RIGA TECHNICAL UNIVERSITY

Aleksei Kuznetsov

HYBRID ANAPOLE STATES AS A PLATFORM FOR NOVEL OPTICAL DEVICES

Summary of the Doctoral Thesis

RTU Press
Riga 2024

RIGA TECHNICAL UNIVERSITY
Faculty of Computer Science, Information Technology and Energy
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Scientific supervisor
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RTU Press
Riga 2024

Kuznetsov, A. Hybrid Anapole States as a Platform
for Novel Optical Devices. Summary of the Doctoral
Thesis. Riga: RTU Press, 2024, 35 p.

Published in accordance with the decision of the Promotion Council
"P- 08" of 24 May 2024,
Minutes No. 31.

This work was supported by the European Social Fund within Project No. 8.2.2.0/20/I/008, “Strengthening of PhD students and academic personnel of Riga Technical University and BA School of Business and Finance in the strategic fields of specialization” of the Specific Objective 8.2.2 “To Strengthen Academic Staff of Higher Education Institutions in Strategic Specialization Areas” of the Operational Programme “Growth and Employment”.

The research was supported by the Doctoral Grant programme of Riga Technical University.

NATIONAL DEVELOPMENT PLAN 2020

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https://doi.org/10.7250/9789934371042
ISBN 978-9934-37-104-2 (pdf)

DOCTORAL THESIS PROPOSED TO RIGA TECHNICAL UNIVERSITY FOR THE PROMOTION TO THE SCIENTIFIC DEGREE OF DOCTOR OF SCIENCE

To be granted the scientific degree of Doctor of Science (Ph. D.), the present Doctoral Thesis has been submitted for defence at the open meeting of RTU Promotion Council on 6 September 2024 at the Faculty of Computer Science, Information Technology and Energy (FCSITE) of Riga Technical University (RTU), 12 Azenes Str., Room 201.

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DECLARATION OF ACADEMIC INTEGRITY

I hereby declare that the Doctoral Thesis submitted for review to Riga Technical University for promotion to the scientific degree of Doctor of Science (Ph. D.) is my own. I confirm that this Doctoral Thesis has not been submitted to any other university for promotion to a scientific degree.

Aleksei Kuznetsov ……………………………. (signature)

Date: ………………………

The Doctoral Thesis has been prepared as a thematically united collection of scientific publications. It comprises 12 scientific articles and publications in conference proceedings proceeding indexed in SCOPUS and WoS databases. The publications are written in English and indexed in SCOPUS, WoS databases; their total volume/number of pages is 95 pages.

CONTENTS

LIST OF ABBREVIATIONS

A

a-Si – Hydrogenated Amorphous Silicon

C

CMOS – Complementary Metal–Oxide–Semiconductor

D

DM – Dipolar Channel Scattering Maxima

E

ED – Electric Dipole

EQ – Electric Quadrupole

F

FDTD – Finite Difference Time Domain Method

FEM – Finite Element Method

H

HA – Hybrid Anapole

M

MD – Magnetic Dipole

MQ – Magnetic Quadrupole

P

PD – Positional Disorder

PML – Perfectly Matched Layer

Q

QNM – Quasinormal Mode

Quasi-BIC – Quasi-Bound States in Continuum

S

SCS – Scattering Cross-Section

SEM – Scanning Electron Microscope

LIST OF SYMBOLS

δ – Kronecker delta
n – unit vector
r – position, m
i – imaginary unit
λ – wavelength, m
c – speed of light in vacuum, m/s
k_0 – wave number, 1/m
k_d – wave number in the environment, 1/m
j_n – n-order spherical Bessel function
p – electric dipole moment, C/m^2
m – magnetic dipole moment, $A \cdot m^2$
Q^e– electric quadrupole moment, $C \cdot m^2$
Q^m – magnetic quadrupole moment, $A \cdot m^3$
σ_{sca} – scattering cross-section, m^2
σ_{eff} – effective scattering cross-section, m^2
$C_{sca}{}^p$ – scattering cross-section of an electric dipole, m^2
$C_{sca}{}^m$ – scattering cross-section of a magnetic dipole, m^2
$C_{sca}{}^{Qe}$ – scattering cross-section of an electric quadrupole, m^2
$C_{sca}{}^{Qm}$ – scattering cross-section of a magnetic quadrupole, m^2
$n(\lambda)$ – real part of the refractive index
$k(\lambda)$ – imaginary part of the refractive index
n_{env} – refractive index of the environment
n_{sub} – refractive index of the substrate
ε_0 – dielectric constant of vacuum
ε_d – dielectric constant of the environment
S_L – lattice unit cell area, m^2
D – lattice constant, m
s – distance between the walls of meta-atoms, m
J_ω – induced electric current density, A/m^2
E_{inc} – amplitude of the electric field of the incident wave, V/m
E_0 – electric field of a normally incident plane wave, V/m
H – height of the cylinder/cone, m
R_{cyl} – radius of the cylinders, m
R_{top} – top radius of the cone, m
R_{bottom} – bottom radius of the cone, m
T – transmission coefficient
t – electric field transmission coefficient
R – reflection coefficient
r – electric field reflection coefficient
A – absorption coefficient

I_{noise} – power obtained (noise) by the spectrometer without any incident light, W/m^2

$I_{substrate}$ – power obtained by the spectrometer when the light is incident on the substrate, W/m^2

$I_{metasurface}$ – power obtained by the spectrometer when the light is incident on the metasurface with the substrate, W/m^2

1. OVERVIEW

1.1. Introduction

In recent years, all-dielectric nanophotonics have begun to develop at a rapid pace [1]–[6]. The popularity of research into high refractive index subwavelength structures is due to the ability to control light at the nanoscale without thermal loss, unlike plasmonic structures [7]–[9]. By carefully tuning the geometry of nanoscatterers and the dispersion of materials, it is possible to excite both electrical and magnetic resonances [9]–[12]. For example, using a combination of resonances makes it possible to obtain the Kerker effects [13]–[19]. Such single particles are called meta-atoms, and their structure is called a metasurface [20]–[22]. With the help of such structures, it is possible to obtain effects that were previously inaccessible with the help of "conventional" materials, for example, artificial magnetism [23]–[25], non-radiative sources [26]–[28], supercavity modes and bound states in the continuum (BIC) [29]–[32], efficient generation of second and third harmonics [33]–[35], sensors [36], [37] or spin-orbit transformation [38], [39].

An intriguing direction in dielectric nanophotonics has become the existence of the so-called non-radiative anapole regime, which was first shown in [40]. The **anapole state** arises due to the destructive interference of the electric and toroidal dipole moments, which causes the particle in the anapole regime to become "invisible" but simultaneously non-trivial fields inside [18], [41]–[47]. Based on the anapole, it has already been proposed to obtain enhanced generation of the second and third harmonics [34], [35], giant photothermal nonlinearities [48], and "dark" lasers [49]. More recently, the next step in anapole electrodynamics, the **hybrid anapole** (HA) regime, has been proposed. This regime represents the simultaneous destructive interference of all dominant multipole moments with their toroidal analogues up to the magnetic quadrupole moment. Hybrid anapoles were first discussed in [50], and only recently, hybrid anapoles emerged in dielectric nanocylinders, which was theoretically shown and experimentally demonstrated in [51]. It was shown that hybrid anapole states are superior to conventional anapoles in both scattering suppression and electromagnetic energy storage. Today, hybrid anapole is gaining popularity and becoming a promising area for research [52]–[55].

As part of this Doctoral Thesis, previously unstudied metasurfaces consisting of silicon particles in a hybrid anapole state were investigated. It was shown analytically and numerically that ultra-weak interaction with the environment naturally leads to unit transmittance without optical phase change. The optical properties of these structures were studied, including their interaction with the environment and how the parameters of the metasurface can be adjusted to preserve its optical properties. Additionally, a method for controlling the optical signal passing through such a structure was demonstrated. For the first time, an anapole state was obtained for particles in the shape of a truncated cone, and the dependence of the anapole state on the conicity was studied. This finding significantly simplifies and reduces the cost of producing new-generation photonic structures.

