

Control of Scattering and Absorption of Light by Multilayer Nanowires

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This thesis is an account of research undertaken in Nonlinear Physics Centre within the Research School of Physics and Engineering at the Australian National University between February 2012 and February 2017 while I was enrolled for the Doctor of Philosophy degree.

The research has been conducted under the supervision of Dr. Andrey E. Miroshnichenko, A. Prof. Ilya V. Shadrivov and Prof. Yuri S. Kivshar. However, unless specifically stated otherwise, the material presented in this thesis is my own original work.

This thesis also contains no material which has been accepted for the award of any other degree or diploma in any institution of learning. It contains no material previously published or written by another person, except where due reference is made in the text.

Ali Mirzaei
22 February 2017



To my beloved parents, Karim and Nasrin, and my lovely sister, Zahra.

Publications and Selected Presentations

Refereed journal articles

- 1) S. Atakaramians, A. E. Miroshnichenko, I. V. Shadrivov, **A. Mirzaei**, T. M. Monro, Y. S. Kivshar and S. V. Afshar. Strong magnetic response of optical nanobers. *ACS Photonics*, 3:972, 2016.
- 2) **A. Mirzaei**, A. E. Miroshnichenko, I. V. Shadrivov and Y. S. Kivshar. Optical Metacages. *Phys. Rev. Lett.*, 115:215501, 2015.
- 3) K. Ladutenko, P. Belov, O. Pena-Rodrguez, **A. Mirzaei**, A. E. Miroshnichenko and I. V. Shadrivov. Superabsorption of light by nanoparticles. *Nanoscale*, 7:18897, 2015.
- 4) **A. Mirzaei**, I. V. Shadrivov, A. E. Miroshnichenko and Y. S. Kivshar. Superabsorption of Light by Multilayer Nanowires. *Nanoscale*, 7:17658, 2015.
- 5) **A. Mirzaei**, A. E. Miroshnichenko, I. V. Shadrivov and Y. S. Kivshar. All-Dielectric Multilayer Cylindrical Structures for Invisibility Cloaking. *Sci. Reports*, 5:9574, 2015.
- 6) **A. Mirzaei** and A. E. Miroshnichenko. Electric and magnetic hotspots in dielectric nanowire dimers. *Nanoscale*, 7:5963, 2015.
- 7) **A. Mirzaei**, A. E. Miroshnichenko, I. V. Shadrivov and Y. S. Kivshar. Superscattering of light optimized by a genetic algorithm. *App. Phys. Lett.*, 105:011109, 2014.
- 8) **A. Mirzaei**, A. E. Miroshnichenko, N. A. Zharova and I. V. Shadrivov. Light scattering by nonlinear cylindrical multilayer structures. *JOSA B*, 31:1595, 2014.
- 9) **A. Mirzaei**, I. V. Shadrivov, A. E. Miroshnichenko and Y. S. Kivshar. Cloaking and enhanced scattering of core-shell plasmonic nanowires. *Opt. Express*, 21:10454, 2013.

Selected conference presentations and proceedings

- 10) **A. Mirzaei**, A. E. Miroshnichenko, I. V. Shadrivov and Y. S. Kivshar. Nanostructuring for enhanced light absorption. *SPIE Micro+Nano Materials, Devices and Applications*, 2015 (Sydney, Australia).
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- 14) **A. Mirzaei**, I. V. Shadrivov, N. A. Zharova, A. E. Miroshnichenko and Y. S. Kivshar. Nonlinear control of enhanced scattering in multi-layer nanowires. *8th International Congress on Advanced Electromagnetic Materials in Microwaves and Optics (METAMATERIALS)*, 211–213, 2014 (Copenhagen, Denmark).
- 15) **A. Mirzaei**, I. V. Shadrivov, A. E. Miroshnichenko and Y. S. Kivshar. Optimization of cloaking in all dielectric multi-layer structures. *8th International Congress on Advanced Electromagnetic Materials in Microwaves and Optics (METAMATERIALS)*, 208–210, 2014 (Copenhagen, Denmark).
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Abstract

In recent decades, nanotechnology has become one of the biggest steps forward in expanding the horizons of science and engineering. Nanotechnology progressively plays more important roles in various modern technologies that are revolutionising human lifestyle. Nano-photonics as one of the fastest growing fields in nanotechnology, is finding its way to become a key tool in various applications. This involves variety of scientific and technological problems, from medical diagnosis and cancer therapy to ultrafast computation and data communication. However, continuously improving cutting-edge technology of optical nanostructures, requires further development of analysis for designing more advanced nanostructures for future generations of optical nano-devices.

The reported progress in nanophotonics, is mainly based on advances in theoretical optics and experimental techniques. Numerical simulations and experiments have made a significant progress in analysing and designing optical nanostructures for various applications. However, they both become considerably expensive in terms of time and material especially when they have to be repeated for several times to optimise a set of parameters. Furthermore, repeatability and measurement challenges in experiments, and robustness and finite precision complications in simulations, yet remain. These restrictions, consequently, limit the exploration possibility for new ideas and solutions for future nanophotonics.

To address this, I introduce a novel, fast and exact approach by employing analytical/semi-analytical solutions and powerful optimisation techniques without the mentioned restrictions. This approach suggests a novel platform for wide exploration of unique possibilities for developing new ideas. I discuss the details of my approach by employing multilayer nanostructures for example applications in optics. To achieve optimal performance, I develop a smart optimisation process that employs the fast analytical solutions within a genetic algorithm. I explain the details of this process that can optimise complicated structures by exploring multi-dimensional parameter space in both linear and nonlinear regimes.

My proposed approach, can generally be applied for different types of nanostructures with different geometries. However, among various introduced components, nanowires have proven themselves to be appropriate candidates for taking important roles in optical devices for different applications. In addition, by studying long nanowires, I analyse optical nanostructures using the developed semi-analytical approach in a two-dimensional platform. Therefore, we can concentrate on developing the main concepts by avoiding

unnecessary complications. In this thesis I provide the complete analysis of nanowire with large aspect ratios, however our further studies prove that the developed design solution and achieved results are not restricted to two-dimensional platform, and are also applicable for three-dimensional structures. I briefly discuss this with some examples, such as nanodisks and nanospheres, even in more complicated configurations and by presence of substrates.

To discuss the details, after a brief introduction in Chapter 1, I first discuss two parallel approaches in Chapter 2: (i) a semi-analytical method to analyse the scattering and absorption of light with single and interfering multilayer nanowires, and (ii) a smart genetic optimisation algorithm, employing the fast semi-analytical solution to search for optimal set of designing parameters.

Then, I focus on developing specific structures based on multilayer nanowire systems. Controlling the light-matter interaction in nanowires allows to engineer the scattering and absorption efficiencies, with the possibility to enhance or suppress the corresponding cross section. As examples, I discuss invisibility cloaking and superscattering of light as two oppositely different effects in Chapter 3. Enhancing the absorption of light on the other hand, is important for improving the efficiency of many optical devices which in its extremum case, can cause superabsorption effect. This is also discussed in detail by the use of single multilayer nanowires in Chapter 3.

By bringing more nanowires together and constructing more complicated systems, the interference between the nanowires can lead to remarkable effects. In Chapters 2 and 4, I explain the analytical solution of multiple scattering problems in nanowire systems. Example structures in Chapter 4 demonstrate that carefully controlling the behaviour of light in nanowire dimer systems can lead us to manage electric and magnetic hotspots, and a complex nanowire system to electromagnetically shield non-isolated areas.

Finally, going beyond the linear regime, I discuss nonlinear effects in multilayer nanowires in Chapter 5, by introducing my novel semi-analytical recipe. By studying an example of nonlinear superscattering of light by a core-shell nanowire and its hysteresis loop and bistability, I demonstrate that my approach is accurate and more than 10^5 times faster than finite difference time domain.

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Introduction

The scattering and absorption of light are the two important aspects of the interaction of light with matter. These phenomena have attracted attention during thousands of years, and have strongly affected our understanding of the world. Gas molecules and suspended nanoparticles in the atmosphere of the earth are scattering sunlight every day, making the sky blue and clouds white, and creating beautiful sunrises and sunsets. On the other hand, absorption of light plays an important role in various natural phenomena such as determining the colour of objects, light detection and generation of thermal or chemical energy. Beyond many examples in nature, recent advances in science and technology have revealed modern applications for controlling the scattering and absorption of light. Newly developed methods for disease diagnosis by scattering of light with plasmonic nanoparticles, advanced sensing systems and highly efficient solar cells are only a few examples.

Having an in-depth understanding of the interaction of light on a microscopic scale is a key tool for more efficient controlling of its behaviour for various applications. Therefore, before discussing the role of scattering and absorption in optical nano-devices, I briefly review their underlying physics in the atomic and molecular scale.

1.1 Physics of scattering and absorption of light

Studying scattering and absorption in small micro- and nano-structures is fundamentally important for interpreting light-matter interaction and discovering new phenomena and applications. Novel particle characterisation techniques have been developed based on the strong dependence of the optical properties of particles on their size, shape, and refractive index. Modern remote sensing, biomedicine, engineering, and astrophysics, all are utilising electromagnetic scattering by small particles. A meaningful interpretation of these phenomena and explanation of observations, require an in depth understanding of the underlying physics of scattering and absorption by small particles [1].

Matter is made of particles with positive and negative electric charges in atomic and molecular scales. Regardless of being in solid, liquid or gaseous form, a particle of any size

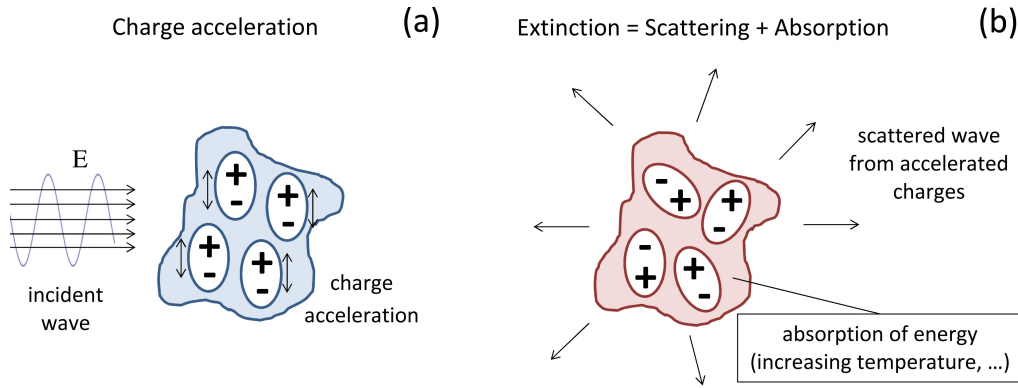


Figure 1.1: Interaction of light with small particles: (a) a part of the incident light's energy interacts with the particle and accelerates electric charges, and (b) absorption in form of thermal energy and re-radiation of light (scattering) from accelerated charges.

from a single electron to a group of many molecules, interacts with light by its charges getting accelerated with the incident wave. The strength of this interaction is a function of the wavelength and the material (and in general environment) properties. In non-negligible interaction of light with particles, the photons' energy causes more polarisation or acceleration of the charges. This is called *extinction* which means transferring the incident light's energy for accelerating charges. The extinction of light generally contributes in two different mechanisms: (i) the accelerated charges re-radiate the electromagnetic energy in all the directions. This secondary radiation which slows the acceleration by transferring the energy into the re-emitted photons, is the *scattering* of light by the particle. (ii) A part of the energy is converted to other forms which are non-radiative (e.g. thermal energy) and is called the *absorbed* energy [1, 2]. Figure 1.1 schematically demonstrates the concept.

Scattering of light as a result of the resonance of discussed electric dipoles, can occur at the same frequency as that of the incident field which caused it to resonate, and this is called *elastic* scattering. However, in practice, the electromagnetic field and material may exchange energy. In this case some photons at a lower frequency are created in secondary radiation (red shift) by transferring a part of the energy from the incident field into the medium in the form of vibrational excited modes (Stokes process). The creation of higher energy photons (blue shift) is also possible through an opposite process where the internal energy of the matter transfers to photons (anti-Stokes process) [3, 4]. This phenomenon is known as *inelastic* or *Raman* scattering which is out of the scope of this thesis.

Basically there are phase differences between the scattered light from the dipole moments in any specific direction [1, 2]. If the dimension of the particle is very small compared to the wavelength, these phase differences are negligible and the scattered field from all the dipole moments are almost in-phase in all the directions. This class of scattering (Rayleigh scattering) is mostly dependent on the wavelength and practically independent from the shape of the scatterer [5]. However, by increasing the size of the particle, these phase differences increase and cause constructive and destructive interference effects of peaks

and valleys in the scattered pattern. In this case the size of the scatterer compared to the wavelength, as well as its material and polarisability, determine the scattering behaviour of the particle. This class of scattering is called *Mie scattering* in the case of spherical scatterers.

Solving a scattering problem directly by considering the secondary waves radiated from all the small dipoles is not practical even for a micrometre-sized particle. However, the same problem can be solved using the concepts of macroscopic bodies without discussing the discrete dipoles in the material construction. This is possible by solving Maxwell's equations with appropriate boundary conditions in systems with known geometry and distribution of the refractive index. For instance, Mie solution describes the scattering of light by a homogeneous sphere illuminated by a planewave in macroscopic scale. Mie theory mathematically explains the electromagnetic fields by decomposing them into multipole expansion of spherical harmonics in the form of infinite series [2, 6]. This completely solves the mathematical problem of the interaction of light with spherical particles and explains the scattering and absorption of different excited harmonics. The cylindrical version of Mie theory is discussed in detail in Chapter 2 to be used for analysing the electric and magnetic fields distribution in nanowire systems.

1.2 Scattering and absorption of light by nanowires

Various nanostructures have been studied to control the behaviour of light for a variety of applications. Among them, nanowires by having a specific geometry and being able to be fabricated out of various materials, have unique optical properties. Nanowires are a group of nanostructures, usually with a symmetric cross-section and high aspect ratio. Studying nanowires as one-dimensional structures with nanoscale-range diameter, facilitates analysing and understanding fundamental concepts about the roles of dimensionality and size for different applications in optics [7]. The length-to-width ratio of nanowires is usually in the range of 10 - 10^3 or even more. Figure 1.2 shows some examples of fabricated nanowires.

The electromagnetic properties of nanowires suggest practical solutions in various applications. For instance, in solar energy harvesting, a proper design of light scattering by nanowires can result in trapping of light and increasing the total absorption as a result of multiple-scattering in the system [8]. This is of significant importance for optimising and improving the overall efficiency of photovoltaic devices. By employing core-shell structure for nanowires, the multiple scattering between the interfaces of different nanowire elements, can be transferred into the construction of a single nanowire between the surfaces of different layers. By adding an additional coating layer over the central core of a nanowire, more parameters become available for more efficient designs. In principle the number of shells can be more than one, creating multi-shell coatings, or multilayer nanowires. In

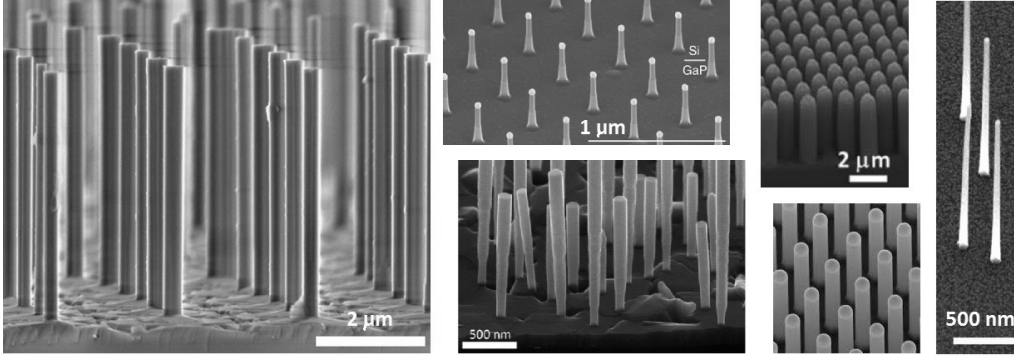


Figure 1.2: Examples of fabricated nanowires with circular cross section and different shapes (references from left to right [9–14]).

this thesis I demonstrate how radially layered nanowires give us a wide range of freedom to control the light behaviour in the near and far field. Then, by different examples it is shown that multilayer configuration makes nanowires capable for various applications from invisibility cloaking and near-zero scattering to highly enhanced scattering and nanoantenna applications, and from resonant solar energy super-absorption to electromagnetic shielding. Discussing axially layered nanowires is beyond the scope of this thesis, however, as is briefly demonstrated later, their efficiency especially in light absorption applications are not as high as in radially layered nanowires.

Multilayer nanowires are practically realisable using various developed techniques for different materials and applications [15–18]. Many techniques have been reported for fabrication of nanowires with single-crystalline core and shell in different temporal regimes [19]. Various aspects of fabrication considerations from vapour-liquid-solid mechanism and wire growth techniques, to using various types of catalyst materials have been discussed for single-material/multilayer nanowires realisation [20–24]. Figure 1.3 demonstrates some examples of realised multilayer nanowires.

