonic Antennas Based Nanocoupler
Andryieuski, A., PhD Student, Department of Photonics Engineering
Lauryinenka, A., Main Supervisor
Malureanu, R., Supervisor
Breinbjerg, O., Examiner
Martin, O. J. F., Examiner
Willatzen, M., Examiner
Forskningsrådsfinansiering
01/06/2008 → 23/11/2011
Award relations: Negative Index Materials and Plasmonic Antennas Based Nanocoupler
Project: PhD

Modelling of Ultrafast Semiconductor Components
Nielsen, J. A., PhD Student, Department of Photonics Engineering
Mark, J., Main Supervisor
Yvind, K., Supervisor
Hvam, J. M., Examiner
Lenstra, D., Examiner
Willatzen, M., Examiner
Forskningsrådsfinansiering
01/01/2003 → 29/10/2007
Award relations: Modelling of Ultrafast Semiconductor Components
Project: PhD

Topology Optimization of Surface Acoustic Wave Devices
Dühring, M. B., PhD Student, Department of Mechanical Engineering
Sigmund, O., Main Supervisor
Jensen, J. S., Supervisor
Hansen, O., Examiner
Willatzen, M., Examiner
Maute, K., Examiner
DTU-lønnet stipendie
01/02/2006 → 21/10/2009
Award relations: Topology Optimization of Surface Acoustic Wave Devices
Project: PhD

Semiconductor Quantum Dot Devices for Optical Signal Processing
Chen, Y., PhD Student, Department of Photonics Engineering
Mørk, J., Main Supervisor
Poel, M. V. D., Supervisor
Öhman, F., Supervisor
Jeppesen, P., Examiner
Manning, R. J., Examiner
Willatzen, M., Examiner
DTU-lønnet stipendie
01/05/2007 → 29/09/2010
Award relations: Semiconductor Quantum Dot Devices for Optical Signal Processing
Project: PhD

Calibrated modelling of ultrasonic fields using Field II
Bæk, D., PhD Student, Department of Electrical Engineering
Jensen, J. A., Main Supervisor
Sams, T., Examiner
Persson, H. W., Examiner
Stepinski, T., Examiner
Willatzen, M., Supervisor
DTU-lønnet stipendie
01/08/2007 → 24/11/2010
Award relations: Calibrated modelling of ultrasonic fields using Field II
Project: PhD

Silicon-based Nanophotonic Structures for Controlling Light
Yang, L., PhD Student, Department of Photonics Engineering
Hvam, J. M., Main Supervisor
Laurynenka, A., Supervisor
Sigmund, O., Supervisor
Melloni, A., Examiner
Willatzen, M., Examiner
DTU-lønnet stipendie
01/11/2006 → 20/04/2011
Award relations: Silicon-based Nanophotonic Structures for Controlling Light
Project: PhD

Light-matter Interaction in Nano-structured Materials
Kristensen, P. T., PhD Student, Department of Photonics Engineering
Mørk, J., Main Supervisor
Lodahl, P., Supervisor
Breinbjerg, O., Examiner
Busch, K., Examiner
Willatzen, M., Examiner
DTU-lønnet stipendie
15/10/2006 → 21/04/2010
Award relations: Light-matter Interaction in Nano-structured Materials
Gain dynamics in quantum dot structures  
Magnúsdóttir, I., PhD Student, Department of Photonics Engineering  
Merk, J., Main Supervisor  
Bischoff, S., Supervisor  
Hvam, J. M., Supervisor  
Bjarklev, A. O., Examiner  
Willatzen, M., Examiner  
Grisen, G., Examiner  
DTU-lønnet stipendie  
01/09/1999 → 28/05/2003  
Award relations: Gain dynamics in quantum dot structures  
Project: PhD

Metal-dielectric-metal waveguides as ultrafast CMOS compatible modulators  
Babicheva, V., PhD Student, Department of Photonics Engineering  
Laurynenka, A., Main Supervisor  
Boltasseva, A., Supervisor  
Willatzen, M., Examiner  
Bozhevolnyi, S. I., Examiner  
Zayats, A. V., Examiner  
Forskningsrådsfinansiering  
15/10/2010 → 11/12/2013  
Award relations: Metal-dielectric-metal waveguides as ultrafast CMOS compatible modulators  
Project: PhD

Quantum Kinetics of charge carriers in quantum dots: applications to slow light and light amplification  
Houmark-Nielsen, J., PhD Student, Department of Micro- and Nanotechnology  
Jauho, A., Main Supervisor  
Merk, J., Supervisor  
Nielsen, T. R., Supervisor  
Mortensen, N. A., Examiner  
Kuhn, T., Examiner  
Pedersen, T. G., Examiner  
Willatzen, M., Supervisor  
Forskningsrådsfinansiering  
15/05/2006 → 20/01/2010  
Award relations: Quantum Kinetics of charge carriers in quantum dots: applications to slow light and light amplification  
Project: PhD

Optical Signal Processing using Four Wave Mixing  
Andersen, L. M., PhD Student, Department of Photonics Engineering  
Rottwitt, K., Main Supervisor  
Willatzen, M., Examiner  
Karlsson, L. M. I., Examiner  
Qian, L., Examiner  
Technical University of Denmark  
01/10/2011 → 26/01/2015  
Award relations: Optical Signal Processing using Four Wave Mixing  
Project: PhD