1.2. Rationale

Directional Huygens sources are of greatest interest in the development of metasurfaces with the ability to control light on the nanoscale. Due to the possibility of simultaneous overlap of electrical and magnetic resonances with different parities, it becomes possible to vary the optical phase of the transmitted radiation with unit transmission [21], [56]–[58]. As a result of the research, a number of applications have already been proposed, such as ultra-thin metalenses [59]–[61], dynamic transmission control [62], anomalous refraction [56], [63], [64], beam steering [65], holograms [66]–[70] and broadband Huygens elements [71].

Huygens metasurfaces must overcome fundamental constraints typically described by the coupling of structural elements [56], [72] to achieve complete control over light manipulation. Meta-atoms in an array interact with each other even at a distance of the order of a wavelength. This significantly complicates the design process, including the design of optical phase changes on individual structural elements. A number of works in metaoptics help solve this problem, for example, through careful optimization of the supercell [73]. This allows the situation to be improved, but the issue of optical phase mapping on individual meta-atoms remained open. All elements of metasurfaces must be carefully adjusted in their position in the structure to minimize interaction. In structures, special attention must be paid to the lattice period, substrate materials, and manufacturing errors – these are all degrees of freedom that interfere with the production of structures. For the reasons stated above, the effectiveness of such devices can be fundamentally limited [72].

For the structures described, highly symmetrical particles with simple geometries, such as spheres, cubes or cylinders, are usually used as meta-atoms, each of which supports a limited set of multipole interactions depending on size, material and aspect ratio, therefore often as auxiliary elements for the configuration of the multipole composition use complications, for example, multilayer structures [74]–[78].

Unfortunately, modern methods for producing dielectric metasurfaces have a number of disadvantages. It is challenging to obtain a metasurface with ideal cylinders; most cylinders have a slight lateral slope [79]–[81], leading to significant property deviations.

This Doctoral Thesis proposes a new concept to create transparent metasurfaces using silicon metasurfaces in a hybrid anapole state. The properties of metasurfaces based on hybrid anapole were studied in detail. The multiresonant nature of the hybrid anapole allows the transmitted optical phase to be varied over a wide spectral and geometric range. Most importantly, unlike Huygens sources, the coupling between particles is practically negligible. Thus, the hybrid anapole particle approaches the ideal of a "true" meta-atom. This capability has been demonstrated, ultra-compact silicon arrays have been developed with particle wall spacing equal to 1/8 of the incident wavelength in the visible, and disordered metasurfaces have been studied that exhibit behavior identical to their periodic counterparts. The effect of the substrate was studied, and transmission window conservation was demonstrated when metasurfaces were applied to a wide range of dielectric materials, potentially facilitating their integration into a chip. As a proof-of-concept application, it was demonstrated that it was possible to modulate the optical phase of an ultrafast Gaussian pulse transmitted with unit efficiency through a highly disordered metasurface deposited on a glass substrate based solely on the optical response of the periodic array. Finally, the influence of conicity on the properties of a hybrid anapole is shown, and for the first time, a hybrid anapole state has been obtained in silicon meta-atoms in the form of truncated cones, which greatly facilitates, simplifies and reduces the cost of fabrication of such structures.

1.3. The aim and theses of the Doctoral Thesis

Summarizing the facts mentioned above about the directions of development of novel optical devices for a wide range of applications based on nanostructured elements, the following **aim of the Doctoral Thesis is proposed:**

To study new optical effects caused by the interaction of high-index weakly absorbing nanoparticles and metasurfaces in a hybrid anapole state with light and to develop models of nanostructural elements for subsequent creation of qualitatively new photonic devices.

To achieve the stated aim, the following theses were proposed:

1. The hybrid anapole state enables the design of ultra-dense silicon metasurfaces without strict adherence to the arrangement order of nanoparticles on diverse substrates, achieving nearly perfect transmission and zero optical phase shift of transmitted radiation.
2. Silicon metasurfaces in the hybrid anapole state can control the phase of optical signals transmitted through the structure under continuous and ultrafast femtosecond pulse irradiation regimes.
3. The hybrid anapole state can be achieved in silicon truncated cone nanoscatterers with symmetry breaking along the main axis.

1.4. The tasks of the Doctoral Thesis

To achieve the set goal of the dissertation and to prove the proposed theses, it is necessary to perform the following **tasks:**

1. To demonstrate nearly perfect transmission and zero optical phase shift of radiation passing through silicon metasurfaces consisting of cylindrical meta-atoms in a hybrid anapole state utilizing numerical methods alongside experimental measurements.
2. To investigate the interaction between silicon metasurfaces in a hybrid anapole state and diverse substrates characterized by varying refractive indices and to show the absence of interaction of such metasurfaces with the surrounding environment.
3. To explore the influence of the distance between particles in a hybrid anapole state on metasurface optical properties and to demonstrate the absence of interaction among meta-atoms during the design of ultra-dense metasurfaces.
4. To study the influence of the disorder of metasurface elements on the optical properties of the structure in a hybrid anapole state and to show the possibility of

maintaining transparency of the structure without strict adherence to the arrangement order of nanoparticles on the substrate.

5. To develop a method for controlling the phase of optical radiation passing through silicon metasurfaces composed of cylindrical meta-atoms in a hybrid anapole state by changing the geometric parameters of meta-atoms in a continuous irradiation regime.
6. To show the possibility of modulation using ultrafast femtosecond pulses passing through a metasurface in a hybrid anapole state by changing the geometric parameters of nanoscatterers with the possibility of a chaotic arrangement of meta-atoms.
7. To study the influence of the conicity of silicon nanoparticles on the resulting optical properties of nanoscatterers in a hybrid anapole state.

1.5. Research methods

To perform the tasks outlined in the Doctoral Thesis and to analyze the problems, mathematical calculations, numerical simulations, and experimental measurements were used. Numerical simulations were implemented in COMSOL Multiphysics, Ansys Lumerical, MATLAB, and Wolfram Mathematica.

Scientific experiments described in the Doctoral Thesis and their results were carried out and discussed at:

- Nanophotonics Research Laboratory (NANO-Photon Lab.) at the Institute of Photonics, Electronics and Telecommunications (IPET) of Riga Technical University (RTU), Riga, Latvia.
- Dynamics of Nanostructures' Laboratory at Tel Aviv University (TAU), Tel Aviv, Israel.
- Advanced Optics and Photonics Laboratory, Nottingham Trent University, Nottingham, UK.
- School of Optics and Photonics, Beijing Institute of Technology, Beijing, China.
- QuasiLab, ITMO University, Saint Petersburg, Russia.
- University of Graz, Graz, Austria.

1.6.Publications and approbation

The results of the author's Doctoral Thesis are presented in **12 scientific articles and conference proceedings** indexed in SCOPUS and WoS databases.

1. **Kuznetsov, A. V.,** Canós Valero, A., Tarkhov, M., Bobrovs, V., Redka, D., Shalin, A. S. "*Transparent hybrid anapole metasurfaces with negligible electromagnetic coupling for phase engineering*," Nanophotonics, Vol. 10, no. 17, pp. 4385–4398, 18 October **2021**.