Fabrication considerations and techniques are not discussed in this thesis, however, experimental data to describe the employed materials is used and practical considerations are taken into account. For instance, the small-size-effect of plasmonic nanostructures and modification of collision frequency has been considered for nanowires with metallic layers and this is discussed in Chapter 2.

1.3 Application of nanowires in optics

After more than nearly two decades of research on optical, electronic, chemical and mechanical properties of nanowires, they are employed in a wide range of applications [27]. The potential applications of single crystalline nanowires are truly impressive, from absorbing oil and killing bacteria in water [28, 29] to magnetic nanowires for construct-

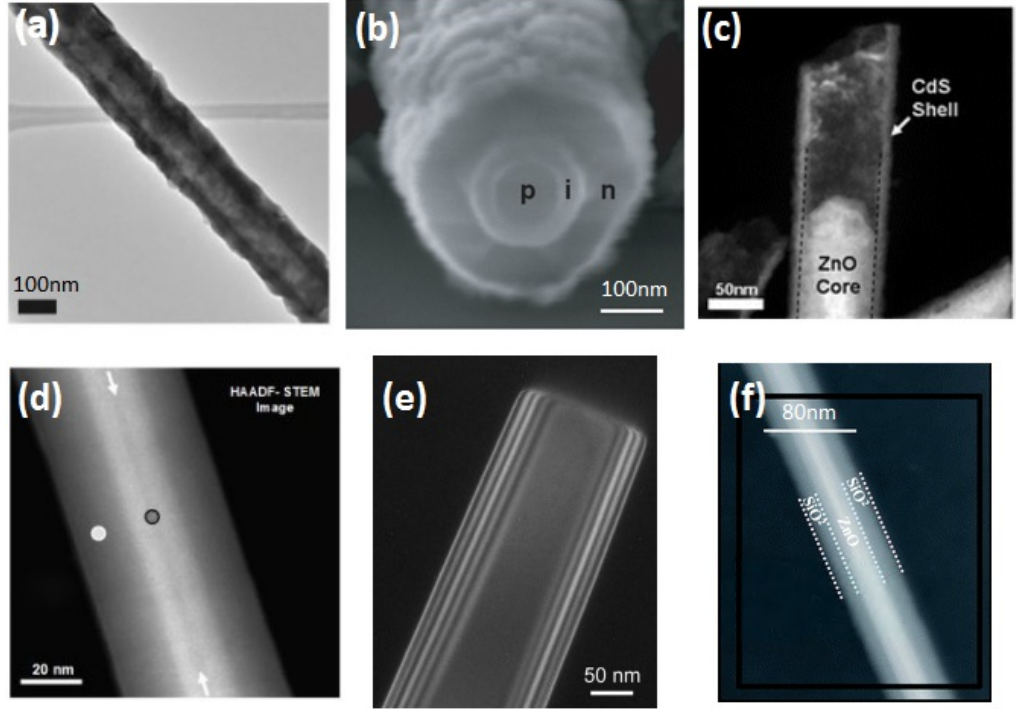


Figure 1.3: Some examples of fabricated multilayer nanowires: (a) a Si/CdS core/shell nanowire [15], (b) a coaxial nanowire with p-type core, intrinsic shell and n-type shell [16], (c) a ZnO/CdS core/shell nanowire fabricated by a two-step chemical solution method [17], (d) a single GaAs/AlGaAs core/shell nanowire [25], (e) n-core, p-shell gallium nitride nanowires [18], and (f) ZnO/SiO₂ single core/shell nanowire [26].

ing long lasting, high efficiency memory devices with low-energy consumption [30]. New types of energy storage systems are introduced based on silicon nanowire electrodes in rechargeable lithium battery technology [31], integrated transistors [32] and electronic programmable nanowire circuits for nano-processors [33] are developed based on semiconductor nanowires.

In optics and photonics nanowires due to their substantial capability for light generation, absorption, detection, etc. are appropriate candidates for studying and controlling the behaviour of light. The range of applications of nanowires in optics is quite vast and covers many topics such as photodetectors and solar cells [34], chemical and gas sensors [35], microcavity lasers and LEDs [36], far-field applications and nanoantennas [37], nonlinear optics [38] and biophotonics [39]. In addition, nanowire-based photonic devices are highly capable for integration and have opened new doors and hopes to achieve fully integrated photonic and on-chip technologies [40].

A wide range of the developed nanowire systems for various optical applications, is a result of their high scattering or absorption efficiencies. In what follows, few examples of application of nanowires, mainly based on scattering and absorption of light, are selected for a brief review. By reviewing the capability of nanowires for controlling the behaviour of

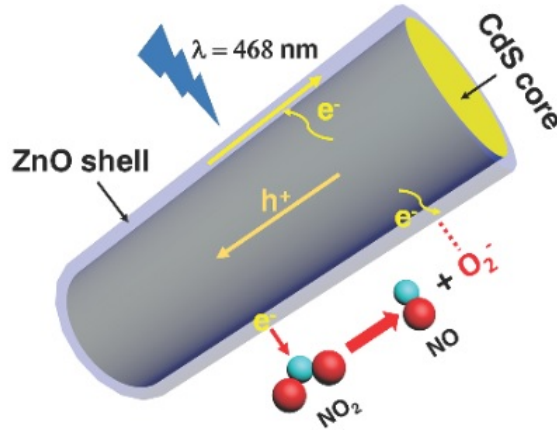


Figure 1.4: Light enhanced NO_2 sensing mechanisms in CdS/ZnO core/shell nanowire-based optoelectronic NO_2 gas sensor [41].

light, the importance of developing a novel solution and necessity of employing a powerful optimisation process for developing more efficient designs are discussed.

Sensing

The large surface-to-volume ratio of nanowires and their versatility for electrical and optical detection have made them highly capable for sensing systems. Their large aspect ratio and sufficient surface area can make them quite sensitive to environmental condition. This is useful for numerous sensing applications by manipulating electrons, photons, plasmons, phonons, and atoms, modifying their electrical and optical properties. For example, uniform CdS/ZnO core/shell nanowires can act as highly sensitive NO_2 sensors. Figure 1.4 demonstrates visible-light-activated gas sensing performance of these nanowires at room temperature [41]. High sensitive Mach-Zehnder interferometer coupled micro-rings based on silicon nanowires have been also experimentally realised with the shift of the resonance wavelength by 111nm per refractive index unit in response to various organic liquids. Such high sensitivity helps to obtain a large measurement range of change in refractive index from 1.0 to 1.538 [42]. Furthermore, optical response of nanowires inherited from the perm-selective nature and made of biocompatible polymer materials, have been reported for humidity and gas sensing. In such a sensor, gas molecules (such as NO_2 and NH_3) are detected by either bonding to nanowires' surface or diffusing into the polymer matrix, resulting in modification of their optical properties. This is not easily possible with other materials such as semiconductor nanowires or glass nanofibres [35]. Light assisted sensing with nanowires, is another interesting feature of nanowire-based sensors. As an example, room temperature ethanol gas sensing is reported by UV light assistance in ZnO/ZnS core/shell nanowires. Using the core-shell configuration under UV illumination, enhances the response to $\text{C}_2\text{H}_5\text{OH}$ gas with respect to ZnO nanowires in the same condition [43].

Apart from semiconductor and polymer nanowires, plasmonic nanowires are also suitable for sensing applications [44]. 70% of the atoms of ultra-thin gold nanowires, for instance, are at the surface, making their optical properties very sensitive to environmental conditions. The strong surface plasmons resonance (SPR) in gold nanowires has enabled surface enhanced techniques such as surface enhanced Raman spectroscopy based sensing [45, 46], for example in single molecule detection [47]. The shift of the SPR peak and its broadening due to high sensitivity of surface plasmon polaritons is the principle of colorimetric sensing [48]. It is also shown that waveguiding properties of polymer nanofibres which are uniaxially embedded with gold nanorods, make it possible to achieve highly efficient excitation of localised SPR, by photon to plasmon conversion with as high efficiency as 70% for a single nanorod [49]. These advances can lead to a compact, low operation power and fast humidity sensor.

In addition, some studies show, even machine learning techniques can be employed for improving the quality of nanowire sensing. Massive parallelism by many sensors, each with its different properties, are considered for example in gas sensing, to operate together. A simultaneous process of their outputs using neural networks can be a big step forward to achieve highly sensitive, smart systems [50]. High performance parallel and precise sensing based on nanowires with high surface-to-volume ratio, can be employed in digital imaging and CCD technology and recording the optical properties of partially polarised light which is reported by integrated aluminium nanowires [51].

In biophotonics, nanowire-based smart probes, can safely penetrate the plasma membrane and enter biological cells. Such nanostructures are potentially useful in high-resolution and high-throughput biosensing. It is shown that visible light can be guided into intracellular compartments of living cells, with a nanowire waveguide attached to the tapered tip of an optical fibre. This facilitates detecting optical signals from sub-cellular regions with high spatial resolution [52]. Low-loss crystalline and amorphous single-nanowires, activated with sensitive dopants, have been also demonstrated to act as highly sensitive and fast chemical and biological sensors with low power consumption [53].

There are many other examples, showing that nanowires are gaining their position in sensing technologies, from hydrogen [54, 55] and explosive material detectors [56] to high-sensitivity accelerometers [57]. Different configuration of nanowires show great promise in sensing applications by modifying their electrical and optical properties. Employing multilayer nanowires by designing optical resonance condition is discussed in Chapter 3, which makes an excellent platform for high performance optical sensing systems.

Solar cells

By increasing the demand for clean energy and decreasing the air pollution and carbon release in the atmosphere, solar energy is drawing more attention and becoming the most

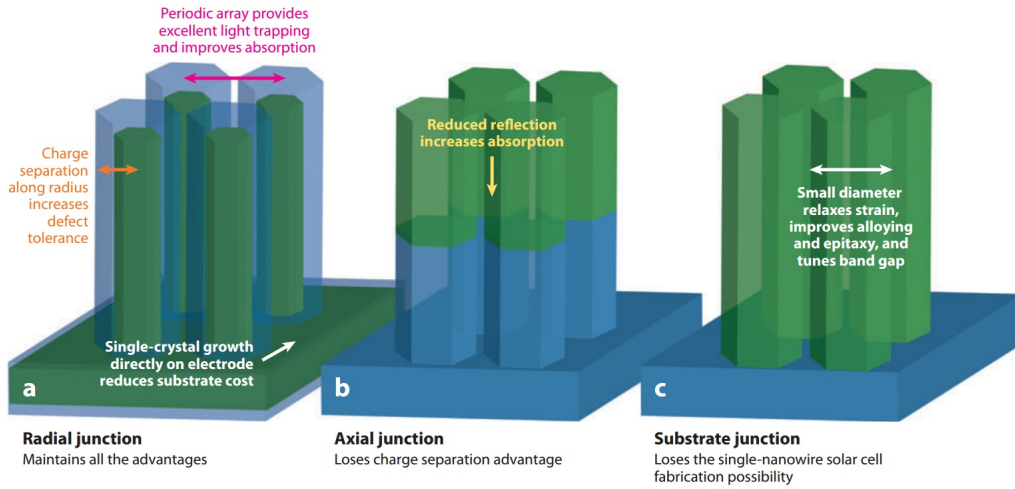


Figure 1.5: Radial vs axial junctions in nanowire solar cells [34].

important alternative for fossil fuels. Solar power generates electricity with no global warming, no pollution and no fuel costs, and it provides cleaner, reliable, and increasingly affordable sources of electricity. Significant efforts and improvements have been reported in making solar cells more affordable and efficient during the recent years. New materials and novel strategies have been introduced to achieve high performance harvesting of solar energy, including nanowire based solutions due to their high surface efficiency.

The geometry of nanowires facilitates light trapping, reducing reflective losses, improving band gap tuning, and increasing defect tolerance with respect to planar wafer-based or thin-film solar cells [34, 58]. Furthermore, vertically aligned silicon nanowires have been shown to be much less sensitive to impurities versus planar Si solar cells [34, 59] (see Fig. 1.5). These advantages do not increase the maximum efficiency of the solar cells above the fundamental limits, but instead they reduce the expense, by lowering the required quantity and quality of material to approach those limits [34, 58]. Another major challenge in the current photovoltaic technology is the fabrication of complex single-crystalline semiconductor devices on low-cost substrates. Nanowires address this, since it is possible to fabricate them on aluminium foil, stainless steel, and conductive glass [34]. With miniaturisation and integrating circuits, nanowire solar cells might also serve as integrated power sources for microelectronic systems.

Various nanowire structures are introduced for use in photovoltaics. Three layer p-type /intrinsic /n-type (p-i-n) silicon nanowire solar cells have been shown to have a maximum power output of up to 200 pW per nanowire device [13, 16] [see Figs. 1.3(b) and 1.6(a)]. Another study shows 19% efficiency improvement by having a nickel-silicide contact over the substrate as Fig. 1.6(b) illustrates.

Photocurrent generation in a single core-shell p-i-n junction GaAs nanowire grown on a silicon substrate, makes it even possible to go beyond the Shockley–Queisser limit [61, 62]. Studies also show that the axial junctions can be more tolerant to doping variations than

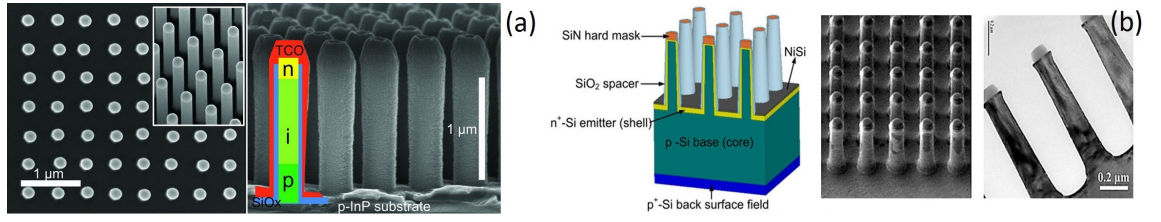


Figure 1.6: Different types of multilayer nanowires for solar cells: (a) InP axial-junction [13] and (b) Si radial-junction [60] nanowire array.

radial junctions, leading to higher electric potential difference between their terminals under certain conditions [63]. However, higher junction area in radially layered structures and more efficient access to the substrate, keep them more efficient than axial junction nanowires [34].

Many other different techniques are developed for improving the efficiency of nanowire solar cells. For instance, 2D conducting materials such as graphene, are reported to serve as the conductive back-contact of the semiconducting nanowires [64]. Another study shows TiO₂ nanowires dye-sensitised solar cells are finding their way to become alternative approaches to traditional p-n junction technology with acceptable efficiencies [65]. Also by making a careful arrangement, trapping of light by an array of silicon nanowires with radial p-n junctions, has been shown to increase the path length of incident solar radiation by up to a factor of 73 [8]. Nanowire solar cell systems show high capability for providing such significantly efficient platforms for resonant-absorption of light. A precise control of scattering and absorption by multilayer nanowires makes it possible to trap light in nanowire systems and to manage resonant super-absorption. This is discussed in detail in Chapter 3 by introducing all-dielectric and hybrid multilayer structures for more efficient light absorption.

Integrated optics

Optical signal processing without electrical currents and radio waves, has been a topic of great interest during the recent years [66]. By increasing the demand for faster data analysis, and storage of rapidly increasing amounts of data, the existent electronic technology will not be able to properly address the future requirements. Electronic integrated circuits have had remarkable success and the prospect of similar success in photonic integrated circuits (PICs) has fascinated photonics researchers since 1969 [67]. The existence of different types of optical components is essential to form light-based integrated circuits and PICs are still facing serious challenges to be practically useful due to difficulties in integration of various optical devices.