Development of nondestructive inspection tools for cultural heritage artefacts with 3D THz imaging  
Dandolo, C. L. K., PhD Student, Department of Photonics Engineering  
Jepsen, P. U., Main Supervisor  
Christensen, M. C., Supervisor  
Willatzen, M., Examiner  
Abraham, E., Examiner  
Gallerano, G. P., Examiner  
Technical University of Denmark  
01/09/2012 → 17/02/2016  
Award relations: Development of nondestructive inspection tools for cultural heritage artefacts with 3D THz imaging
**All-optical transistor / Optisk transistor**  
Heuck, M., PhD Student, Department of Photonics Engineering  
Merk, J., Main Supervisor  
Kristensen, P. T., Supervisor  
Willatzen, M., Examiner  
Manning, R. J., Examiner  
Santaguestina, M., Examiner  
Technical University of Denmark  
01/01/2010 → 15/08/2013  
Award relations: All-optical transistor / Optisk transistor  
Project: PhD

**Modeling of Coupled Nano-Cavity Lasers**  
Skovgård, T. S., PhD Student, Department of Photonics Engineering  
Mørk, J., Main Supervisor  
Gregersen, N., Supervisor  
Abram, I., Examiner  
Willatzen, M., Examiner  
Technical University of Denmark  
01/10/2008 → 19/04/2012  
Award relations: Modeling of Coupled Nano-Cavity Lasers  
Project: PhD

**Extreme nonlinear THz optics of metals**  
Tarekegne, A. T., PhD Student, Department of Photonics Engineering  
Jepsen, P. U., Main Supervisor  
Iwasczuk, K., Supervisor  
Willatzen, M., Examiner  
Johnston, M. B., Examiner  
Kampfrath, T., Examiner  
Technical University of Denmark  
15/03/2014 → 23/08/2017  
Award relations: Extreme nonlinear THz optics of metals  
Project: PhD

**QUEENS: QUantum dot Energy level Engineering for laser applications on InP and Si platforms**  
This project is dedicated to the research of quantum dot (QD) epitaxial growth on both indium phosphide (InP) and silicon (Si) based platforms with the aim of creating superior gain material emitting in the 1.5-1.6 μm wavelength range. The majority of the proposed research is quite fundamental but will have noticeable impact to device applications for our everyday life in the near future. Diverse areas like telecommunication, optical coherence tomography including medical applications, sensing, computer and network clock-distribution, THz generation, and metrology can benefit from the materials investigated.  
The projected research covers two directions. The first is the development of QDs which possess desired electronic and optical properties in the InP based material system, i.e. tailoring the energy level structure and wave functions in the dots. Manipulating the shape, chemical composition and surroundings of the nanostructures is the key to achieving the set goals. In the frame of the project I will implement two different approaches to design and grow high optical quality arrays of QDs. Those approaches are self-assembled quantum dot growth and selective area growth using block copolymer lithography. The second direction of the research is the deployment of the highly efficient QD gain material to a silicon platform. The development of epitaxial growth technology of III-V materials on Si combines the benefits of high optical quality III-V QD gain material with low cost silicon photonics, which is a key platform to push towards increased integration, higher speed and lower energy consumption.  
Semenova, E., Project Manager, Department of Photonics Engineering, Nanophotonic Devices  
Yvind, K., Project Participant, Department of Photonics Engineering, Nanophotonic Devices  
Almdal, K., Project Participant, Center for Nanostructured Graphene, Department of Micro- and Nanotechnology, Amphiphilic Polymers in Biological Sensing  
Viazmitnov, D., PhD Student, Department of Photonics Engineering, Nanophotonic Devices  
Shikin, A., PhD Student, Department of Photonics Engineering, Nanophotonic Devices  
Kadkhodazadeh, S., Project Participant, Center for Electron Nanoscopy, DTU Danchip  
Ottaviano, L., Project Participant, Department of Photonics Engineering, Nanophotonic Devices  
Willatzen, M., Project Participant, Department of Photonics Engineering  
Barrettin, D., Project Participant, UNICUSANO Università degli Studi Nicola Cusano - Telematica Roma, Rome -Italy
Activities:

Presentation title: "A valence force field-Monte Carlo algorithm for quantum dot growth modeling".
Period: 24 Jul 2017 → 28 Jul 2017
Shima Kadkhodazadeh (Other)
Elizaveta Semenova (Other)
Morten Willatzen (Other)
Alessandro Pecchia (Other)
Matthias Auf de Maur (Other)
Daniele Barettin (Speaker)
Center for Electron Nanoscopy
DTU Danchip
Department of Photonics Engineering
Nanophotonic Devices
Centre of Excellence for Silicon Photonics for Optical Communications
Degree of recognition: International
Documents:
nusod17paper59
Links:

Related event

17th International Conference on Numerical Simulation of Optoelectronic Devices (NUSOD17)
24/07/2017 → 28/07/2017
Kgs. Lyngby, Denmark
Activity: Talks and presentations › Conference presentations