2. **Kuznetsov, A. V.,** Canós Valero, A., Shamkhi, H. K., Terekhov P., Ni, X., Bobrovs V., Rybin M. V., Shalin A. S. "*Special scattering regimes for conical all-dielectric nanoparticles*, " Scientific Reports, Vol. 12, p. 21904, 30 November **2022**.
3. **Kuznetsov, A. V.,** Canos Valero, A., Shalin, A. S. "*Optical properties of a metasurface based on silicon nanocylinders in a hybrid anapole state*, " Proceedings of the 5th International conference on metamaterials and nanophotonics "METANANO 2020", Vol. 2300, No. 1, p. 020075, online, December **2020**.
4. **Kuznetsov, A. V.,** Canos Valero, A. "*Non-Huygens transparent metasurfaces based on the novel Hybrid anapole state*, " Proceedings of the 6th International conference on metamaterials and nanophotonics "METANANO 2021", Vol. 2015, No. 1, p. 012079, online, November **2021**.
5. **Kuznetsov, A. V.,** Canos Valero, A., Terekhov, P. D., Shamkhi, H. K. "*Various multipole combinations for conical Si particles*," Proceedings of the 6th International conference on metamaterials and nanophotonics "METANANO 2021", Vol. 2015, No. 1, p. 012080, online, November **2021**.
6. Shalin, A. S., **Kuznetsov, A. V.,** Bobrovs, V., Valero, A. C. "*Novel Hybrid anapole state and non-Huygens' transparent metasurfaces*," Proceedings of the 4th International Smart NanoMaterials Conference 2021: Advances, Innovation and Applications "SNAIA 2021", Vol. 2172, No. 1, p. 012001, Paris, France, February **2022**.
7. Terekhov, P. D., **Kuznetsov, A. V.,** Canos Valero, A., Shamkhi, H. K., Ni, X., Bobrovs, V., Rybin, M. V. Shalin A. S. "*Various Scattering Regimes of Truncated Cone Particles*," Proceedings of the CLEO: Applications and Technology 2023, San Jose, USA, 7–12 May **2023**.
8. **Kuznetsov, A. V.,** Bobrovs, V. "*Existence of the Hybrid Anapole for Si Conical Nanoparticles*," Proceedings of 12th International Conference on Computer Science Online Conference "CSOC 2023", Lecture Notes in Networks and Systems, Vol. 772, pp. 397–401, online, 3–5 April **2023**.
9. **Kuznetsov, A. V.,** Bobrovs, V. "*Superscattering Regime for Si Conical Nanoparticles for the Different Directions of Excitation*," Proceedings of 12th International Conference on Computer Science Online Conference "CSOC 2023", Lecture Notes in Networks and Systems, Vol. 723, pp. 254–258, online, 3–5 April **2023**.
10. Babich, N., **Kuznetsov, A.,** Bobrovs, V., Kislov, D. "*Optomechanical Manipulation of Nanoparticles in Hybrid Anapole State*," Proceedings of 12th International Conference on Computer Science Online Conference "CSOC 2023", Lecture Notes in Networks and Systems, Vol. 723, pp. 237–243, online, 3–5 April **2023**.
11. **Kuznetsov, A. V.,** Bobrovs, V. "*Transverse Kerker Effects in All-Dielectric Conical Nanoparticles,*" Proceedings of the 7th Computational Methods in Systems and Software 2023 (CoMeSySo2023) conference, Vol 909, pp. 278–281, online, **2024**.

12. **Kuznetsov, A. V.,** Bobrovs, V. "*Generalized Kerker Effects in All-Dielectric Conical Nanoparticles*," Proceedings of the 7th Computational Methods in Systems and Software 2023 (CoMeSySo2023) conference, Vol. 909, pp. 283–287, online, **2024**.

Results of the Doctoral Thesis have been presented at **15 international conferences.**

1. **Kuznetsov, A. V.,** Canos Valero, A., Shalin, A. S. "*Investigation of the optical properties of a metasurface based on silicon nanocylinders in a hybrid anapole state*," 3rd School on Advanced Light-Emitting and Optical Materials "SLALOM 2020", Saint Petersburg, Russia, 29–30 June **2020**.
2. **Kuznetsov, A. V.,** Canos Valero, A., Shalin, A. S. "*Optical properties of a metasurface based on silicon nanocylinders in a hybrid anapole state*," 5th International conference on metamaterials and nanophotonics "METANANO 2020", online, December **2020**.
3. **Kuznetsov, A. V.,** Canos Valero, A., Terekhov, P. D., Shalin, A. S. "*Study of the optical properties of a metasurface based on silicon nanocylinders in a hybrid anapole state*," International scientific conference of students, graduate students and young scientists "Lomonosov-2020", online, 10–27 November **2020**.
4. **Kuznetsov, A. V.,** Canos Valero, A., Terekhov, P. D., Shamkhi,H. K., Shalin, A. S. "*Investigation of various multipole combinations of silicone conical nano-scatterers*," 4th School on Advanced Light-Emitting and Optical Materials "SLALOM 2021", online, 28–30 June **2021**.
5. **Kuznetsov, A. V.,** Canos Valero, A., Terekhov, P. D., Shamkhi, H. K., Shalin, A. S. "*Investigation of various multipole combinations of silicone conical nano-scatterers*," Summer School on Photonics of 2D materials "METANANO SCHOOL 2021", Saint Petersburg, Russia, 19–23 July **2021**.
6. **Kuznetsov, A. V.,** Canos Valero, A. "*Non-Huygens transparent metasurfaces based on the novel Hybrid anapole state*," 6th International conference on metamaterials and nanophotonics "METANANO 2021", online, November **2021**.
7. **Kuznetsov, A. V.,** Canos Valero, A., Terekhov, P. D., Shamkhi, H. K. "*Various multipole combinations for conical Si particles*," 6th International conference on metamaterials and nanophotonics "METANANO 2021", online, November **2021**.
8. Shalin, A. S., **Kuznetsov, A. V.,** Bobrovs, V., Valero, A. C. "*Novel Hybrid anapole state and non-Huygens' transparent metasurfaces*," 4th International Smart NanoMaterials Conference 2021: Advances, Innovation and Applications "SNAIA 2021", Paris, France, February **2022**.
9. Terekhov, P. D., **Kuznetsov, A. V.,** Canos Valero, A., Shamkhi, H. K., Ni, X., Bobrovs, V., Rybin, M. V., Shalin, A. S. "*Various Scattering Regimes of Truncated Cone Particles*," CLEO: Applications and Technology 2023, San Jose, USA, 7–12 May **2023**.
10. **Kuznetsov, A. V.,** Bobrovs, V., Shalin, A. S. "*Quasi-BIC on a Hybrid anapole regime in silicon metasurfaces*," The 9th International Conference on Antennas and Electromagnetic Systems "AES 2023", Torremolinos, Spain, 5–8 June **2023**.

11. **Kuznetsov, A. V.,** Bobrovs, V. "*Existence of the Hybrid Anapole for Si Conical Nanoparticles*," 12th International Conference on Computer Science Online Conference "CSOC 2023", Lecture Notes in Networks and Systems, online, 3–5 April **2023**.
12. **Kuznetsov, A. V.,** Bobrovs, V. "*Superscattering Regime for Si Conical Nanoparticles for the Different Directions of Excitation*," 12th International Conference on Computer Science Online Conference "CSOC 2023", online, 3–5 April **2023**.
13. Babich, N., **Kuznetsov, A.,** Bobrovs, V., Kislov, D. "*Optomechanical Manipulation of Nanoparticles in Hybrid Anapole State*," 12th International Conference on Computer Science Online Conference "CSOC 2023", online, 3–5 April **2023**.
14. **Kuznetsov, A. V.,** Bobrovs, V. "*Transverse Kerker Effects in All-Dielectric Conical Nanoparticles*," 7th Computational Methods in Systems and Software 2023 (CoMeSySo2023) conference, online, **2024**.
15. **Kuznetsov, A. V.,** Bobrovs, V. "*Generalized Kerker Effects in All-Dielectric Conical Nanoparticles*," 7th Computational Methods in Systems and Software 2023 (CoMeSySo2023) conference, online, **2024**.

1.7. Structure of the Doctoral Thesis

The Thesis is prepared as a thematically unified set of publications based on the developed theoretical models of novel optical devices for a wide range of applications.

CHAPTER 1: OVERVIEW. This chapter describes the scope of the Doctoral Thesis. It formulates the main research hypotheses and the importance of the novelty of research related to the silicon metasurface in hybrid anapole. This chapter also presents a brief description of the Thesis structure. The list of publications and presentations at international conferences is also displayed in this chapter.

CHAPTER 2: METHODOLOGY. This chapter describes the basic methods and tools used for modelling and explaining the effects that occur during the interaction of radiation with metasurfaces in a hybrid anapole state. Three main stages are outlined.

CHAPTER 3: MAIN RESULTS. This chapter represents publications which reflect the main results obtained during the research and application of the optical properties of metasurfaces in hybrid anapole state. The results of the Doctoral Thesis were published in **12** publications indexed in the Scopus and WoS databases, including **two** articles in highly rated international scientific journals; the total Impact Factor is **13.3** (5-year Journal Impact Factor) with a total of **43** (13/03/2024) citations in journals indexed in Scopus.

CHAPTER 4: FINAL REMARKS. This chapter presents the main conclusions and discusses the challenges and their solutions regarding theoretical and practical applications of metasurfaces in the hybrid anapole state.

2. METHODOLOGY

The chapter provides the main methods for studying the optical properties of the structures described in the Doctoral Thesis.