On the other hand, the concept of the realisation of highly integrated collection of nanowire elements for lasing and light emitting, wave-guiding, nonlinear pulse conver-

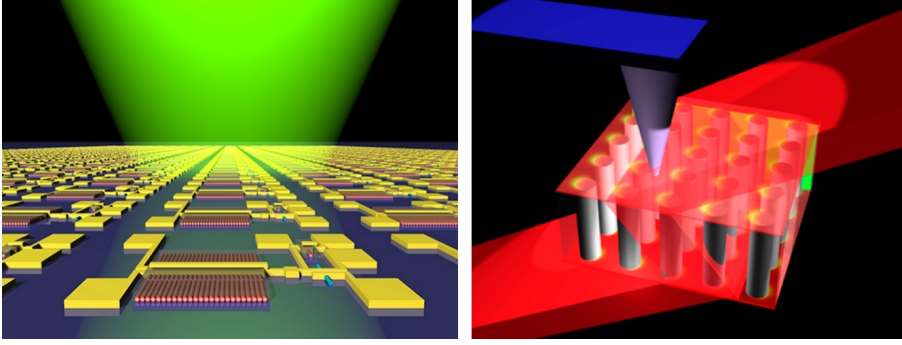


Figure 1.7: Schematics of future all-optical integrated circuits based on nanowire components [74, 75].

sion and photo-detection has made a promising perspective for future integrated optics. This image of ultra-compact photonic devices is based on the high capacity of nanowire-based components for high integration. Such a circuitry constructed from thousands of building blocks (as demonstrated schematically in Fig. 1.7 in a small scale), offers numerous opportunities for development of nanowire-based digital optical components for next-generation PICs [27]. For example, gap-variable couplers with micro-electromechanical silicon-nanowire-waveguide switches, have been introduced for optical switching [68–71]. All optical switching systems and logic gates are also demonstrated to have higher speed functionality in nanowire-based systems. A new type of logic gate has been reported comprising of simple networks of silver nanowires operating by controlling the polarisation and phase of the input optical signals [72]. As another example of all-optical switching, individual subwavelength CdS nanowire cavities, have been shown to be suitable for switching through stimulated polariton scattering, and a functional NAND gate is introduced based on these switches [73]. In the boundary of optical integration and sensing, hybrid photon-plasmon circuits by integrating silver nanowires with optical fibres are demonstrated experimentally by an all-fibre resonator and a Mach-Zehnder interferometer in optical communication frequency range [76]. Better nanoscale confinement and on-chip guiding of optical signals have been demonstrated by integrating multiple plasmonic waveguides with polymer optical nanowires [77].

By the rapid advances in variety of nanowire systems, from lasing to sensing and waveguiding to optical signal detection, nanowires are demonstrated to be reliable and capable building blocks for constructing PICs. Improving the compactness of the elements in PICs is one of the key points for realisation of more sophisticated photonic integration. The use of a high refractive index contrast in multilayer nanowires can highly confine the light propagation as an effective solution. This, together with single-mode operation of nanowire elements, can restrict their dimensions to sub-micron scale, making them capable to construct more compact components [78, 79]. By integrating more photonic components in small areas, employing a proper shielding structure between them becomes more critical. In this thesis by presenting my developed techniques to control the behaviour of light by multilayer nanowires, some efficient designs applicable in integrated optics are introduced.

In Chapter 4 a novel flexible, thin, symmetric and frequency selective shielding structure is discussed, which has a great capability to isolate nano-components in PICs.

1.4 Engineering optical properties of nanowires, and outlook of the thesis

Reviewing the role of nanowires in various applications, reveals their high capability for efficient solutions for optical systems. Developing novel designs which can employ more of these capabilities, is significantly important for improving the performance of optical nano-devices. However, this may require developing novel approaches without the limitations of the typical methods, which can analyse nanowire systems from a different point of view.

The typical routes for studying nanowire systems are numerical simulations and direct experiments, particularly for complex systems. In spite of their considerable benefits in investigation of nanostructures such as nanowires, none of them provide deep insight into underlying fundamental physics. Experiments are usually expensive in terms of time and material, especially when several parameters need to be optimised. Numerical methods have also limitations such as finite precision and are very time consuming. Furthermore, both experiments and numerical simulations can overlook nontrivial results and they often cannot explore the whole parameter space of a problem. Thus, it is important to develop fast and accurate methods, particularly for complex composite structures involving several constituents.

To address this, in this thesis, I suggest a novel semi-analytical approach to study nanowires for efficient engineering and optimising the behaviour of light. This approach employs a precise and fast semi-analytical solution for long nanowires and benefits a smart optimisation algorithm. I discuss my developed techniques for controlling the scattering and absorption of light, by examples of single and multi-element nanowire systems. Our further studies show that these techniques and the achieved results in two-dimensional platform, are also applicable for similar three-dimensional structures [80, 81].

In this study, there are some assumptions in technical discussions to prevent unnecessary complications, letting us concentrate on developing and analysing the main concepts. In summary, we assume (unless stated otherwise):

- The nanowires are long enough to be studied in a two-dimensional platform. Consequently, this is followed by:
 - Nanowires axes are parallel;
 - All the fields are propagating in the plane perpendicular to nanowires axes;

- One of the electric or magnetic fields vector is set and remains parallel to nanowires axes, determining TM or TE polarisation of the fields respectively;
- Being *multilayer* is defined in the radial direction (uniaxial with circular cross section);
- The effect of mechanical, thermal, chemical, and environmental parameters on the studied structures is negligible;
- All fields maintain the same polarisation and frequency as the incident wave.

The technical content of this thesis is mainly based on the information already published during my PhD (listed in my publications list). I review the analytical solutions for nanowires and Mie-type scattering in cylindrical systems, and the developed genetic optimisation algorithm [82] in Chapter 2. These are used as the key tools in the rest of the thesis to develop different structures, based on either a single nanowire in Chapter 3 [82–86], or in more complicated designs in Chapter 4 [87, 88]. Later in Chapter 5 it is demonstrated that semi-analytical solutions are not limited to linear structures [84].

Semi-analytical Approach

By increasing the demand for more efficient and precise designs for various applications, multi-parameter optimisation has become significantly important. Efficient optimisation techniques usually require hundreds or thousands of repeated analyses to gather enough data to conclude the optimised set of parameters' value. The high cost of repeating experiments, in terms of time, material and equipment expenses, makes experimental optimisation a practically difficult process, especially if a set of parameters should be optimised. On the other hand, acceptable meshing still remains a challenge in numerical techniques. By increasing the meshing precision to achieve more precise results, they become substantially time consuming especially for being repeated for many times as a part of optimisation purposes. Furthermore, none of experiments and numerical simulations provide us information about underlying physics of the studied structures such as behaviour of different harmonics. They can overlook nontrivial results and are not suitable for large parameter space exploration. This consequently prevents us from optimally controlling the behaviour of light.

Therefore for precisely designing and effectively optimising nanostructures in a multi-dimensional parameter space for a wide range of applications, we need to develop a fast solution which is accurately repeatable. Employing such an approach in a flexible and smart optimisation process, can basically lead a randomly suggested model to become an optimised and precisely functioning design. I managed to develop such an approach by the use of analytical and semi-analytical solutions and a smart genetic algorithm. This approach is used to study and optimise the optical properties of multilayer nanowires for different applications. The developed code in C++ is capable of analysing single nanowire systems or multi-element compounds and to optimise them in a multi-dimensional space. Mie-like solution to solve multipole expansion and multiple scattering problems is employed by expansion of the fields into cylindrical harmonics.

In this chapter the analytical and Mie-like solution for analysing cylindrical structures is reviewed and the mechanism of the optimisation process used in the rest of the thesis is explained. Decomposition of the fields into superposition of cylindrical harmonics, solving the boundary value problems, and the expansion coefficients are discussed. I start by

solving the wave equations in a single nanowire in Section 2.1 and discuss cross sections in Section 2.2 and plasmonic small size effect in Section 2.3. This is followed by a solution to systems consisting of more than one nanowire in Section 2.4. Finally in Section 2.5, the developed genetic optimisation algorithm is introduced which is employed for optimising the optical properties of nanowire systems.

2.1 2D Mie theory

The basics of light-matter interaction by particles and the response of positive and negative charges to incident electromagnetic fields was discussed in Chapter 1. The response of every single electric dipole contributes in the overall response of a particle, but as was mentioned, calculating and considering all the microscopic responses even in a micrometre scale particle and by having powerful computation facilities is not practical. Therefore we use macroscopic analysis to investigate the scattering and absorption of light by particles.

Mie-theory for analysing spherical particles was first introduced in 1908 by Gustav Mie [6] to explain the colourful effects of colloidal gold solutions. In Mie-theory, the Maxwell's equations are used for mathematical derivation of the incident, scattered and internal fields. These expressions take the form of an infinite series expansion of vector spherical harmonics [6, 89–91]. Nowadays, the interest in Mies theory is much broader, from interstellar dust, near-field optics and plasmonics to engineering subjects such as optical particle characterisation or nano-medical applications. Mie theory can be applied in many areas as scattering particles are often considered as homogeneous isotropic structures or can be approximated in such a way. However, I developed a novel semi-analytical approach based on Mie solution for highly nonlinear structures which experience inhomogeneous correction in refractive index [84]. This approach is separately discussed in Chapter 5.

The same concept of Mie-theory based on expansion of fields into spherical harmonics, is applicable on cylindrical structures by similar expansion of the fields into infinite series of cylindrical harmonics. As the focus of this thesis is studying nanowires and cylindrical structures, reviewing the original spherical fields' expansion is out of the scope of this thesis. We focus on investigating cylindrical Mie-like scattering solution which is discussed in detail in this chapter.

We start with decomposition of a planewave into cylindrical harmonics in a single nanowire system. Figure 2.1 demonstrates the general geometry of the problem, the planewave (propagating along x) and the cross section of a multilayer nanowire. We study TE and TM polarisations by assuming the magnetic and electric fields polarised parallel to the axis of the cylinder in z direction respectively [89, 90].

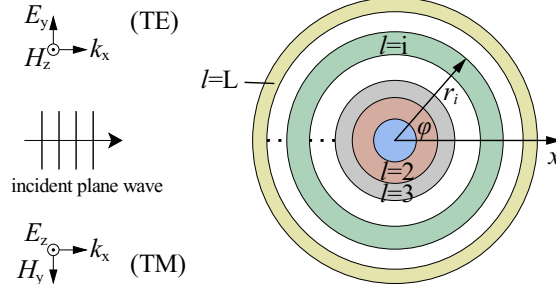


Figure 2.1: Schematics of the problem: A multi-layer cylindrical nanowire along z axis and TM/TE polarised planewave propagating in x direction.

TE polarisation

In TE polarisation (magnetic field polarised parallel to the nanowire's axis), the magnetic field of the incident planewave can be expressed as $\mathbf{H}^{Inc} = \hat{\mathbf{a}}_z H_0 \exp[-i\omega t + ik_0 r \cos(\varphi)]$, where $\hat{\mathbf{a}}_z$ is the unit vector in direction of z axis, H_0 is the incident magnetic field amplitude ($E_0 = \eta_0 H_0$ where $\eta_0 = [\mu_0/\epsilon_0]^{\frac{1}{2}}$ is the free space impedance) and ω is angular frequency. The incident planewave, then can be written as a superposition of cylindrical Bessel functions as [89, 90]:

$$\mathbf{H}^{Inc} = \hat{\mathbf{a}}_z H_0 \sum_{n=-\infty}^{+\infty} i^n J_n(k_0 r) \cos(n\varphi), \quad (2.1)$$

where $k_0 = 2\pi\lambda^{-1}$ (λ is the wavelength), J_n and $H_n^{(1)}$ are the n -th order Bessel function and Hankel functions of the first kind, respectively; n is the mode number, r is the radius and φ is the azimuthal angle in cylindrical coordinate.

In an L -layered cylindrical structure as is demonstrated in Fig 2.1, the total fields can be presented as a function of r and φ as:

$$\mathbf{H}_z(r, \varphi) = \hat{\mathbf{a}}_z H_0 \sum_{n=-\infty}^{+\infty} i^n \left[\tau_n^l J_n(\beta_l r) + \rho_n^l H_n^{(1)}(\beta_l r) \right] \cos(n\varphi), \quad (2.2)$$

$$\mathbf{E}_\varphi(r, \varphi) = \hat{\mathbf{a}}_\varphi E_0 \sum_{n=-\infty}^{+\infty} \frac{i^{(n+1)}}{\sqrt{\epsilon_l(\lambda)}} \left[\tau_n^l J_n'(\beta_l r) + \rho_n^l H_n^{(1)'}(\beta_l r) \right] \cos(n\varphi), \quad (2.3)$$

$$\mathbf{E}_r(r, \varphi) = \hat{\mathbf{a}}_r E_0 \sum_{n=-\infty}^{+\infty} \frac{ni^n}{k_0 r \epsilon_l(\lambda)} \left[\tau_n^l J_n(\beta_l r) + \rho_n^l H_n^{(1)}(\beta_l r) \right] \sin(n\varphi), \quad (2.4)$$

in which $\beta_l = k_0 \sqrt{\epsilon_l(\lambda)}$ where $\epsilon_l(\lambda)$ is the dielectric constant in layer l at wavelength λ , τ_n^l and ρ_n^l are n -th mode expansion coefficients in the l -th layer which are found by solving the boundary condition equations for the tangential components H_z and E_φ . Additionally, we put $\rho_n^1 = 0$ to avoid singularity of Hankel functions at the origin, and $\tau_n^{L+1} = 1$ for each mode, to describe the incident plane wave expansion through the cylindrical waves

(see Eq. 2.1).

TM polarisation

Similar to TE polarisation, with electric field parallel to the axis of the nanowire, we can write the incident planewave as $\mathbf{E}^{Inc} = \hat{\mathbf{a}}_z E_0 \exp[-i\omega t + ik_0 r \cos(\varphi)]$ and write its decomposition as [89, 90]:

$$\mathbf{E}^{Inc} = \hat{\mathbf{a}}_z E_0 \sum_{n=-\infty}^{+\infty} i^n J_n(k_0 r) \cos(n\varphi) \quad (2.5)$$

Therefore in an L -layered cylindrical structure, the total fields in layer l can be presented as:

$$\mathbf{E}_z(r, \varphi) = \hat{\mathbf{a}}_z E_0 \sum_{n=-\infty}^{+\infty} i^n \left[\tau_n^l J_n(\beta_l r) + \rho_n^l H_n^{(1)}(\beta_l r) \right] \cos(n\varphi), \quad (2.6)$$

$$\mathbf{H}_\varphi(r, \varphi) = -\hat{\mathbf{a}}_\varphi H_0 \sum_{n=-\infty}^{+\infty} i^{(n+1)} \sqrt{\epsilon_l(\lambda)} \left[\tau_n^l J_n'(\beta_l r) + \rho_n^l H_n^{(1)'}(\beta_l r) \right] \cos(n\varphi), \quad (2.7)$$

$$\mathbf{H}_r(r, \varphi) = -\hat{\mathbf{a}}_r H_0 \sum_{n=-\infty}^{+\infty} \frac{ni^n}{k_0 r} \left[\tau_n^l J_n(\beta_l r) + \rho_n^l H_n^{(1)}(\beta_l r) \right] \sin(n\varphi). \quad (2.8)$$

The boundary condition equations for the tangential components in TM polarisation is defined by making E_z and H_φ components equal, in both sides of all the boundaries.

Similar to Mie solutions, the effective number of excited modes can be truncated based on the size parameter $M = k_0 r_L + (k_0 r_L)^{1/3} + 2$ in which r_L is the radius of the outer layer (see Ref [2] for example). Then, by solving the set of equations for the boundary conditions ($2 \times L \times M$ equations), we can find $2LM$ unknown amplitudes of the cylindrical modes, letting us find electromagnetic field distribution in the whole space.

2.2 Cross-sections

To characterise scattering and absorption properties of nanoparticles, it is convenient to use the scattering cross-sections (SCS) and absorption cross-sections (ACS) respectively, which are defined as: $\sigma^s = P^{sct}/I_0$ and $\sigma^a = P^{abs}/I_0$, where P^{sct} and P^{abs} are the scattered and absorbed power and I_0 is the incident power density, and in 2D case, all per unit length. SCS and ACS of nanowires can be studied in cylindrical coordinates, and be represented as a superposition of different cylindrical modes. This decomposition can generally be represented as $\sigma^{s/a} = \sum_{n=-\infty}^{+\infty} \sigma_n^{s/a}$, in which $\sigma_n^{s/a}$ is a single mode SCS/ACS (positive and negative order harmonics) and n is the mode number [2]. The spectral

behaviour of every mode is a function of the size and material parameters of the particle.

In a single nanowire, the mode degeneracy of the positive and negative orders appears due to the azimuthal symmetry. They are equal and add together across the spectrum, which leads to doubling the absorption of every harmonic with respect to the single-mode value (except for $n = 0$ mode). Also from energy conservation for non-radiating modes, the σ^a can be written as $\sigma^a = \sigma^e - \sigma^s$, where σ^e is the extinction cross-section (ECS).

By solving the boundary value equations and obtaining the expansion coefficients, the σ^s which is defined as the ratio of the total scattered power to the intensity of the incident plane wave, can be found as:

$$\sigma^s = \frac{2\lambda}{\pi} \sum_{n=-\infty}^{+\infty} |\rho_n^{L+1}|^2. \quad (2.9)$$

The extinction cross section is defined as the ratio of the sum of the total scattered and absorbed powers to the intensity of the incident plane wave, and can be expressed as:

$$\sigma^e = \frac{2\lambda}{\pi} \sum_{n=-\infty}^{+\infty} \text{Re}\{\rho_n^{L+1}\}. \quad (2.10)$$

Therefore the ACS for each mode is found by

$$\sigma_n^a = \sigma_n^e - \sigma_n^s. \quad (2.11)$$

Also, it is possible to introduce *normalised cross-section* (NSCS, NACS and NECS for normalised SCS, ACS and ECS, respectively) as,

$$\hat{\sigma} = \frac{\pi}{2\lambda} \sigma. \quad (2.12)$$

It can be shown that the single mode limit of $\hat{\sigma}_n^s$ and $\hat{\sigma}_n^e$ is equal to unity and $\hat{\sigma}_n^a$ is limited to 0.25, similar to spherical nanostructures [92].