Currently, the main tools for studying the optical properties of nanostructures are numerical methods (e.g., finite element methods, discrete dipole approximation, finite difference methods, etc.). These methods primarily involve solving Maxwell's partial differential equations [82] and calculating electric and magnetic fields at each point in the system. They take into account all geometric and material characteristics of the structure under consideration, such as the shape of particles, their size, spatial position, structure of the incident beam, etc. These methods are implemented in commercial scientific software products (COMSOL Multiphysics, Ansys Lumerical, CST, etc.) and have been rigorously tested by the global scientific community. The results of their application are widely presented in the literature.

However, although numerical methods have proven excellent in engineering calculations, they cannot compete with analytical approaches when it is necessary to understand the physics of a phenomenon and, most importantly, to determine the range of parameters in which unusual new phenomena can be observed. Therefore, in addition to the aforementioned numerical methods, this dissertation employs multipole decomposition, which is convenient for studying anapole states of various orders [83].

The method of multipole decomposition of the reflection and transmittance coefficients of the metasurface was also used, allowing for a qualitative analysis of the optical response of the system [10].

In addition to multipole analysis, the method of searching for eigenmodes in the COMSOL Multiphysics optical module was also used. This method is based on solving Maxwell's equations for electromagnetic fields in structures. It involves using the wave equation and boundary conditions to determine the propagation of electromagnetic waves in optical systems. The method relies on the numerical solution of the full Maxwell’s equations, including those for electric and magnetic fields. To find eigenmodes, one must solve the eigenvalue problem, which depends on the type of structure. Solving these equations allows for determining the characteristics of the eigenmodes, such as frequency and field distribution.

Thus, the method encompasses the physical principles of wave optics and mathematical techniques for the numerical solution of Maxwell's equations, enabling the study and optimization of electromagnetic fields in optical structures.

The primary material for nanoscatterers was the dispersion of the refractive index, measured experimentally and chosen as a high-index dielectric material for particles and metasurfaces in the Doctoral Thesis (unless otherwise indicated) (Fig. 2.1).

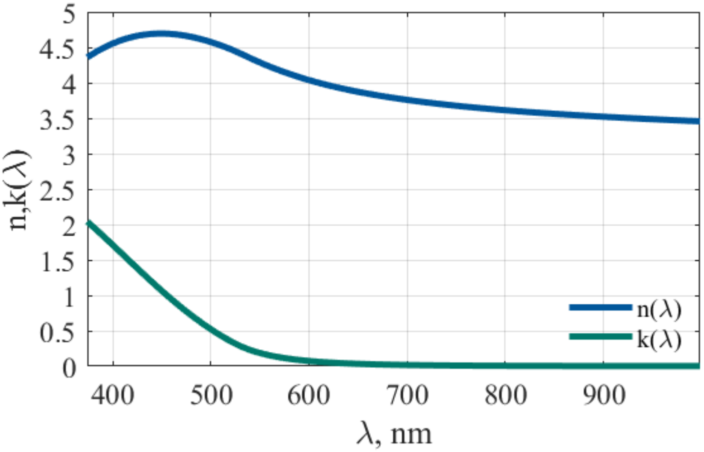

Fig. 2.1. Real (n) and imaginary (k) parts of the experimentally measured refractive index of hydrogenated amorphous silicon (a-Si) as a function of wavelength.

There were two sets of samples. The first set was fabricated by the Advanced Optics and Photonics Laboratory at Nottingham Trent University, Nottingham, UK, represented by Prof. Mohsen Rahmani. The second set was fabricated by the School of Optics and Photonics at Beijing Institute of Technology, Beijing, China, represented by Prof. Huang Lingling.

To verify the numerical results obtained, experimental samples of metasurfaces with different lattice parameters and different radii of meta-atoms were used. The experimentally measured refractive index dispersion of hydrogenated amorphous silicon was used as a material for numerical calculations Fig. 2.2.

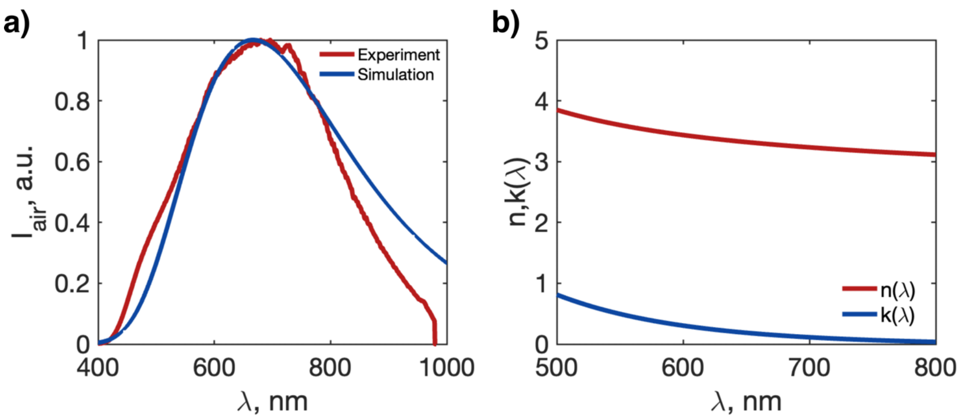

Fig. 2.2. **a)** – Intensity of incident radiation in free space versus wavelength. **b)** – Real (n) and imaginary (k) parts of the experimentally measured refractive index of amorphous hydrogenated silicon (a-Si) as a function of wavelength.

The effective scattering cross-section in this Doctoral Thesis was determined by Eq. (2.1):

$$\sigma_{\text{eff}} = \frac{\sigma_{\text{sca}}}{\pi R_{\text{cyl}}^{2}}, \tag{2.1}$$

where

σ_{eff} – effective scattering cross-section, m^2;

σ_{sca} – scattering cross-section, m^2;

R_{cyl} – radius of the cylinders, m.

The arrangement of metasurface samples is shown in Fig. 2.3. The series was manufactured separately and consisted of 18 metasurfaces (6 different geometric configurations under 3 different manufacturing regimes) with more detailed parameters selected, consistent with theoretical calculations. There is also one additional sample on which a thin film of silicon is deposited at the same height as the height of the metaatoms.

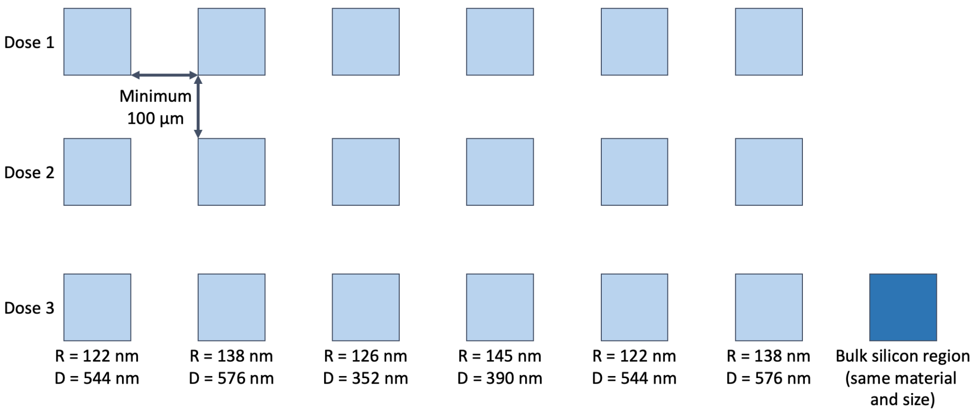

Fig. 2.3. Pattern on the sample. Layout of samples with different geometric parameters of meta-atoms, periods, and different manufacturing regimes.

The geometric parameters with the number of samples of the metasurfaces are shown in Table 2.1.

Table 2.1

Parameters of Metasurfaces

Number of samples	Radius of cylinder, nm	Period of metasurface, nm
1	138	576
2	122	544
3	145	390
4	126	352
5	138	576
6	122	549

Transmission spectra of these metasurfaces were measured in the range of 400–1000 µm, the light source was a halogen lamp, and the detector was an OceanInsight QEpro spectrometer. The light was focused onto the metasurface and collected after it using identical 40× lenses.