2.3 Plasmonic small-size effect

It is well known that small nanoparticles may have dielectric constants quite different from those of bulk materials. Confinement of electrons' motion in conductive nanowires becomes more significant when their diameter decreases to the mean-free-path of free electrons in bulk material and less. In long multilayer nanowires in particular, when the thickness of a plasmonic layer becomes comparable to the electron mean free path or smaller, the collision frequency is modified. This causes considerable changes in the nanowire conductivity and in the optical properties by getting strong influence of the surface. By making a nanowire thinner, the electrons reach the surface faster causing an increase in the rate of their

scattering. This random way of electron scattering can cause the coherence of overall plasmon oscillation to disappear and result in increasing its bandwidth [93, 94].

To take this size-dependent effect into account, we modify the collision frequency of the Drude model γ , making the following replacement: $\gamma_{small-particle} = \gamma_{bulk} + V_f/d$, where V_f is the Fermi velocity. d is the characteristic size of the metallic structure [93, 94] which here, in multilayer nanowires discussion refers to the thickness of a metallic shell or diameter of a metallic rod. However, as is discussed later, Drude's model does not describe accurately the experimental data for noble metals in the visible spectrum. For longer wavelengths these discrepancies can be reduced by using appropriate values of ϵ_∞ , γ and ω_p (ϵ_∞ is the relative permittivity for high frequencies in bulk material, where electrons cannot follow excitation and the illumination does not see free electrons anymore). This, however, still does not describe the parameters of plasmonic materials well enough for higher frequencies, namely above the interband transition frequency [95].

To obtain the corrected dielectric permittivity of metals in nanoparticles using experimental data, we use real (ϵ_r) and imaginary (ϵ_i) parts of bulk materials to achieve exact γ_{bulk} and ω_p by using the Drude formula as follows:

$$\gamma_{bulk} = \frac{\omega \epsilon_i}{(\epsilon_\infty - \epsilon_r)} \quad , \quad \omega_p^2 = \omega^2 \frac{(\epsilon_\infty - \epsilon_r)^2 + \epsilon_i^2}{\epsilon_\infty - \epsilon_r}. \quad (2.13)$$

Then by calculating $\gamma_{small-particle}$ we recover the value of ϵ using Drude's model (one also can use the approximation $\epsilon_{small-particle} = \epsilon_{bulk} + i[\omega_p^2 V_f]/[\omega^3 d]$) [83].

2.4 Multiple scattering

In a multi-element systems constructed of more than one nanowire (see Fig. 2.2), we first solve the boundary condition equations for individual wires separately and find the expansion coefficients. Solving the boundary value equations gives us ${}_s^c \tau_n^l$ and ${}_s^c \rho_n^l$ coefficients, where the left-subscript 's' indicates the single nanowire and superscript 'c' refers to the nanowire 'c' (therefore ${}_s^c \tau_n^l$ and ${}_s^c \rho_n^l$ indicate the expansion coefficients for mode 'n' in layer 'l' of nanowire 'c', independent of interference effect of other nanowires - because of subscript 's'). Then we employ multiple scattering problem solution, to consider the interaction between the nanowires [91, 96, 97]. The scattered field from one cylinder becomes an incident wave on another in addition to the incident planewave. Using the translation additional theorem, we can rewrite the scattered fields in the form of Hankel function, to the new form of a superposition of incident Bessel functions as [98]

$$e^{-in\theta_2} H_n(kr_2) = (-1)^n \sum_{m=-\infty}^{+\infty} H_{m+n}(kd) J_m(kr_1) e^{im\theta_1}, \quad (2.14)$$

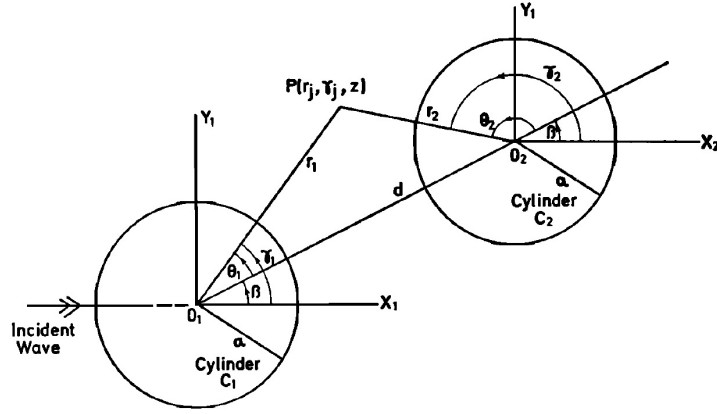


Figure 2.2: The geometry of the multiple scattering problem. Two nanowires are parallel to each other and perpendicular to the direction of incident planewave propagation [96].

where θ is the angle between the nanowires centre-to-centre line and the direction of each centre to the observation point [96, 97] as Fig. 2.2 demonstrates. This procedure leads the modified expansion coefficients ${}^c_m \rho_n^{air}$ for each nanowire in which the left-subscript 'm' indicates the case of multiple scattering between the cylinders. By having ${}^c_m \rho_n^{air}$, we calculate the fields inside the nanowire 'c' independent of the other nanowires by solving the boundary conditions and obtain new ${}^c_m \tau_n^l$ and ${}^c_m \rho_n^l$ coefficients for each layer of the multilayer nanowire 'c'.

Cross sections

The total cross sections are modified in multiple scattering regime due to the interference of the fields. The total value of σ^e and σ^s can be expressed as:

$$\sigma^e = \frac{2\lambda}{\pi} \sum_{c=1}^W \sum_{n=-\infty}^{+\infty} Re\{ {}^c_m \rho_n^{L+1} e^{-i\beta R_c \cos \phi_c} \}, \quad (2.15)$$

and

$$\sigma^s = \frac{2\lambda}{\pi} \sum_{c=1}^W \sum_{n=-\infty}^{+\infty} \left[|{}^c_m \rho_n^{L+1}|^2 - Re\{ conj({}^c_m \rho_n^{L+1} e^{-i\beta R_c \cos \phi_c}) (1 - \frac{{}^c_m \rho_n^{L+1} e^{-i\beta R_c \cos \phi_c}}{{}_s \rho_n^{L+1}}) \} \right], \quad (2.16)$$

where 'W' is the number of the nanowires, R_c and ϕ_c indicate the position of nanowire 'c' and $e^{-i\beta R_c \cos \phi_c}$ is the phase of the incident wave (propagating in x direction) at the site of nanowire 'c' with respect to a reference frame.

2.5 Genetic algorithms

In the introduction of this chapter the importance of an effective optimisation for designing high performance optical systems was discussed. In optimisation problems, we basically have a set of variables with their defined range of variation and one or more functions based on these parameters which are going to reach their maximum or minimum, or to be set at specific optimum points with respect to each other. The optimised value of parameters can tune the system in locally optimum situation, which means by a small change in any of the parameters we will lose the optimal condition. Or we may find a set of parameter values to tune the system in a globally optimised condition which means there is no other set of allowed values for a better functionality.

Different optimisation methods have been introduced and applied for different problems. Here, genetic algorithms are chosen as they are significantly effective optimisation procedures based on mimicking ‘natural selection’. Genetic algorithms (GAs) are used for finding a global extremum of multi-dimensional target functions within the defined parameter space. These adaptive algorithms have been employed in a variety of scientific and engineering problems forming computational models of evolutionary systems [99–103]. GAs are also employed for optimisation of various electromagnetic properties of optical devices and systems [104–111] and specifically scattering problems [112–117].

Here, I briefly outline the algorithm that is used in my simulations. Figure 2.3 demonstrates the principles of a GA. Figure 2.3(a) shows how genetic algorithms are based on natural selection. First, a ‘generation’ of ‘individuals’ are generated which are not necessarily including an optimised individual. But undergoing the rest of the procedure is the way that can lead to a generation which includes one or more acceptably optimised individuals. The individuals of each generation population compete with each other and only the higher ranked individuals can survive to generate the next generation.

To start, we form arrays of similar variables that we aim to optimise, which in our case can be thickness of the layers in a multilayer structure, material of the layers, nanowire location or the wavelength for instance. By the defined analogy of GAs in computer science [99–101], we call these sets of parameters as ‘chromosomes’, while each variable within these chromosomes is a ‘gene’. In Fig 2.3(b) a three-gene chromosome structure has been shown. We generate a large number of random chromosomes, as individuals of the first generation. Next, we choose random pairs of these individuals to act as ‘parents’, then we apply ‘crossover’ and ‘mutation’ processes to generate ‘offspring’ for the next generation.

The crossover process involves breaking parents’ chromosomes and swapping their heads and tails between the two chromosomes to form two new offspring chromosomes with the same number of genes [118]. Figure 2.3(b) shows how crossover can be performed by breaking the chromosomes in randomly chosen points. Here, a one-point-crossover method

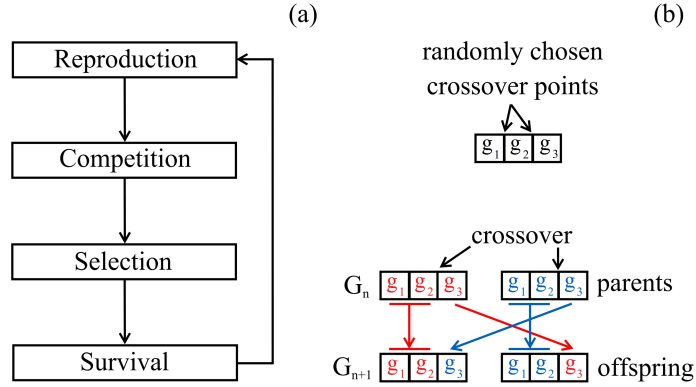


Figure 2.3: (a) General flow of a genetic algorithm based on natural selection, and (b) crossover process which is applied on three-gene chromosomes. Chromosomes of parents are divided into two parts (head and tail) which are then swapped to generate offspring by having their properties. The crossover point is chosen randomly. G_n and g_{1-3} indicate generation n , and different genes, respectively.

is used while it is also possible to use two-point-crossover to break parents' chromosomes into three parts and swap only the middle part's genes for generating offspring. Mutation is the process of randomly change of genes' value (every couple of generations) to maintain 'genetic diversity' [119]. In our problem, mutation implies changing the physical properties of nanowires, such as material or the thickness value of a layer, wavelength, etc.

Next, we sort the individuals of offspring generation based on how close they are to our defined goal. Mathematically this means that we need a 'fitness function' in order to evaluate each individual in the population by assigning 'fitness values'. Then, a random quantity of the individuals with the lowest fitness values, is removed from the population and replaced with additionally generated offspring of the best parents (the population of parents' generation should also be evaluated based on the fitness function). The best individual during all the generations is saved to randomly enter to the next generations (if a better individual than the current best one is identified, the new one replaces the current one). 'Tabu search' technique should also apply to find the local optimum value [120]. The local search technique can also be applied for some random individuals in periodically chosen generations. By finalising the offspring generation, they act as parents and the procedure continues as Fig. 2.3(a) suggests, until the best individual of the last generation satisfies some defined conditions based on fitness function to be qualified enough to stop the procedure.

Figure 2.4 demonstrates how a genetic algorithm is applied on a nanowire system. Two four-layer nanowires are shown as parents, generating the next generation with crossover and mutation. A set of available materials can be defined for the genetic algorithm to choose among them randomly to construct different layers of the nanowires.

Apart from high level of flexibility and comprehensive exploration of parameter space

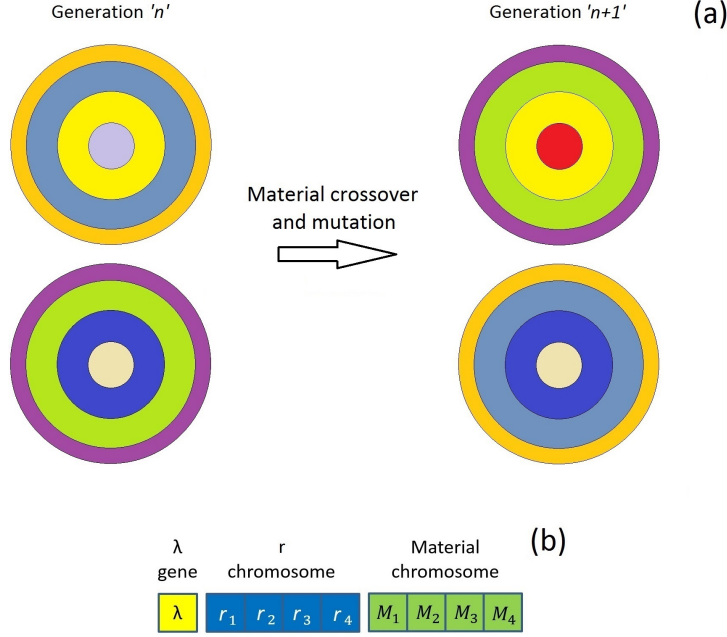


Figure 2.4: (a) An example of crossover and mutation in two four-layer individuals (optimisation of a single nanowire system). Parent and offspring nanowires are compared in two generations. The radii of the layers are the same in both parent nanowires but the materials differ. The first two layers, and the third and fourth layers of each nanowire in parents' generation, are swept to produce offspring nanowires. The core of one the offspring is randomly changed to another available material during a mutation of its gene. (b) A more general formation of chromosomes.

with such an algorithm, controlling practical considerations is significantly important. Therefore several steps to check the parameter values have been considered in the developed code. In each generation and during offspring generation, several conditions based on material properties are applied on choosing permitted materials for the adjacent layers to make sure about practical realisation possibilities. Size parameters and location of nanowires are continuously controlled to prevent them from overlapping and also keeping the predefined space between them. Also plasmonic small size effect and dielectric constant corrections are applied on metallic layers before calculating fitness values. The developed computer code used to achieve the results presented in this thesis, has a smart controlling procedure which checks all the required conditions and in case of any conflict, modifies the parameter values to the nearest acceptable set of values. It also controls the optimisation process not to be trapped in unwanted loops which may occur during the program execution. This helps the optimisation process to decide about how to continue calculations without requiring to manually stop it and correct the variables value. By employing the described analytical solution along with this smart optimisation process, analysing hundreds and thousands of structures becomes possible within a reasonable amount of time, which facilitates obtaining of highly precise optimised designs.

Some other novel and innovative techniques have been developed in this GA. For instance, all the population of the current generation are removed after several hundred

or thousand generations, followed by starting over by choosing new randomly generated individuals, similar to what was done for the first generation. The difference is that in this technique some previously found best individuals are used along with the new generation. Our observations demonstrate that this technique extends the random coverage of the parameter space in order to find the globally maximum fitness value. As another example, my developed code let us suggest some individuals among the population of the first generation, if there are already known good sets of guessed parameters [82].

Note!

In case of optimising a system with more than one nanowire, every individual is a multi-element system, containing the same number of nanowires. Therefor the total number of analysed nanowires is the number of nanowires defined in the original problem to be optimised, times the number of the population. In any case, every individual is analysed independent of the others.

Generally, the developed genetic algorithm used in this thesis, optimises four type of parameters:

- (i) the wavelength (λ),
- (ii) size parameters (r_l),
- (iii) materials used in the multilayer structure construction (ϵ_l), and
- (iv) the location of each nanowire (R_c, φ_c) to optimise the multiple scattering properties,

in which 'l' is the layer number and 'c' is the nanowire index. Chromosomes are defined as arrays including the genes of radii, wavelength, dielectric constants of the composed layers, and the location of the nanowire. Here I note that for preventing more complications, in optimising multi-element systems all the nanowires of each individual have been considered similar structures, which is more practical for realisation purposes.

In this chapter, I discussed the Mie-like scattering and multipole expansion method to analysis light-matter interaction in cylindrical structures. Moreover, multiple scattering problem for multi-element systems composed of multilayer nanowires was discussed. Different parameters such as extinction, absorption and scattering cross-sections, and the small size effect in plasmonic particles were discussed and mathematically explained. The general concept of genetic algorithms and the details of the optimisation process used in this thesis were introduced. My C++ code is based on the materials of this chapter and an additional developed approach which is discussed in Chapter 5. The described Two-dimensional analysis leads to an acceptable simplification of many scattering and absorption problems with less complications compared to similar three-dimensional problems and eases developing new solutions and ideas. Later, it is shown that the achieved results and the introduced approach are also applicable for three-dimensional structures.

Single Nanowires

In this chapter, the scattering and absorption of light by single multilayer nanowires are studied. I demonstrate that the total scattering of such structures can be suppressed leading to optimal invisibility cloaking. Moreover, I show that by overlapping the scattering or absorption resonances of different modes, it becomes possible to achieve enhanced effects, superscattering or superabsorption, respectively.

Here, both plasmonic and all-dielectric configurations are analysed by employing experimental material data in nanowires' construction. The full analytical method and the developed genetic algorithm described in Chapter 2 are used to optimise the optical properties of nanowires by adjusting the material, multilayer size parameters and the wavelength, for different polarisations.

Section 3.1 contains discussions about scattering of light by single nanowires. In Section 3.1.1 scattering cancellation and invisibility of nanowires [85] and in Section 3.1.2 the opposite effect, superscattering of light by nanowires [82] are discussed. In Section 3.1.3, nanowires with both scattering cancellation and enhancement properties are introduced using an example of a hybrid structure [83]. This is followed by studying the absorption of light by single nanowires and the superabsorption effect [86] in Section 3.2.

3.1 Scattering of light

We discuss the scattering of light by single nanowires in two different regimes: i) suppressed scattering which can result in invisibility cloaking, and ii) enhanced-scattering (superscattering effect). Then the coexistence of both the effects in one nanowire is discussed in the visible spectrum.

3.1.1 Invisibility

Subwavelength multi-layer structures may demonstrate very unusual optical properties which can be employed for engineering functional metadevices [121]. In particular, it was shown that multi-shell plasmonic nanoparticles may possess highly unusual scattering characteristics related to the reduced scattering attributed to invisibility cloaking and scattering cancellation [122–124]. One of the approaches to achieve nearly ideal invisibility is based on the so-called Transformation Optics [125–127], which relies on a coordinate transformation. Using transformation optics necessitates the use of materials having inhomogeneous anisotropic permittivity and permeability. This is not achievable without using metamaterials [128, 129], which normally have narrow bandwidth, high losses and other practical complications for optical frequencies. Therefore other approaches were developed including using non-magnetic materials [130], carpet cloaks [131], optical ‘Janus’ devices [132] and flattened Luneburg lenses [133].

Another technique is scattering cancellation with plasmonic or dielectric multilayer structures. One of the first examples was demonstrated by Kerker for core-shell spherical particles consisting of metallic core and dielectric shell [134]. The out-of-phase electric dipole polarisabilities of subwavelength metallic and dielectric parts lead to total scattering cancellation in the far-field. Later this approach was widely used for various layered plasmonic structures [135–140]. It has been shown that by using this approach and employing normal materials (isotropic, homogeneous and non-magnetic media), the scattering cross section can be minimised, thus providing invisibility of perfect electric conductor (PEC) cores. This is mostly achieved by a considerable number of layers [113, 117, 141, 142]. Cloaking by a few layers of lossless, epsilon-near-zero materials was also reported to cloak a PEC core with a plasmonic structure [113] which is not yet experimentally available. Generally, plasmonic materials make it easier to control the SCS, but they introduce prohibitively high losses near plasmonic resonance frequencies. This issue becomes less crucial far from the resonances, where reduction of the SCS can also be achieved [143]. One of the solutions to this problem is the use of nearly lossless dielectric materials to control SCS, and this is the focus of this section.

The possibility to realise a structure which is invisible in the optical range raises several important questions. (i) Is it possible to use real conventional materials to control SCS practically? (ii) How many layers are required to achieve the best invisibility possible? (iii) Can we design all-dielectric structures to exhibit lossless invisibility in the optical range? Here in this section these questions are answered, and it is shown that one can achieve up to 80 fold total scattering suppression. Then, it is demonstrated that the optimum invisibility is achievable with three or even smaller number of dielectric shells [85].

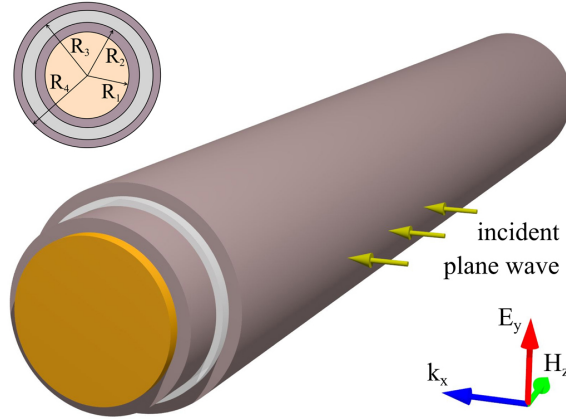


Figure 3.1: Geometry of the problem: cloaking of a cylindrical scatterer with a multi-layer all-dielectric coating. The plane wave is incident from the side and the magnetic field is parallel to the structure's axis.

All-dielectric structures for invisibility

Figure 3.1 shows general schematics of the problem, a cylindrical multilayer structure illuminated by a plane wave incident normal to the structure axis. The telecommunication wavelength of $1550nm$ is used by considering some randomly chosen, commonly used materials in studying optical structures, such as AlAs, TlBr and GaAs [144, 145] for the core.

We start with TE polarisation where the incident electromagnetic plane wave is propagating along the x axis, with the magnetic field polarised along the cylinder axis. Similar to Section 2.1, it is assumed that our multi-layer structure contains L layers, and it is placed in free space. This is followed by the electromagnetic fields decomposition into a superposition of cylindrical harmonics.

According to Eq. (2.9) and by taking into account $|\rho_{L+1}^n| = |\rho_{L+1}^{-n}|$ degeneracy for a single nanowire due to the azimuthal symmetry, the SCS can be expressed as a function of mode amplitudes as [89, 90]

$$\sigma^s = \frac{2\lambda}{\pi} \left(|\rho_{L+1}^0|^2 + 2 \sum_{n=1}^{+\infty} |\rho_{L+1}^n|^2 \right). \quad (3.1)$$

Invisibility implies that the SCS of the whole structure is minimised (the studied dielectric materials are almost lossless in telecommunication frequency). We aim to achieve this by the proper design of multilayer dielectric shells. To do so, the GA from Section 2.5 is employed to search for the optimal values of materials permittivity as well as layers' radii to minimise the total scattering at a given wavelength. We first define the material and the radius of the scatterer (core) as the input of our optimisation process. A set of materials is also defined according to the working wavelength ($\lambda = 1550nm$) and experimental

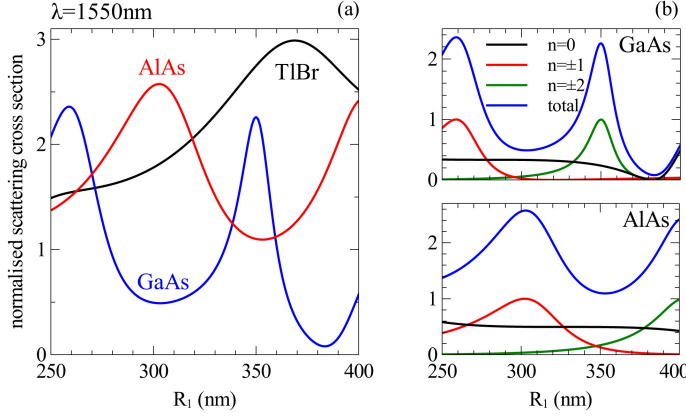


Figure 3.2: (a) Dependence of the normalised scattering cross-section on the cylinder radius for three different materials at 1550nm , and (b) decomposition of the total scattering cross-section into contributions from different multipoles for GaAs and AlAs nanowires. The radii of nanowires are chosen such that their NSCS reaches maximum at $\lambda = 1550\text{nm}$ ($r_{\text{AlAs}} = 303\text{nm}$, $r_{\text{TlBr}} = 369\text{nm}$ and $r_{\text{GaAs}} = 261\text{nm}$).

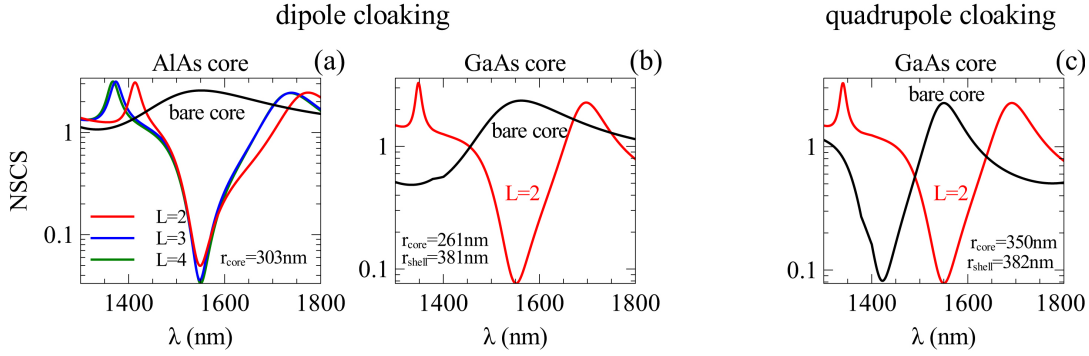


Figure 3.3: Suppression of the total scattering cross section for two different core materials. The core radii are chosen based on Fig. 3.2 to have the maximum SCS to be cancelled. (a,b) Demonstration of SCS suppression for dipolar resonance and (c) similar results for quadrupole cloaking, indicating the efficiency of the approach for different multipolar orders.

data [144, 145] from which the GA chooses dielectric constants randomly to form the layers in the shell. To employ the genetic algorithm to minimise the scattering cross section, we define the fitness function as

$$F(r_{1-L}, \varepsilon_{1-L}) = \min\{\hat{\sigma}^s(r_1, \dots, r_L, \varepsilon_1, \dots, \varepsilon_L)\} \quad (3.2)$$

where r_l represents the outer radius of the l -th layer. The GA searches the parameter space by calculating fitness values and then removes and replaces the individuals with lower fitness values (the fitness value of an individual shows how close it is to the ideal properties the GA is looking for, as explained in 2.5).

We aim to suppress the total SCS of the resonant dielectric core. Therefore, to begin and to make more challenges for our optimisation process, we choose a radius of the core r_1 such that the nanowire exhibits the maximum of SCS at $\lambda = 1550\text{nm}$. Figure 3.2(a) shows

Table 3.1: Optimisation of the invisibility of AlAs, TlBr and GaAs nanowires by multi-shell structures (silicon and fused-silica). The red numbers indicate repeated values which do not improve the optimisation process as compared to previously found results. The green numbers represent the optimised SCS and size parameters. Adding more layers to the optimised shells does not reduce the SCS any further. The core radii r_1 are chosen based on Fig. 3.2 to have the maximum SCS without dielectric shells. The superscript ‘§’ indicates the bare core while ‘†’ and ‘‡’ indicate the shells’ sequence starting with silicon and fused-silica, respectively.

	Core	Config.	SCS	r_1	r_2	r_3	r_4	r_5
AlAs		1 [§]	2.575	303				
		2 [†]	0.05	303	431			
		2 [‡]	2.575	303	303			
		3 [†]	0.05	303	431	431		
		3 [‡]	0.036	303	309	432		
		4 [†]	0.033	303	346	355	433	
		4 [‡]	0.036	303	309	432	432	
		5 [†]	0.033	303	346	355	433	433
		5 [‡]	0.033	303	303	346	355	433
TlBr		1 [§]	2.988	369				
		2 [†]	0.359	369	496			
		2 [‡]	2.988	369	369			
		3 [†]	0.359	369	496	496		
		3 [‡]	0.181	369	392	503		
		4 [†]	0.170	369	402	426	504	
		4 [‡]	0.181	369	392	503	503	
		5 [†]	0.170	369	402	426	504	504
		5 [‡]	0.170	369	369	402	426	504
GaAs		1 [§]	2.353	261				
		2 [†]	0.076	261	381			
		2 [‡]	2.353	261	261			
		3 [†]	0.076	261	381	381		
		3 [‡]	0.076	261	261	381		

the normalised scattering cross section as a function of nanowires’ radius for different materials. Figure 3.2(b) shows the decomposition of the SCS into contributions from different order modes, namely monopole, dipole and quadrupole. Contributions from higher order modes are negligible.

The genetic algorithm uses a database of several dielectric materials, and it chooses the ones that are more suitable for cloaking. I noticed that the GA always chooses two types of materials with the lowest and highest dielectric constants to form the highest possible index contrast between the shell layers, which in our database are fused-silica and silicon. Materials with dielectric constant values in between are not chosen by the GA and adding such materials to our set does not help improving the cloaking quality. Figure 3.3 shows the reduction of the SCS that can be achieved by coating the nanowires by dielectric layers. Black curves correspond to the SCS of the nanowire without shells. Figure 3.3(a) shows how the scattering cross-section of AlAs nanowire can be reduced by

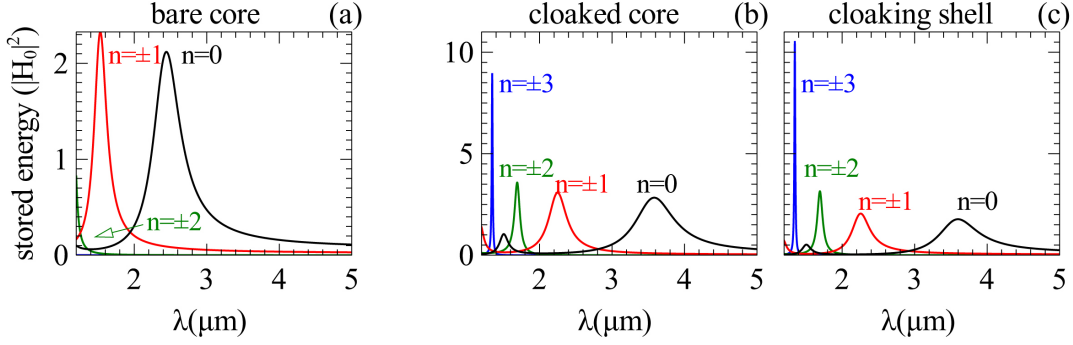


Figure 3.4: Stored energy. The values are normalised to $|H_0|^2$ and shown inside (a) the bare core, (b) the cloaked core and (c) the cloaking shell. Coating the silicon layer causes a red-shift in the resonance of all modes.

adding more shells. Even 1 shell ($L=2$) reduces the SCS by a factor of 50. Adding up to 3 shells allows the SCS to be reduced by 80 times. Figure 3.3(b) demonstrate that the SCS of the GaAs nanowire can be reduced by a factor of 30. In both cases the main contribution to the scattering cross-section is given by the dipole mode excitation in the structure. To show the wide applicability of the GA approach, a thicker GaAs core is also considered with radius of 350nm . For such a nanowire, at the telecommunication wavelength, the main contribution to the SCS is given by the quadrupole mode according to 3.2. Figure 3.3(c) shows that the scattering induced by the quadrupole mode can be also suppressed by an appropriate choice of cloaking shell. The detailed optimisation results for dipolar cloaking are summarised in Table 3.1. I note that for a simple core-shell structure, analytical expressions exist for the optimum shell size to compensate the SCS induced by individual modes, however, such expressions do not exist for the total SCS, nor for the case of multilayer structures. Therefore this approach provides a more universal solution to cloaking optimisation problems.

Now we would like to understand the physical origin of the observed invisibility. One of the obvious reasons could be that the reduction of scattering is caused by a shift of the resonance of the core caused by adding a dielectric layer. To have more in-depth physical interpretation of the optimisation process, we calculate the stored energy inside the core and the shell of the introduced GaAs/Si core/shell structure separately for different modes, as demonstrated in Fig. 3.4. To calculate the stored energy in layer ‘ l ’ of a multi-layer nanowire, we use

$$W_l^n = \frac{1}{4} \int_l [\epsilon_l (|E_r^n(r, \varphi)|^2 + |E_\varphi^n(r, \varphi)|^2) + \mu |H_z^n(r, \varphi)|^2] dv, \quad (3.3)$$

in which n is the mode number. Figure 3.5 demonstrate the spectrum of expansion coefficients in this structure for different modes and how the variation in real and imaginary parts of the coefficient shown in Fig. 3.5(a) for every layer, causes scattering cancellation in Fig. 3.5(b) demonstrated separately for each mode. This is explainable directly by the materials in Section 2.1 which our GA is employing.