The diameter of the focusing area was about 15 μm; the spectrum was taken from the center of the structure. The light incidence is normal, the light is unpolarized. Experimental transmission of the metasurface is calculated by spectrometer software using Eq. (2.2):

$$T = \frac{I_{\text{metasurface}} - I_{\text{noise}}}{I_{\text{substrate}} - I_{\text{noise}}}, \tag{2.2}$$

where

I_{noise} – power obtained (noise) by the spectrometer without any incident light, W/m^2;

$I_{\text{substrate}}$ – power obtained by the spectrometer when the light is incident on the substrate, W/m^2;

$I_{\text{metasurface}}$ – power obtained by the spectrometer when the light is incident on the metasurface with the substrate, W/m^2.

The experimentally measured refractive index dispersion of hydrogenated amorphous silicon (a-Si) of the second set of samples was used as a material for numerical calculations (Fig. 2.4).

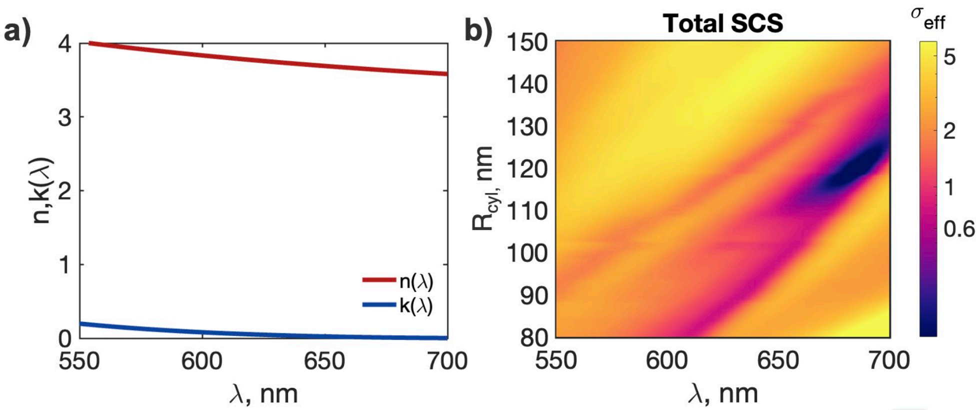

Fig. 2.4. **a)** – Real (n) and imaginary (k) parts of the experimentally measured refractive index of amorphous hydrogenated silicon (a-Si) as a function of wavelength. **b)** – Numerically calculated evolution of the hybrid anapole for a single nanoparticle as a function of radius and wavelength.

As for the previous set, Fig. 2.4 b) shows a distinct hybrid anapole scattering dip for a single cylindrical particle with different radii.

3. MAIN RESULTS

This Doctoral Thesis proposes a new concept to create transparent metasurfaces using silicon metasurfaces in a hybrid anapole state. The properties of metasurfaces based on the hybrid anapole were studied in detail. The multiresonant nature of the hybrid anapole allows for variation of the transmitted optical phase over a wide spectral and geometric range. Importantly, unlike Huygens sources, the coupling between particles is practically negligible. Thus, the hybrid anapole particle approaches the ideal of a 'true' meta-atom. This capability has been demonstrated through the development of ultra-compact silicon arrays with particle wall spacing equal to 1/8 of the incident wavelength in the visible spectrum, and disordered metasurfaces have been studied that exhibit behavior identical to their periodic counterparts. The effect of the substrate was studied, and conservation of the transmission window was demonstrated when metasurfaces were applied to a wide range of dielectric materials, potentially facilitating their integration into chips. As a proof-of-concept application, it was demonstrated that it was possible to modulate the optical phase of an ultrafast Gaussian pulse transmitted with unit efficiency through a highly disordered metasurface deposited on a glass substrate based solely on the optical response of the periodic array. Finally, the influence of cones on the properties of a hybrid anapole is shown, and for the first time, a hybrid anapole state has been obtained in silicon meta-atoms in the form of truncated cones, greatly facilitating, simplifying, and reducing the cost of creating such structures.

The detailed results are presented in Papers 1, 3, 4, 6, 8, and 10 in Appendices.

The main result of these scientific papers is the theoretical description, numerical simulation and experimental confirmation of the optical properties of silicon metasurfaces consisting of cylinders in a hybrid anapole state.

This Doctoral Thesis discovered that the recently identified non-scattering hybrid anapole regime can also be achieved in conical nanoparticles, in addition to elliptical and cylindrical ones. It is shown how adjusting geometric parameters enables the manipulation of anapole regimes for different multipoles, thereby achieving a hybrid anapole regime. The Doctoral Thesis represents a step forward in nanophotonics, allowing for the exploration of more complex shapes and fine-tuning of effects achievable with individual nanoscatterers. This research significantly reduces the cost of developing photonic devices and opens new avenues for practical applications in next-generation photonics. The findings of this Doctoral Thesis have potential applications in various research fields, such as creating diverse dielectric nanoantennas in the form of resonator chains compared to chains of spheres or cylinders. They also pave the way for metasurfaces capable of achieving optical effects that were previously unattainable.

The detailed results are presented in Papers 2, 5, 7, 9, 11, and 12 in **Appendices**.

The main contribution of these papers is the theoretical description and numerical simulation of the hybrid anapole state in truncated silicon nanocones.

Unfortunately, at this moment, the measured materials have not yet been published, so this subsection demonstrates the obtained results.

First, it was necessary to demonstrate the existence of a hybrid anapole regime in single silicon nanoparticles for experimentally measured refractive index dispersion, shown in Fig. 2.2.

Figure 3.1 shows the results of numerical simulation.

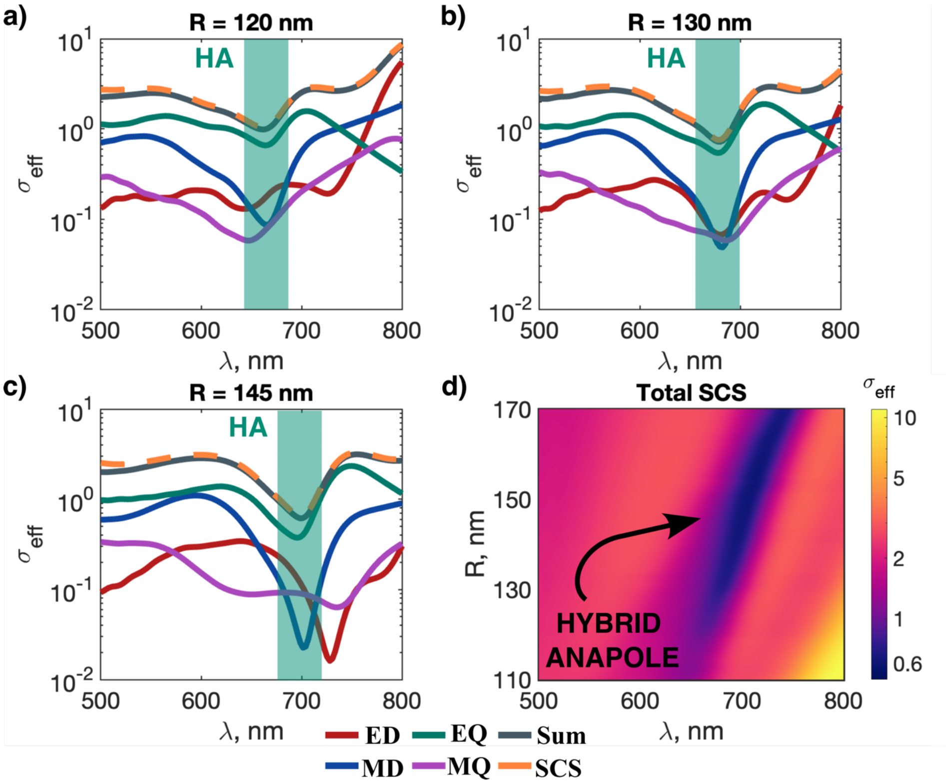

Fig. 3.1. Numerically calculated evolution of the hybrid anapole for a single nanoparticle as a function of radius and wavelength. **a)–c) –** Multipole decompositions of the SCS (semilogarithmic scale) for selected radius R_{cyl}. In all calculations, the height of the nanoparticle was kept constant (H = 370 nm). **d)** – Total SCS as a function of radius and wavelength.

Figure 3.1 a)–c) shows the numerically calculated multipole decomposition of a single cylinder-shaped nanoscatterer for different radii for the experimentally measured refractive index. The hybrid anapole scattering dip changes with different geometric parameters but is still present for the parameters shown. Figure 3.1 d) demonstrates at what geometric parameters an anapole dip will occur in such a silicon particle.