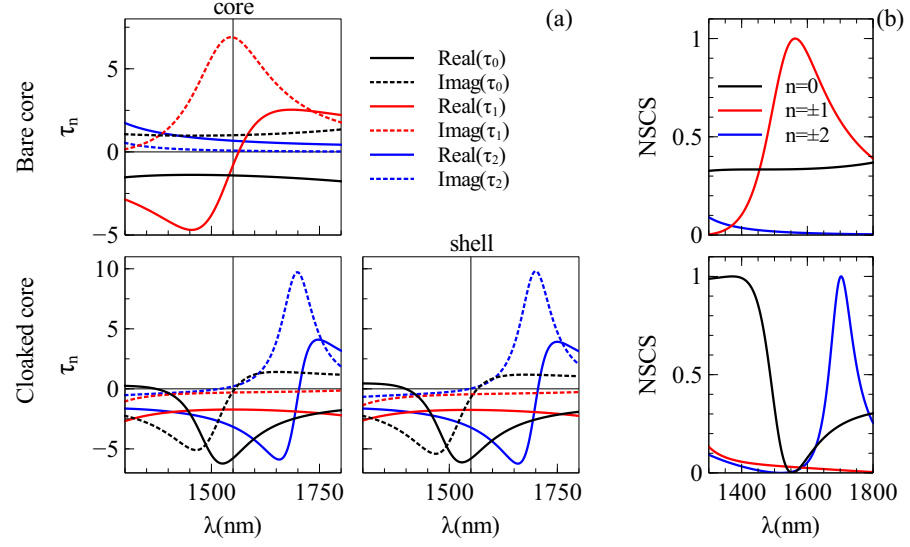


Figure 3.5: (a) The spectrum of the expansion coefficients inside the GaAs-Si nanowire in two cases of the bare core and the core-shell structure. The coefficients are plotted separately for each layer. (b) The normalised scattering cross section for the bare and cloaked GaAs core.

Indeed, if we take a single dielectric shell and change its radius continuously, as presented in Fig. 3.6, all the resonances linearly shift with the shell thickness. Importantly, the optimal minimal SCS [see Fig. 3.7] is achieved near the resonant conditions of both core and shell as indicated by the dotted lines in Figs. 3.6 and 3.7. The peculiarity is that while the initial resonances are shifted towards longer wavelengths, different resonances appear at the given wavelength [see Fig. 3.4]. Similar to Kerker's original approach [134], we have two out-of-phase resonant modes excitations of the core and shell which compensate each other in the far-field, resulting in scattering cancellation, with one important difference that now we are dealing with dielectric materials only.

Table 3.1 also illustrates that by adding more layers, the SCS saturates. Values shown in red in the table indicate configurations found by the GA that repeat results obtained for a smaller number of coating layers. After obtaining the optimised design (the green numbers in the table), the GA merges newly added layers to the previously existing ones and decreases the number of layers to the optimised design. In case of the GaAs scatterer, this saturation happens by coating the first silicon layer. The invisibility of AlAs and TlBr cores saturates when adding three dielectric layers. This is in contradiction with the effective medium theory (EMT) for cloaking with anisotropic materials which predicts better invisibility with increasing number of isotropic layers [146–148].

The field profiles of bare nanowires and core-shell structures with cores made of AlAs and GaAs are calculated in both near and far field regions using the optimised parameters from Table 3.1 and they are shown in Fig. 3.8. The comparison between the far field profiles in bare and invisible structures reveals the drastic suppression of scattering and shows how the invisibility of the structures are obtained using only one or three coating

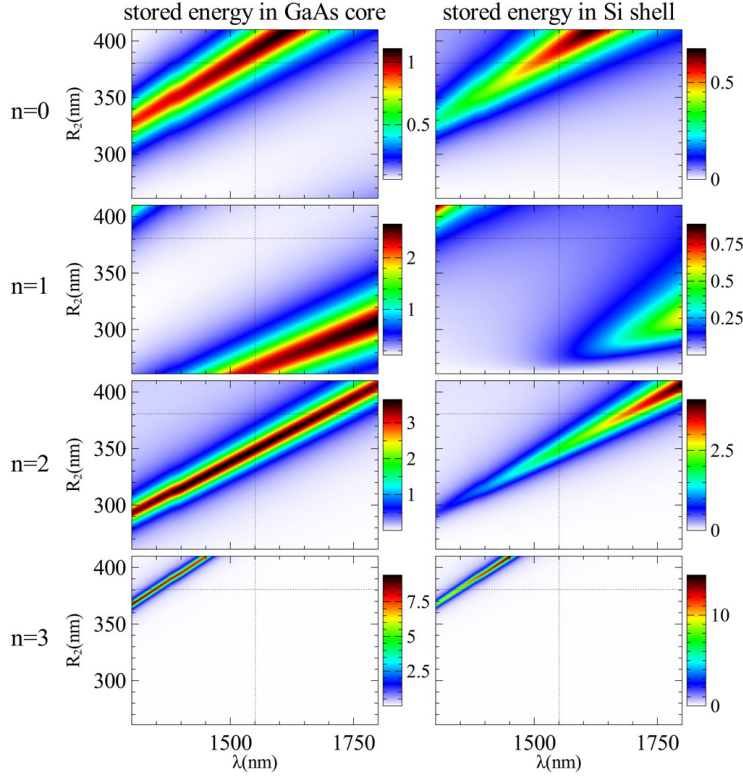


Figure 3.6: Spectral variation of stored energy of different modes in GaAs-Si core-shell structure with changing r_2 . In the plots, r_2 starts from 261nm , which indicates zero thickness of the shell (bare core).

layers.

The fitness function can be also defined based on the scattering cancellation in TM polarisation by having electric field parallel to the axis of nanowires. Similar results demonstrated in Fig. 3.9 are obtained in TM polarisation showing excellent scattering suppression of a GaAs nanowire covered by just one layer of a silicon shell. This figure shows the same procedure as Fig. 3.2 to choose a radius for the GaAs core that makes the maximum scattering without the Si shell, for better demonstration of the discussed solution's high performance.

3.1.2 Superscattering

In addition to cloaking, it was shown that multi-layer nanoparticles can exhibit an enhanced scattering, or *subwavelength superscattering* [149], when the scattering cross-section of a subwavelength structure exceeds substantially its geometrical cross-section and can be made very large. This effect can be very important for practical applications in photovoltaics and solar cells, sensing and biomedicine [150–155].

Superscattering of light can be achieved by engineering an overlap of resonances of

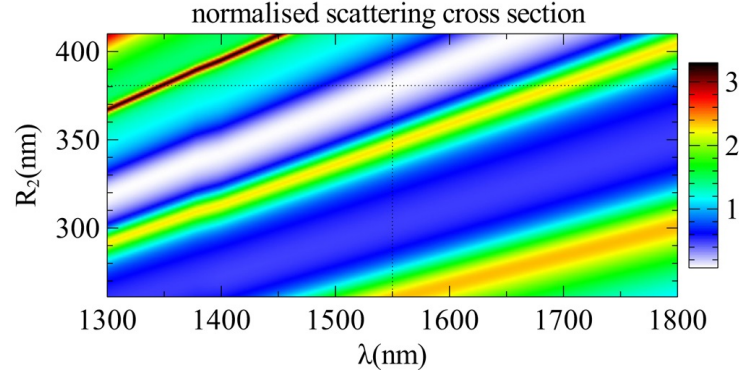


Figure 3.7: Spectrum of the scattering cross-section of the GaAs-Si nanowire with changing r_2 . The shell radius starts from 261nm which corresponds to the bare core structure. Dotted lines show the optimal parameter values.

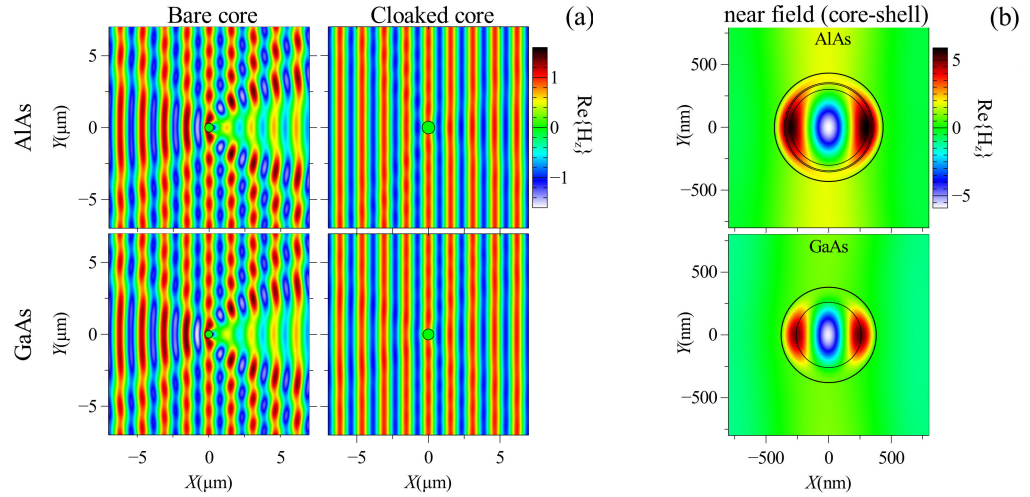


Figure 3.8: (a) Far field profiles of magnetic field for bare and invisible nanowires and (b) the field profiles inside the structures in invisibility regime. Optimised radii of core-shell structures are illustrated in Table 3.1.

different modes at the same wavelength [156, 157], and this effect is very sensitive to the material parameters being drastically suppressed by material losses. A design and optimisation of such systems remain a real challenge, so the big question is how to engineer a nanoscale structure to achieve the superscattering effect at any desired wavelength.

To address this, the developed genetic algorithm is employed for maximising the scattering cross section of multilayer plasmonic nanowires and demonstrate that the superscattering can be realised at any given wavelength, for realistic material parameters.

In Fig. 3.10 a general schematics of the problem is shown with the incident plane wave propagates along the x axis. Due to similarities between TE and TM polarisation, we investigate the superscattering effect only in TE polarisation with the magnetic field polarised parallel to the cylinder axis. The goal is maximising the total SCS at an arbitrarily chosen wavelength by optimising the size parameters in a three-layer nanowire. Here, to

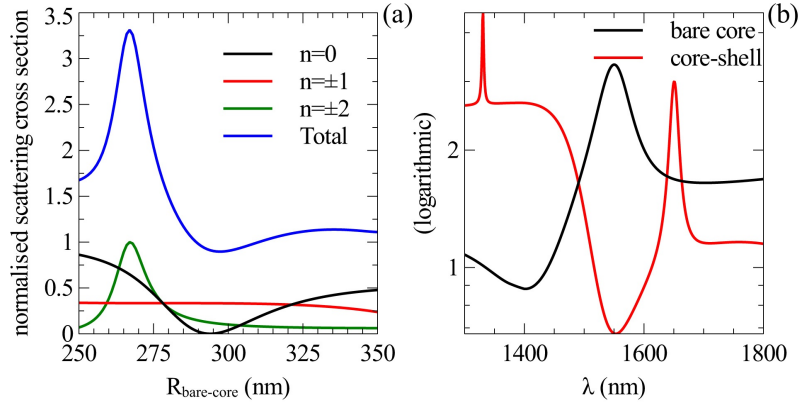


Figure 3.9: Cloaking a GaAs core with a Si shell under TM polarisation (electric field parallel to the axis of the structure). (a) The radius of the bare core is chosen to have the maximum SCS ($r_{\text{core}} = 267\text{nm}$) to be cancelled (similar to Fig. 3.2), and (b) suppression of the total SCS by adding a Si shell similar to Fig. 3.3(c) ($r_{\text{total}} = 382\text{nm}$).

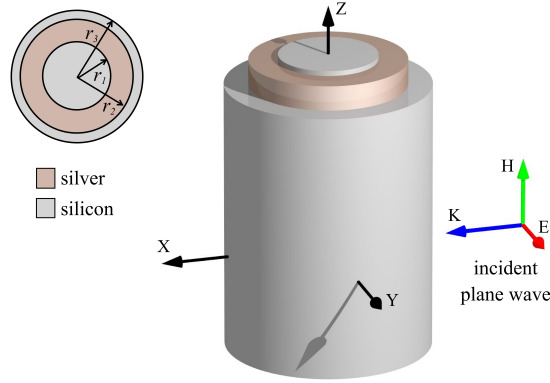


Figure 3.10: Geometry of the problem: A three layer structure made of silicon and silver. The plane wave is illuminating from side with magnetic field parallel to the structure's axis.

simplify the problem, particular materials are chosen, such as silver and silicon, as shown in Fig. 3.10, using material data obtained from optical experiments [144]. We keep the thickness of the layers as the variables to be optimised and limit the outer radius of the structure to 87nm to make the outcome comparable with previously published results of investigation superscattering effect in nanowires [83, 149].

For superscattering problem we define the following fitness function in our genetic algorithm

$$F_i(r_1, r_2, r_3) = \max\{\hat{\sigma}^s(\lambda_{\text{opt}}, r_1, r_2, r_3)\}, \quad (3.4)$$

where i indicates an individual, varying from 1 to the population number of each generation in our GA (50) and λ_{opt} is the wavelength at which we want to optimise the SCS and $\hat{\sigma}^s$ is calculated from Eqs. (2.9) and (2.12). The fitness function is used to evaluate each individual to assign fitness values.

The results of the optimisation are shown in Fig. 3.11. This figure demonstrates that in

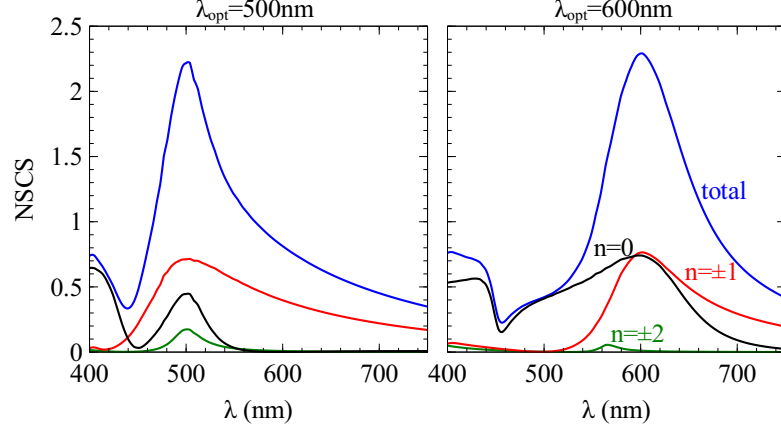


Figure 3.11: Spectrum of the NSCS of optimised superscattering structures at different wavelengths. Shown is the total cross-section, as well as contributions of the first three modes. The size parameters are listed in Table 3.2.

optimal superscattering regimes, several multipole resonances overlap at λ_{opt} . This effect is considerable in the case of $\lambda_{opt} = 500\text{nm}$, when the resonances of *three* different modes are overlapped. The contribution of the quadrupole mode becomes weaker for longer wavelength as it's shown in Fig. 3.11. This is caused by narrowing of the silver layer (see Table 3.2 for parameters). It can be also confirmed by comparing the amplitudes of the electric fields corresponding to different multipoles, presented in Fig. 3.12(a). According to this figure the quadrupole mode has the largest amplitude at this particular wavelength, $\lambda_{opt} = 500\text{nm}$.

In Fig. 3.12(b) the far-field profiles for the structure are shown which are optimised for $\lambda = 500\text{nm}$. Shown are field profiles at two different wavelength: 500nm (superscattering) and 440nm (weak scattering). The weak scattering regime is chosen such that SCS is minimal for our structure. Figure 3.12(b) clearly demonstrates that in the superscattering regime the particle creates a large shadow behind the structure, and the shadow is much larger than the physical size of the particle.

It is also interesting to look at the far-field radiation pattern of the optimised structures. Fig. 3.13 demonstrates the variation of the far-field radiation pattern with wavelength, for multilayer structures optimised for different wavelengths. One can notice that at the optimal wavelength, the total scattering is maximal along with the directivity. Such relation between total scattering and directivity can be understood by using the optical theorem, according to which the overall extinction is proportional to the forward scattering. Stronger scattering leads to better directivity, making the optimised multilayer structures good candidates for subwavelength optical nanoantennas.

Table 3.2 summarises the parameters of several optimised structures. The results show that the shift of superscattering spectrum is mostly controlled by tuning the outer radius of the silver layer r_2 . This can intuitively be understood from the total field profile shown

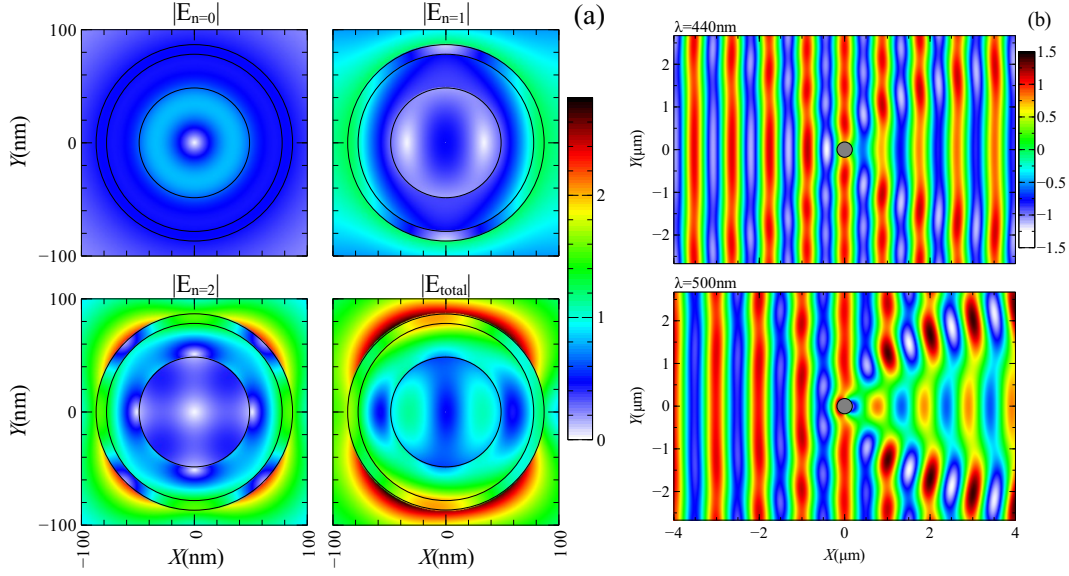


Figure 3.12: Field profile of the optimised structure at $\lambda = \lambda_{opt} = 500nm$. (a) Electric field profile for the first three modes as well as the total electric field. (b) The far field distribution for at two different wavelengths, $440nm$ and $500nm$ showing weak scattering and super scattering regimes. The plane wave is incident from left and the final field profile is calculated using first ten modes within the structure.