The height H of the resulting cylinders was H = 370 nm. Figure 3.2 shows scanning electron microscope (SEM) images of the metasurfaces.

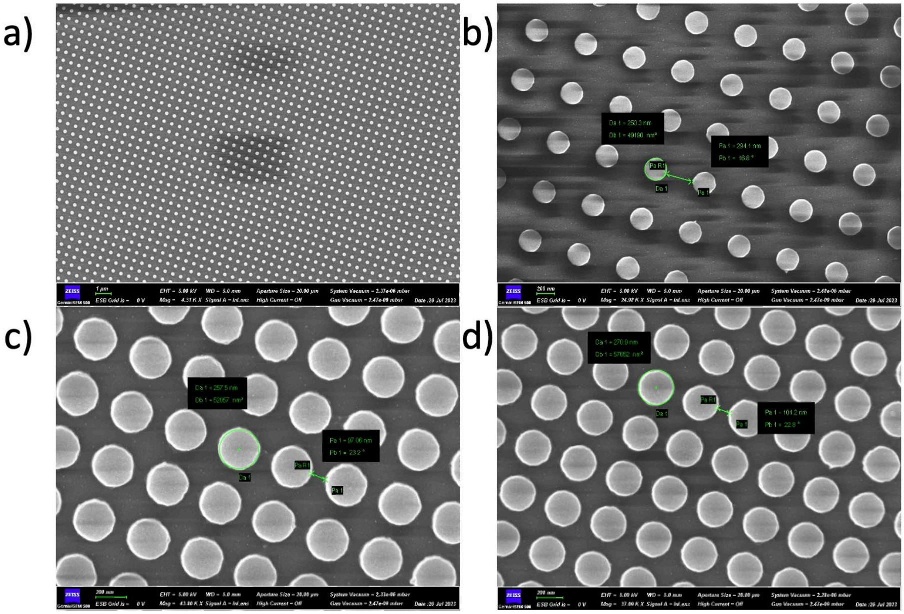

Fig. 3.2. Example SEM image of a metasurface. **a)** – General view of the metasurface with a distance between the walls of meta-atoms s = 300 nm. **b)** – Metasurface with a distance between meta-atoms s = 300 nm and radius R_{cyl} = 125 nm. **c)** – s = 100 nm and R_{cyl} = 130 nm. **d)** – s = 100 nm and R_{cyl} = 135 nm.

The transmission spectra of these metasurfaces were measured in the range of 400–1000 µm (Fig. 3.3).

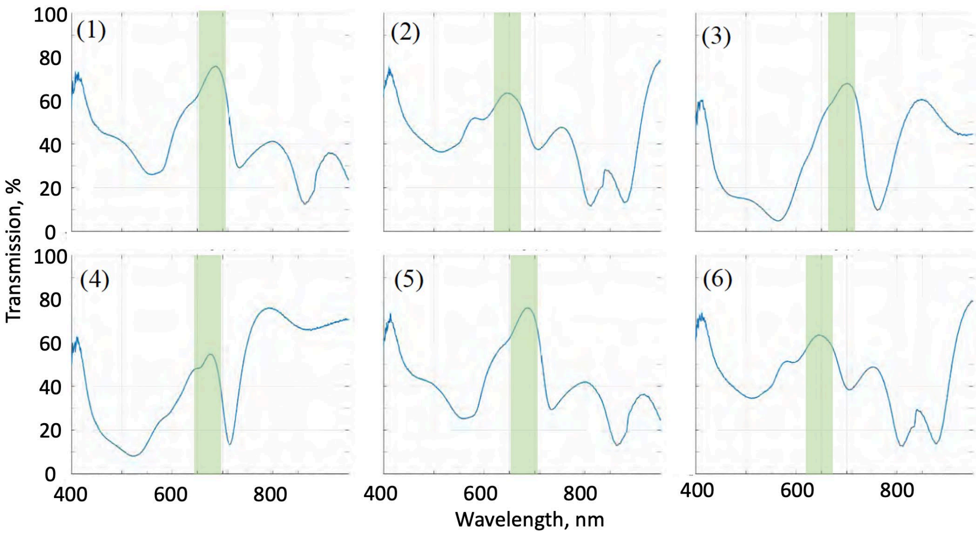

Fig. 3.3. Measured transmittance spectra for silicon metasurfaces in the hybrid anapole regime for metasurfaces with different periods s and radius R_{cyl}. The numbering corresponds to Table 2.1.

In the spectral response, a feature is visible in the range of 650–700 nm, corresponding to the hybrid-anapole state (maximum transmission, corresponding to the minimum of scattering). A comparison of conventional metasurfaces and superdense ones shows that the hybrid anapole peak of transmission almost does not change its spectral position.

To prove that this is indeed a hybrid anapole state, Figure 3.4 shows a multipole decomposition.

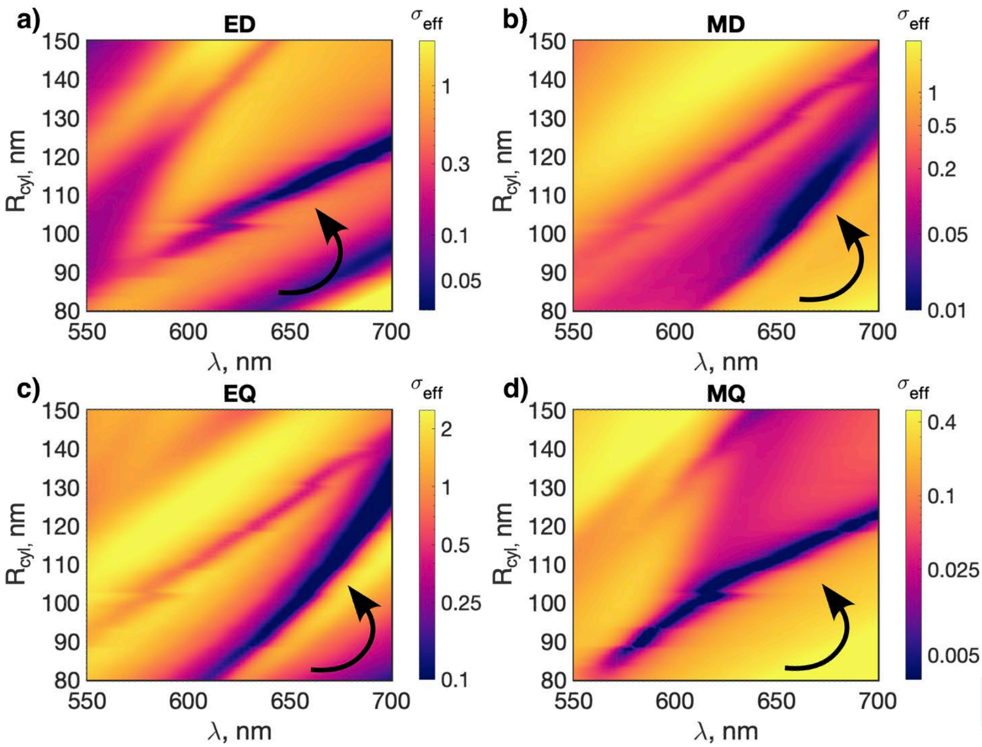

Fig. 3.4. Evolution of the SCS of each multipole (in log scale): a) ED, b) MD, c) EQ, d) MQ, as a function of wavelength and radii. The arrow indicates the anapole state of each of the multipoles.

Figure 3.4 shows anapole lines that intersect in parameter space in a certain region, which is called the hybrid anapole state.

Using such particles, metasurfaces with two different radii and three different configurations were experimentally obtained: usual, dense and disordered (Fig. 3.5).