Table 3.2: Results of the superscattering optimisation for a three-layer plasmonic structure (see Fig. 3.10) for several wavelengths. All dimensions are in nm.

λ_{opt}	r_1	r_2	r_3	$NSCS_{max}$
450	43	83	87	1.909
500	49	78	87	2.211
550	49	72	87	2.261
600	47	66	87	2.290
650	36	58	87	2.287

in Fig. 3.12(a). Indeed, we observe that the field amplitude is the largest near the outer layer, and if we assume that the overall size of the structure is constant (see Table 3.2), then variation of outer radius of metallic layer r_2 , will affect the field stronger than if we change the radius of the internal silicon layer r_1 .

Table 3.2 also illustrates high flexibility of multilayer nanowires and capability of the developed approach for controlling their optical properties in any given frequency. It shows that by a precise optimisation, even with a fixed set of materials and only by adjusting the size parameters, multilayer nanowires are highly capable of showing frequency selective enhanced scattering properties for various optical applications.

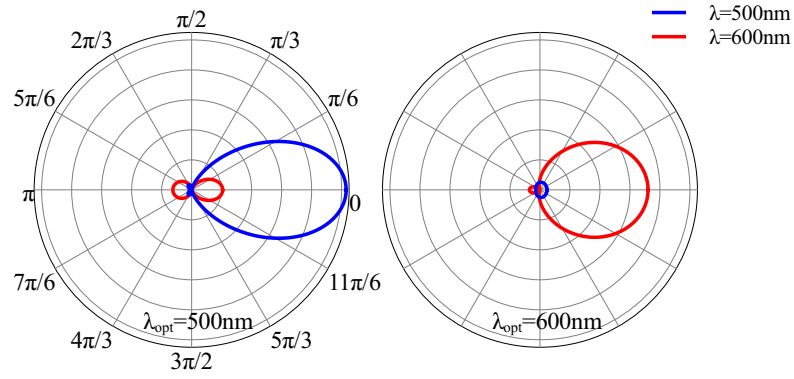


Figure 3.13: Far field radiation pattern of structures optimised for different wavelengths. The plane wave is incident from left. Both panels have the same radial tick steps.

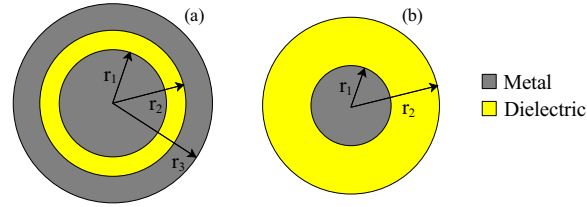


Figure 3.14: Schematic view of (a) double-shell and (b) core-shell nanowires.

3.1.3 Can invisibility and superscattering live together?

Invisibility cloaking and superscattering effect have been shown for different nanoparticles with different structure, and very often under the assumption of low losses. In previous sections we studied these two seemingly different phenomena, and wonder if these dissimilar effects of the anomalous scattering, i.e. the suppressed and enhanced scattering (cloaking and superscattering) may exist for realistic parameters and in one type of structure.

Cloaking of metal-dielectric cylindrical structures has been investigated experimentally by combining geometrically resonant metallic and semiconductor nanostructures with highly functional hybrid devices that derive their properties from the near-field coupling via intermodal interference and local negative polarisability [136, 138, 158]. In this section, these interference effects are analytically studied by considering the role of realistic material dispersion and losses on both superscattering and cloaking of multi-shell nanowires. First, I analyse the scattering properties of a three-layer structure shown in Fig. 3.14(a) and demonstrate that for realistic parameters the previously predicted superscattering regime is drastically suppressed. Then, using experimental data, a simpler design of a nanoplasmonic structure is introduced as is shown in Fig. 3.14(b) which demonstrates both superscattering and cloaking effects in the visible frequency spectrum.

Here, TE polarisation is chosen by following the analytical approach of Section 2.1.

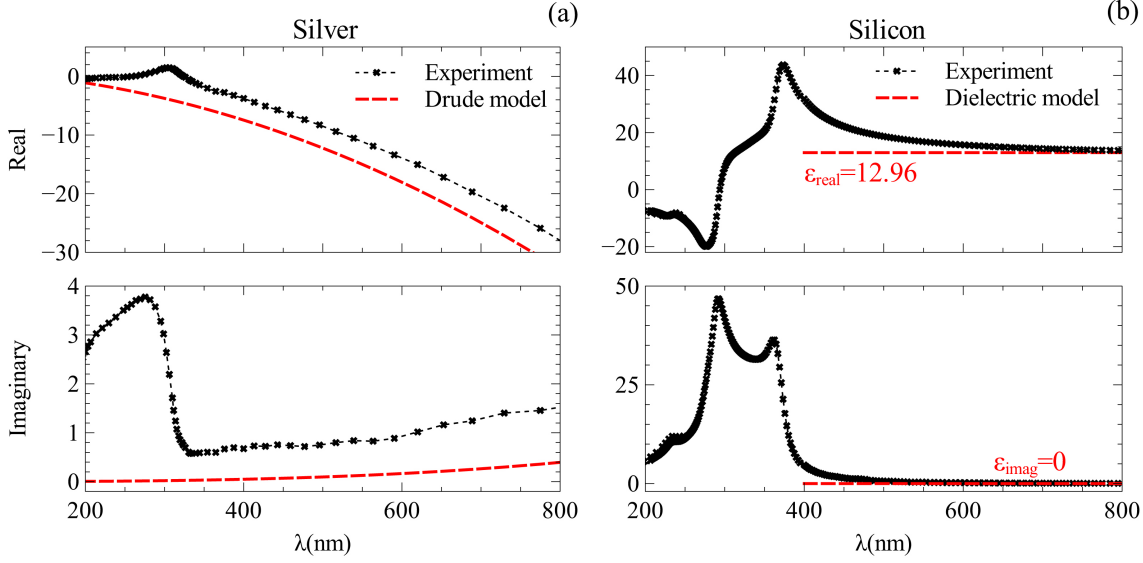


Figure 3.15: Real and imaginary parts of dielectric permittivity of bulk (a) silver and (b) silicon. (a) Comparison of the permittivity for silver with experimental data and modelled with the Drude formula. (b) Silicon experimental data vs. commonly used a constant value of 12.96.

Employing multi-layer structures with plasmonic materials, the value of SCS can be significantly enhanced by employing multiple scattering channels. To achieve this, we need to design a nanostructure with a significant contribution of different channels *at a same frequency* by overlapping the frequencies of at least two different resonances [149, 157].

Metals are known to be strongly dispersive in the optical frequency spectrum. Therefore, it is important to use accurate models for describing metal properties in order to obtain realistic results. Here, we compare the results obtained by using Drude's model for silver (this model was employed in [149]) with the results obtained by using the experimental data from [144]. In addition, for shorter wavelengths the permittivity of some common dielectrics also becomes dispersive and this effect will contribute to the light scattering.

Superscattering of a double-shell structure shown in Fig. 3.14(a) has been studied previously in [149], where $\epsilon_d = 12.96$ is used as permittivity of the dielectric layer, as well as Drude's model for the permittivity of silver, $\epsilon = \epsilon_\infty - \omega_p^2 / (\omega^2 + i\gamma\omega)$, where $\epsilon_\infty = 1$, $\omega_p = 1.37 \cdot 10^{16}$ rad/sec and $\gamma = 2.74 \cdot 10^{13}$ rad/sec are plasma and bulk collision frequencies respectively (using additional surface damping as is followed). These dependences are shown by dashed lines in Fig. 3.15(a). The radii of the shells, $r_{1,2,3}$, are 47.9nm, 77.3nm, and 87.6nm, respectively.

Taking the plasmonic small size effect and the additional surface damping into account, the calculated NSCS as well as contributions to scattering from the first three modes, is shown in Fig. 3.16(a), and these results coincide with those of Fig. 4(a) in [149] (shown in a wider wavelength range). However, Fig. 3.15(a) indicates that Drude's model does not describe accurately the experimental data for silver in the visible spectrum. For longer

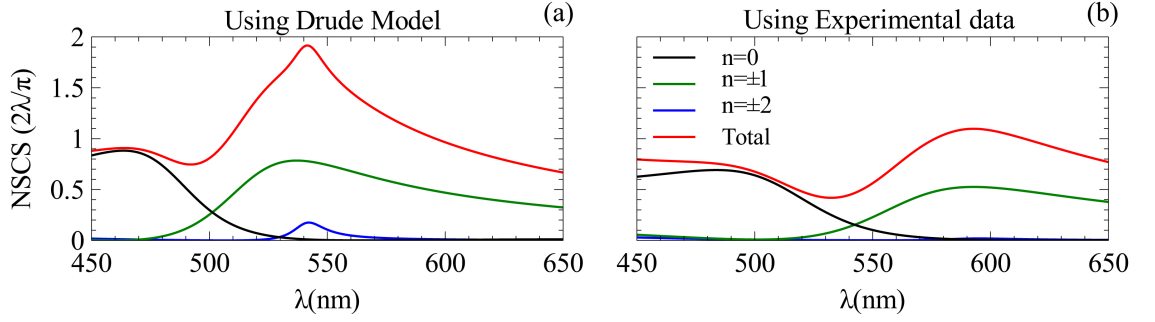


Figure 3.16: NSCS of the 3-layer structure, using (a) Drude’s model and (b) experimental data.

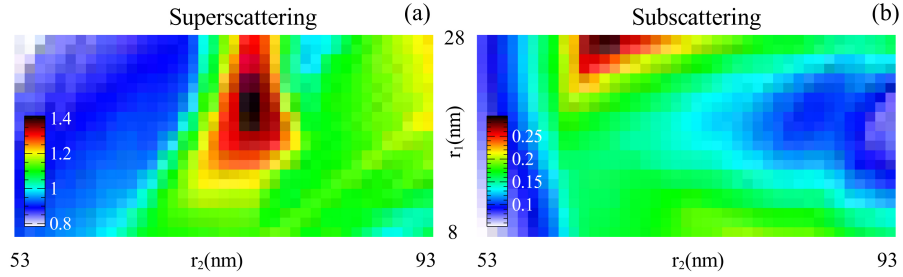


Figure 3.17: (a) Maximum and (b) minimum values of NSCS of core-shell nanowire versus radii r_1 and r_2 in the visible wavelength region ($380\text{nm} - 750\text{nm}$) using experimental data.

wavelengths these discrepancies can be reduced by using appropriate values of ϵ_∞ , γ and ω_p . This, however, still does not describe the parameters of silver well enough for higher frequencies, namely above the interband transition frequency [95]. To demonstrate the importance of using accurate values of $\epsilon_l(\lambda)$ in numerical simulations, below we study the light scattering by the same structure but using Palik’s data for $\epsilon_{silver}(\lambda)$ [144] and compare the results with those obtained using Drude’s approximation.

Figure. 3.16 shows the NSCS for a three-layer nanowire with the Drude model and Palik’s experimental data for the metallic layer. The superscattering effect observed for Drude’s model [Fig. 3.16(a)] completely disappears when the experimental data is used as is shown in Fig. 3.16(b). This demonstrates the importance of using material realistic parameters. Moreover, at lower wavelengths, permittivity of dielectrics may also become significantly dispersive, as shown in Fig. 3.15(b) for silicon. In what follows, the realistic dispersive data is used for both silver and silicon, with a linear interpolation between experimental points where needed.

Here, the obtained results raise an important question: *Is it still possible to observe enhanced scattering with layered nanowires for realistic materials?* Or, what is the realistic variation of the SCS of layered nanowires? To answer these questions we analyse the scattering properties of a simpler core-shell metal-dielectric structure shown in Fig. 3.14(b), which has silver core and silicon outer shell. In Fig. 3.17 maximum and minimum NSCS are plotted within the frequency range of interest as a function of radii r_1 and r_2 . We observe that the maximum NSCS close to 1.4 can be achieved in this structure. Moreover,

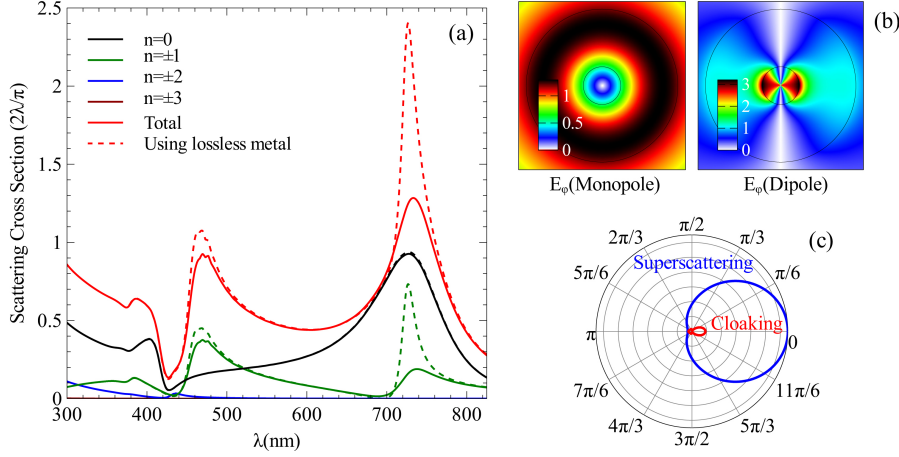


Figure 3.18: (a) NSCS of a core-shell structure with cloaking and superscattering properties at 427nm and 733nm , respectively. Dotted lines show the results for the case of lossless metal. (b) Field profile (dipole and monopole modes) as the absolute values of E_ϕ normalised to the incident wave amplitude in superscattering regime using realistic parameters and (c) far-field radiation pattern of the nanowire with plane-wave excitation from left.

if we take the values $r_1 = 18\text{nm}$ and $r_2 = 73\text{nm}$, then both enhanced and suppressed scattering can be observed simultaneously. In particular, for such a choice of parameters, the NSCS is 0.135 at 426.9nm and 1.284 at 733.2nm . Corresponding NSCS is shown in Fig. 3.18(a) as a function of wavelength. The suppressed scattering is associated with the cloaking phenomenon, where the scattering of all modes is simultaneously and significantly reduced [122, 135]. At the same time, at the frequency of enhanced scattering, both monopole and dipole modes are at resonance. Remarkably, if we calculate NSCS neglecting metal losses [shown by dashed curves in Fig. 3.18(a)], we obtain that losses predominantly suppress the dipole mode without affecting much the monopole mode. This effect originates from stronger overlap of the dipole mode with metallic part of the nanowire as shown in Fig. 3.18(b). Also as the dipole mode has a higher quality factor than the monopole mode, the light resides longer in the dipole mode of the nanowire and material loss has a higher impact in this mode. We also compare the directionality of the scattering in both the regimes, as shown in Fig. 3.18(c). In both cases, scattering occurs predominantly in the forward direction with a significant difference in amplitude which is quite attractive for applications to optical antennas.

Figure 3.19 shows the near-field and scattered-field distribution inside and outside the nanowire in both enhanced and suppressed scattering regimes. In enhanced scattering regime the near-field exhibits superposition of monopole and dipole modes inside the nanowire as was expected from scattering cross section in this regime from Fig. 3.18(a). Comparing Figs. 3.18(b) and (d) indicates how differently a core-shell nanowire can control the behaviour of light in a relatively small spectral range simultaneously.