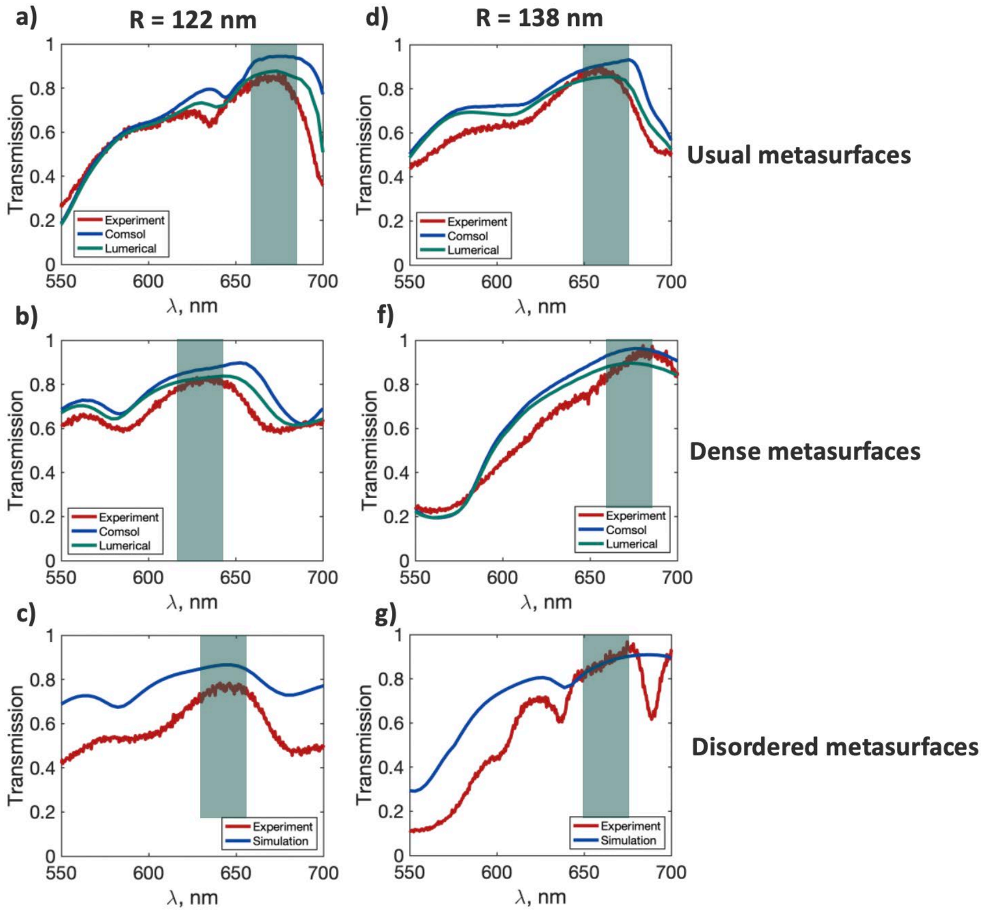

Fig. 3.5. Measured transmittance spectra for silicon metasurfaces in the hybrid anapole regime for metasurfaces with different periods, s, and structures without strict adherence to the arrangement order of nanoparticles for radius (a–c) R_{cyl} = 122 nm and (d–g) R_{cyl} = 138 nm.

The main result of this part of the Doctoral Thesis is that the experimental results were compared with numerical simulations of metasurfaces for the current refractive index and radii. The numerical and experimental curves are quite similar. Transmission has a maximum, which indicates a hybrid anapole state in these metasurfaces.

The results obtained in the Thesis were used in:

- LZP project "*Dynamics of non-scattering states in nanophotonic (DNSSN)*" No. lzp-2021/1-0048
- LZP project "*Novel non-Hermitian singularities in all-dielectric nanostructures (NEO-NATE)*" No. lzp-2022/1-0553

4. FINAL REMARKS

In this final chapter, the main achievements of the presented Doctoral Thesis are discussed in **Section 4.1,** the main conclusions are discussed in **Section 4.2,** and **Section 4.3** gives a perspective for future research.

4.1. Main achievements of the Doctoral Thesis

The main achievements of the Doctoral Thesis can be summarized as follows:

1. A model of a metasurface has been developed, comprising silicon cylindrical meta-atoms that sustain a hybrid anapole state at a specific wavelength. It has been demonstrated that such a metasurface is transparent and does not alter the optical phase of the radiation passing through it at the anapole wavelength.
2. The practical implementation of metasurfaces will inevitably require the presence of a substrate. It can play an important role in the optical response and introduces magnetoelectric coupling. In sharp contrast to conventional resonances, hybrid anapole is extremely stable when applied to a substrate. In the studied nanocylinder with a hybrid anapole state (in contrast to conventional anapoles or Huygens sources), complete transmission is achieved due to the overlap of the resonant Mie and Fabry–Perot modes. The Mie modes can be associated with standing waves arising between the side walls of the resonator cavity, and the Fabry–Perot modes are mainly formed by standing waves between the upper and lower walls. Consequently, variations in the reflectivity of the substrate affect mainly the amplitude of the Fabry–Perot modes, while the Mie modes remain almost unchanged. However, in the presence of a significant contrast between the particle and the substrate, the hybrid anapole state changes insignificantly. However, as the refractive index of the substrate approaches the refractive index of the nanoparticle (the disappearance of the contrast and, accordingly, the leakage of the Fabry–Perot mode into the substrate), the hybrid anapole state gradually transforms into a conventional electric dipole anapole, still retaining a strong decrease in scattering.

   To study this phenomenon, transmission, reflection, and absorption were obtained in the hybrid anapole state for a metasurface deposited on a series of hypothetical substrates with refractive indices varying from 1 to 2. For numerical simulations, the experimentally obtained refractive index dispersion for amorphous silicon was used.

   A gradual narrowing of the bandwidth is found, mainly due to the redshift of high-order Bloch modes. It is important to note that the total transmittance of the metasurface itself remains close to 100 % in the vicinity of the hybrid anapole wavelength, even for a refractive index of 2.

   Unlike in the case of a single particle, in the case of a metasurface, the Mie and Fabry–Perot modes are coupled. As noted above, when the contrast decreases, the Fabry–Perot mode leaks into the substrate, and the hybrid anapole degenerates into a regular anapole. In the presence of significant contrast, the hybrid anapole state-induced passband is very resistant to changes in the refractive index of the substrate. These results clearly show that the metasurface can be directly deposited on ordinary glass (SiO_2) or another substrate without additional design steps and provide full transmittance as well as optical phase control.

As a result, the contrast between the refractive indices of the elements of the metasurface and the substrate is maintained, and the hybrid anapole metasurface is insensitive to various substrate materials, which greatly simplifies the experimental implementation of the proposed structures.

A unique advantage of the hybrid anapole metasurfaces studied in this Doctoral Thesis compared to traditional Huygens metasurfaces is the stability of their characteristics to changes in the arrangement of particles due to the fact that in the hybrid anapole state, the individual elements of the hybrid anapole metasurface (meta-atoms) practically do not interact with each other. In this case, the effective multipoles of meta-atoms on the substrate are almost identical to the multipoles of an isolated particle. This means that even at very small distances, they are not affected by the scattered fields of neighbors, unlike a conventional nanoantenna, for example, in the Kerker effect, the optical response of which is highly dependent on the presence and location of neighbors.

3. It was demonstrated that hybrid anapole retains its properties even at very small distances (down to 6 % of the diameter of individual meta-atoms) between the elements of the metasurface. Successful suppression of reflection has been achieved for such closely packed metasurfaces. Importantly, the optical phase of the transmitted field also remains virtually unchanged. Besides its academic significance, this result sets the stage for implementing ultra-small pixels compared to what has been achieved on other platforms thus far, which is crucial, for instance, for holographic applications.
4. It was demonstrated that, unlike traditional periodic Huygens metasurfaces, hybrid anapole metasurfaces are practically insensitive to the disordering of meta-atoms. This was shown through a series of numerical calculations. It was found that the hybrid anapole state exhibits remarkable resistance to significant deviations from an ideal periodic lattice precisely because it is largely unaffected by its neighbors, rendering their arrangement insignificant. Additionally, it is worth noting that the proposed metasurface exhibits high field concentrations within the meta-atoms, characteristic of anapole regimes. Therefore, disordered hybrid anapole metasurfaces represent a fundamentally new and flexible platform for enhancing the interaction of light and matter at the nanoscale. This property of hybrid anapole metasurfaces presents a unique opportunity for their utilization in nonlinear optics, such as the generation of multiple harmonics.

It is noteworthy that such metasurfaces can be produced quite simply without the need for complex optimization methods or careful arrangement of meta-atoms. This is particularly crucial in the manufacturing of large metasurfaces, as maintaining strict periodicity of meta-atoms on a large scale poses significant challenges. The complexity increases as the size of the metasurface grows, ultimately imposing a technological upper limit on its size. In contrast, hybrid anapole metasurfaces are not bound by such restrictions and can have practically unlimited dimensions.

5. A new mechanism was introduced to achieve 100 % transmission and control the optical phase of the transmitted wave, based on the physics of a non-radiating state – a hybrid anapole. With future practical implementation in mind, the radius of the cylinder was chosen as the parameter to control the optical phase of the radiation. This choice was made because changing the radius of meta-atoms can be relatively easily realized using well-established fabrication techniques, such as electron beam lithography followed by reactive ion etching.

   Using numerical methods, a 'map' was created that related the specific transferred optical phase to the geometric parameter of the meta-atom. Such a map allows us to select a meta-atom that produces a specific optical phase while maintaining complete transparency of the metasurface. The transmittance and optical phase were calculated for a hybrid anapole metasurface with small distances between meta-atoms for various radii and wavelengths. Thanks to the map, it is possible to set the operating wavelength and observe a well-defined optical phase change for a set of radii within the hybrid anapole transparency window.

   Thus, a method was demonstrated to control the optical phase of radiation transmitted through the structure by varying the radii of meta-atoms. In the studied case, the optical phase change primarily occurs due to an increase in the contribution of the electric quadrupole moment, which is significantly minimized by the electric quadrupole anapole. With the assistance of 2D maps, it becomes possible to select a specific optical phase delay for hybrid anapole nanocylinders of a given radius while maintaining complete transparency of the structure.

6. The possibility of modulating the optical phase of an ultrafast Gaussian pulse in transmission mode using a disordered hybrid anapole array on the surface of a glass substrate was investigated. Strong disorder in the plane was chosen to illustrate the system's independence from the arrangement of particles. Subsequently, a time-domain finite-difference time-domain (FDTD) simulation of the incoming x-polarized Gaussian pulse with a duration of 600 fs was conducted. The nanoparticle radius values ranged from 125 nm to 135 nm to fall within the range covered by hybrid anapole states.

   As expected from previous calculations, the optical phases transferred by periodic and disordered metasurfaces were almost identical. Transmission remained above 85 %, as confirmed by full-time profiles. Alternatively, although generally less practical, the device can also be wavelength-controlled. It was demonstrated that the interaction of Mie and Fabry–Perot modes enables additional optical phase modulation of the beam. An ultrafast optical phase modulator based on a disordered hybrid anapole array was numerically implemented. The results suggest the possibility of flexible design of meta-atoms without the need for time-consuming optimization steps.

7. The influence of sample non-ideality on effects in dielectric nanoscatterers was investigated, and a quantitative study was conducted on the influence of taper ($1 - R_{top}/R_{bottom}$) on the resulting optical properties of the nanocavity. Specifically, the impact of the cone shape on the hybrid anapole regime in single nanoparticles and metasurfaces based on them was meticulously examined. It was found that the hybrid anapole state in cylinders is disrupted when changes are made to the shape due to alterations in the particle's symmetry. In such cases, previously closed channels open, leading to additional interactions between the resonator modes. Furthermore, the feasibility of achieving a hybrid anapole regime in conical particles was demonstrated for the first time, offering new opportunities for the design of photonic devices with more precise tuning of optical properties, thanks to the additional degree of freedom provided by the truncated cone radius

4.2.Main conclusions

1. It has been demonstrated that metasurfaces in the hybrid anapole state exhibit nearly perfect transmittance and do not induce alterations in the optical phase or amplitude of transmitted radiation at the wavelength corresponding to the hybrid anapole state.
2. As a result of parametric modelling, changing the dielectric properties of the substrate (with the refractive index varying in the range of 1 to 2), transmission spectra, and maps of the spatial distribution of electromagnetic fields inside and outside the meta-atom were calculated. It was demonstrated that in the presence of a contrast between the significant refractive index of the particle and the substrate, the hybrid anapole state remains extremely stable. However, as the refractive index of the substrate approaches that of the nanoantenna, leakage of the Fabry–Perot mode into the substrate was observed, causing the hybrid anapole to gradually transition into an electric dipole anapole.
3. It is shown that the same effect makes it possible to create metasurfaces in the hybrid anapole state with a very dense packing of meta-atoms (the distance between the walls is up to 6 % of the diameter of individual meta-atoms). Meta-atoms in the hybrid anapole state do not interact with each other.
4. The transmission spectra of metasurfaces were calculated for both perfectly ordered arrangements of meta-atoms and disordered configurations. Upon comparing the obtained spectra and optical phase curves of the transmitted field, it is demonstrated that hybrid anapole metasurfaces are insensitive to the disordering of meta-atoms. Meta-atoms in the hybrid anapole state are not influenced by their neighbors.
5. A method has been developed to control the amplitude and optical phase of the field passing through the metasurface in the hybrid anapole state. Through parametric numerical modelling (varying the radii of the nanocylinders), electromagnetic fields passing through the metasurface in the hybrid anapole state were analyzed. A map

was then constructed linking the transmitted optical phase with the geometric parameter of the meta-atom. This map allows for the selection of the geometric parameter that produces a desired optical phase while maintaining complete transparency of the metasurface.

6. A numerical simulation of an ultrafast optical phase modulator utilizing a disordered array in a hybrid anapole state was conducted with a pulse duration of approximately 600 fs. Through alterations in the shape of the meta-atoms, control over the pulse passing through the structure was achieved. The results suggest the capability to flexibly design metadevices without the need for time-consuming optimization steps, achieving exceptionally high resolution.
7. The effect of changing the conicity on the resonances responsible for the hybrid anapole regime was demonstrated. Adjustment of the conicity effectively disrupts the fundamental symmetry of the particles and opens previously inaccessible channels, resulting in additional interactions between cavity modes. Understanding this effect may become crucial for future applications that leverage the unique properties of the hybrid anapole, such as metasurface engineering and sensing.

   Moreover, beyond the already established configurations of cylinders and ellipsoids in the hybrid anapole regime, the potential for achieving the hybrid anapole state in nanocones has been explored. Nanocones offer a simpler and easier-to-manufacture platform for implementing multipole interference effects. It was demonstrated that the hybrid anapole regime is sustained in nanocones, even with changes of up to 30 % in the upper radius, albeit with a slight frequency shift of the resonance. Consequently, the library of all-dielectric nanostructures supporting the hybrid anapole regime has been expanded.

4.3. Further outlook

Metasurfaces in the hybrid anapole state offer a promising platform for various photonic effects and applications owing to their unique properties. Current research can be expanded in the following directions:

- Exploration of new photonic effects based on anapole metasurfaces, such as the attainment of high-quality quasi-bound states in the continuum using hybrid anapoles. This could serve as a promising platform for developing ultrasensitive sensors of a new generation.
- Development of a model for a controllable optical structure comprising silicon metasurfaces in a hybrid anapole state, 2D materials, and substrates. Each element would interact with the others, enabling the creation of a selectively transparent structure for controlling optical radiation passing through it.
- Investigation of optical forces acting on non-scattering single silicon particles in the hybrid anapole regime when irradiated with various forms of beams.

ACKNOWLEDGMENT

I would like to thank the following people for their invaluable assistance with this Doctoral Thesis, without whom I would not have been able to complete this research:

- Many thanks to my scientific supervisor, Professor Vjačeslavs Bobrovs, for his invaluable contribution to this Thesis. None of this would have been possible without his support, genuine interest in research, and the opportunities for development he provided.
- I am grateful to my scientific consultant, Professor Alexander Shalin, for the fruitful scientific discussions and his unique approach to research and consultation.
- I thank my colleague, Dr. Denis Kislov, for his patience, knowledge, and the skills he shared with me.
- I am deeply appreciative of Dr. Adria Canos Valero for the experience he imparted during my studies, his patience and wisdom, and for helping me take my first small steps in big science.
- I extend my gratitude to Associate Professor Toms Salgals for his friendliness, support in critical situations, the experience he passed on to me, and the skills he helped me develop.
- I also thank my colleagues, Dmitry Redka and Alexander Krotov, for their adventurous spirit, friendliness, and the valuable advice they provided.
- Many thanks to my family, who supported me in all my endeavors and helped me through the most difficult situations.
- I am grateful to all my colleagues who encouraged me not to give up, shared their scientific experience, engaged in discussions, and provided support and skills essential to this work.
- Finally, many thanks to all the participants who took part in the study and made it possible.

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