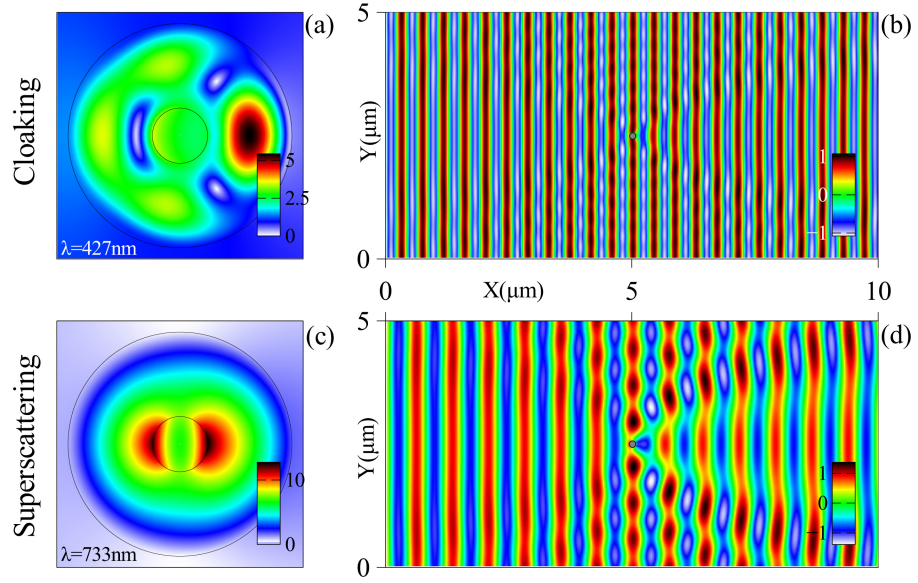


Figure 3.19: Distribution of the magnetic field in cloaking (a,b) and superscattering (c,d) regimes for the plane wave incident from the left. The internal field profiles in (a,c) are shown as the absolute values of the total field H_z normalised to the incident wave amplitude. (b,d) Real part of H_z . The small grey circle in the plots (b,d) corresponds to the nanowire.

3.2 Superabsorption of light

In this section, I suggest a new strategy for tailoring and enhancing the absorption of light by multilayer nanowires, due to an overlap of different resonant modes. This approach can be employed for a design of multiband tunable optical absorption across a wide spectral range for both TE and TM polarisations.

Light absorption and its enhancement in nanostructures, is fundamentally important and can be used in various applications. In medicine, the absorption of infrared light by noninvasive cell-tracking nanoparticles leads to the improvements in the cancer diagnostics techniques [159]. In physics, quantum-engineered superabsorption is used for improving optical sensors and light harvesting technologies [160]. Solar cells and thermophotovoltaic devices also benefit from larger light absorption [161].

To achieve higher absorption, various strategies and geometrical designs have been analysed. Perfect absorbers [162], omnidirectional absorption by reflectionless impedance matching in periodic arrays and nanoscale gratings [163], and spatial trapping of resonances in semiconductors to improve the energy conversion [164] have been studied. Wide-band thin super-absorption, using hyperbolic metamaterials [165] and black-bodies [166] using plasmonic resonances are also introduced. One important technique to obtain higher absorption by nanostructures is spectrally overlapping several absorption resonances, for example by using Mie and leaky/guided modes in nanowires [167], or by overlapping the resonances from different polarisations [168, 169]. Enhancement of the absorption for

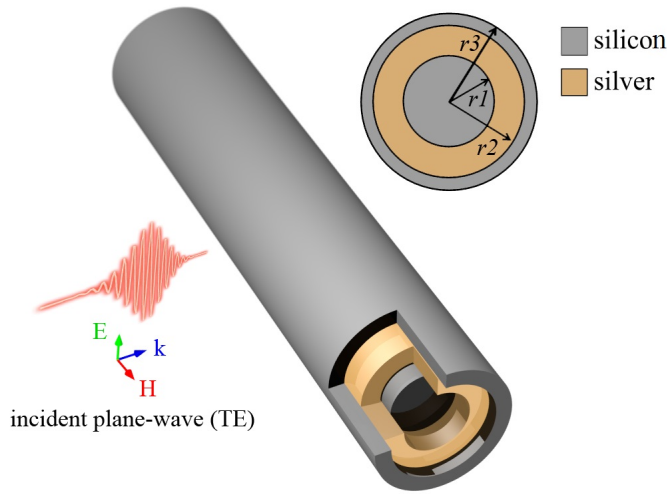


Figure 3.20: Schematics of the problem: electromagnetic plane wave is incident on a multilayer nanowire whose layers are made of silicon and silver.

one polarisation (either TE or TM) has been also suggested by utilising two resonant modes [168]. However, to the best of my knowledge, the strategy for overlapping multiple resonances and its tunability was not comprehensively studied before our work in neither plasmonic nor all-dielectric structures.

Here, I introduce a highly tunable approach for overlapping various absorption resonances of different modes, in either TE or TM polarisations. By using experimental data for material parameters [144, 170], superabsorption by multilayer nanowires is designed and analysed with the total absorbed energy being substantially larger than that achieved in homogeneous structures of the same size. Herein, by adding one plasmonic (silver) or dielectric (aluminium arsenide) shell to a silicon nanowire, an overlap of up to four different absorption resonances of the same polarisation is demonstrated. The substantially enhanced absorption occurs mostly in the semiconductor layers which is important for photovoltaics and solar-cell applications. Figure 3.20 demonstrates a schematic of the problem.

As is explained in Section 2.2, the absorption cross-section can be presented as a superposition of absorption contributions from different cylindrical modes. The spectral behaviour of absorption of each mode is a function of the size and material parameters of the nanowire. In a single nanowire, mode degeneracy of the positive and negative orders appears due to the azimuthal symmetry. Their contribution to the absorption is equal across the spectrum, except for $n = 0$ mode. The absorption spectrum also depends on material parameters. In solid metallic nanowires the absorption is considerable only close to the plasmonic resonance frequency and relatively small everywhere else. In solid dielectric nanowires, several resonances exist, but they are well spaced in the frequency domain, so that the overlap between them is not substantial. To overcome these restrictions of enhancing the absorption, I introduce multi-mode absorption

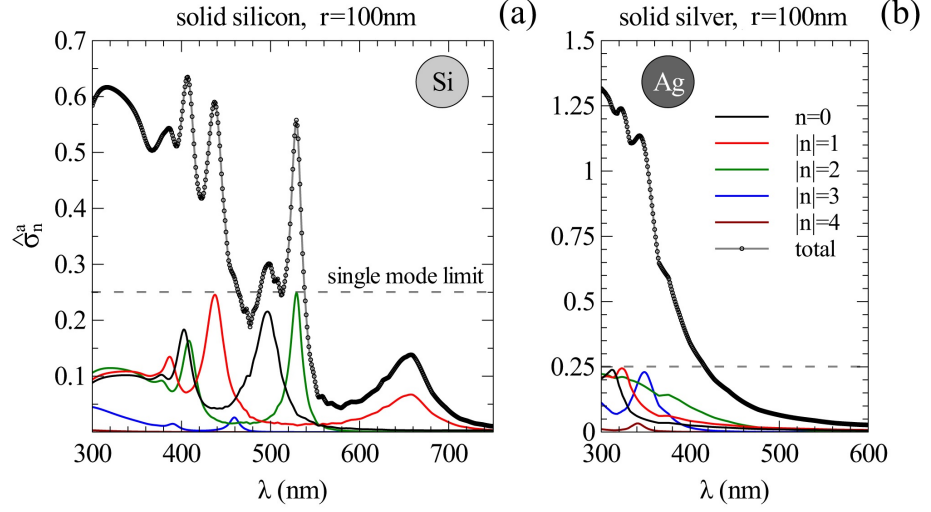


Figure 3.21: Spectrum of the total normalised absorption cross-section for TE polarisation, as well as contributions of individual modes for solid (a) silicon and (b) silver nanowires. The figure shows non-overlapped absorption resonances of different modes in solid dielectric and their concentration close to the plasmonic resonance wavelength in metallic nanowires.

approach, aiming at a design of structures that have several resonances co-existing at a selected frequency. To achieve this, we engineer multilayer nanostructures whose absorption is enhanced far beyond the single-mode limit. The genetic optimisation algorithm (discussed in Section 2.5) is used by defining a fitness function for a three-layer nanowire as $F(r_1, r_2, r_3) = \max\{ACS(\lambda_{opt}, r_1, r_2, r_3)\}$, where λ_{opt} indicates the operating wavelength. This optimisation process allows the design of enhanced absorption at any selected wavelength, or even simultaneously for several frequency bands.

From the energy conservation, following the analysis of Section 2.1, for non-radiating modes, the σ^a can be written as $\sigma^a = \sigma^e - \sigma^s$, where σ^e and σ^s are extinction and scattering cross-sections, respectively. We follow the procedure of Section 2.3, and use $\epsilon_\infty = 4.96$ for silver [144]. It can be shown that the single mode limit of $\hat{\sigma}_n^s$ and $\hat{\sigma}_n^e$ is equal to unity and $\hat{\sigma}_n^a$ is limited by 0.25, similar to spherical nanostructures [92]. To overcome this limit, we propose to overlap several resonances at a given frequency, so that the combined absorption of multiple resonances is larger than that for a single mode. We call such regime as superabsorption. Clearly, this only becomes possible, when absorption of each of the involved resonances is high enough, and it is shown below, that by using numerical optimisation it becomes possible to design structures that outperform single resonance limit at any desired wavelength within visible frequency range.

To have a better understanding of spectral distribution of σ^a , ACS of solid silicon and silver nanowires is analysed in Fig. 3.21 for TE polarisation and similarly this can be done for TM polarisation. The results for a solid silicon nanowire in Fig. 3.21(a) suggest that the absorption resonances of different modes are spread over a wide spectral range, and the total ACS is almost limited to the summation of positive and negative orders of

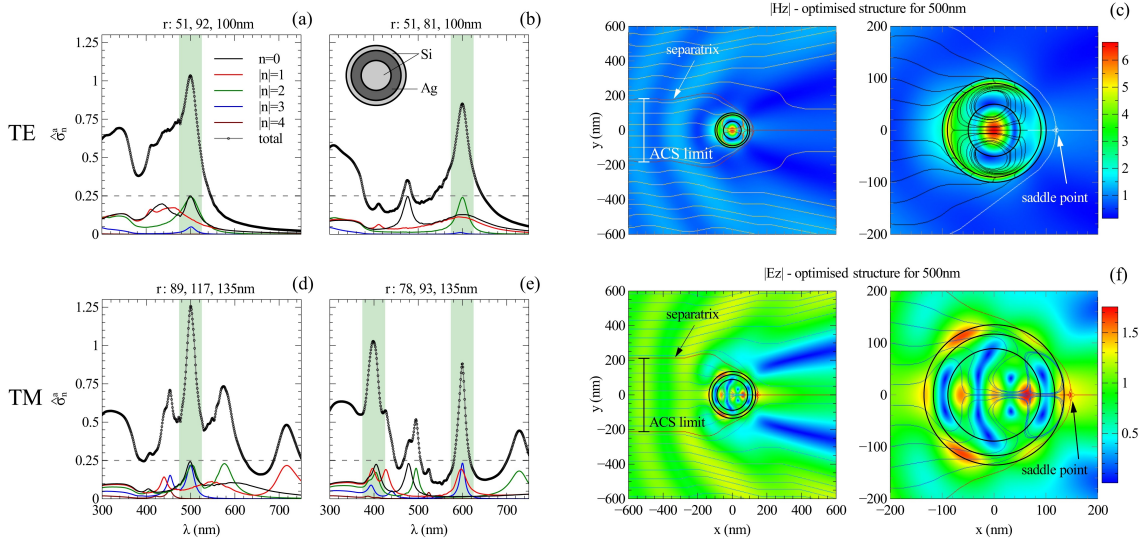


Figure 3.22: Optimised nanowires for multiband absorption for both polarisations for Si-Ag-Si configuration. Figures (a, b, d and e) correspond to different multilayer structures with the radii of the layers shown above panels. Outer radius is fixed at 100nm and 135nm for TE and TM polarisations, respectively (the same as Fig. 3.21). (c) and (f) demonstrate field profiles and energy flow lines. The light is trapped and absorbed in the semiconductor material.

a single harmonic. Figure 3.21(b) shows that in a solid silver nanowire, the absorption resonances are concentrated near the plasmonic resonance wavelength, and ACS is rapidly decreasing to the values under the single-mode limit for the rest of the spectrum. Spectra with similar features characterise solid nanowires for TM polarisation.

As the next step, we analyse multilayer structures for the example of Si-Ag-Si geometry, for both TE and TM polarisations. The key strategy to enhance the absorption efficiency of a nanostructure is to increase the number of supported resonances while maintaining the same particle size [168, 171], which also provides a meaningful comparison of the ACS in multilayer structure with that of the solid nanowires. The results for the absorption enhancement by multilayer nanowires are demonstrated in Fig. 3.22. The results for two different nanowires are presented in Fig. 3.22 for both polarisations, showing overlapping of absorption resonances of different modes.

Figure 3.22(b) demonstrates a superabsorption effect due to the overlap of the resonances of four different modes at $\lambda = 600\text{nm}$. By using the optimisation techniques, it is also possible to design structures that demonstrate the enhanced absorption for several wavelengths. For example, Fig. 3.22(e) also shows a specific configuration for which simultaneous superabsorption is obtained for two different wavelengths within the visible range.

Comparing Figs. 3.21 and 3.22 reveals that we can obtain single-band or multi-band enhanced absorption at wavelengths for which none of the solid nanowires show considerable absorption. Figure 3.22 also demonstrates a possibility of tuning the superabsorption

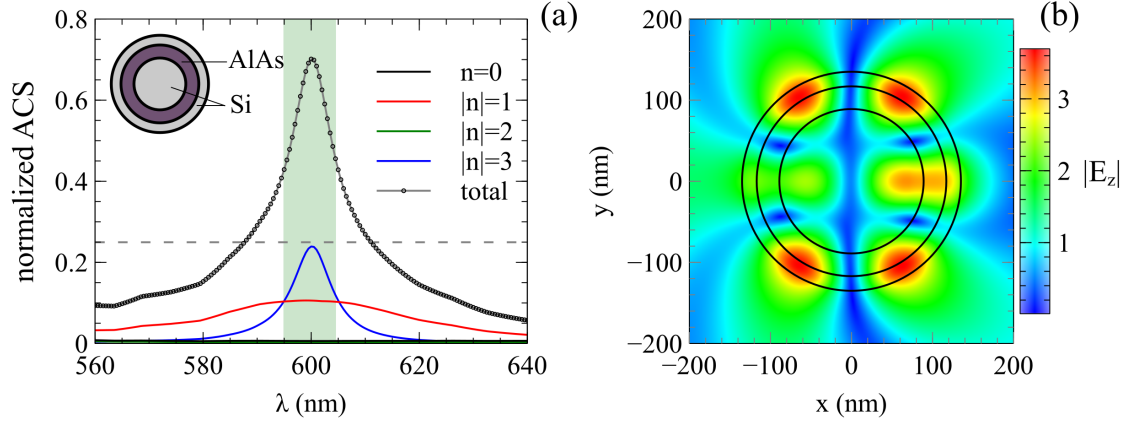


Figure 3.23: (a) Superabsorption effect tuned at $\lambda = 600\text{nm}$ in an all-dielectric nanowire made of Si and AlAs layers (TM polarisation). The radii are 75, 115 and 135nm . (b) The electric field profile and the enhanced absorption of light in the silicon layers due to the losslessness of AlAs in 600nm .

effect in multilayer structures to a desired wavelength. Figures 3.22(a, b) for TE polarisation and Figs. 3.22(d, e) for TM polarisation are for two different multilayer structures with different layer thickness that can demonstrate the superabsorption effect in different parts of the spectrum, while having a fixed external radius.

Figures 3.22(c, f) demonstrate the field profile in the structures which are optimised for the superabsorption effect at $\lambda = 500\text{nm}$. The profiles show trapping of light in semiconductor layers, which for the example of TM polarisation [Fig. 3.22(f)] leads to 78% of the enhanced absorption to occur in silicon.

The energy flow streamlines show how the nanowires absorb light, effectively collecting light from the area that is larger than the geometrical cross-section of the nanowire. To have an in-depth interpretation, we calculate the Poynting vector singular points known as saddle points [172, 173]. The energy flowing close to these points define the separatrices, which in this case have the meaning of the interfaces separating the regions where the energy flows into the nanowire and the region where the energy flows past the nanoparticle. The separatrices are highlighted in Figs. 3.22(c, f). Some part of the energy propagating into the nanowires may escape out again without being absorbed. Therefore, the separatrices indicate the upper limit for the absorption cross-section. In the presented nanowires designed for superabsorption at $\lambda = 500\text{nm}$ for TE and TM polarisations, ACS is equal to $\sigma_{TE}^a = \hat{\sigma}_{TE}^a \times 2\lambda/\pi = 1.0344 \times 2\lambda/\pi = 330\text{nm}$ and $\sigma_{TM}^a = 1.2569 \times 2\lambda/\pi = 400\text{nm}$, respectively. Comparison of these results with the ACS limit shown in Figs. 3.22(c, f), suggests that almost maximum possible energy is absorbed by the nanowires (more than 90% and 94%, for TE and TM polarisations, respectively). Relatively strong absorption of both TE and TM waves in the cylindrical structures can be achieved by compromising absorption of each individual polarisation. We expect that a less polarisation sensitive effect can be achieved in a more symmetric structure such as a sphere.

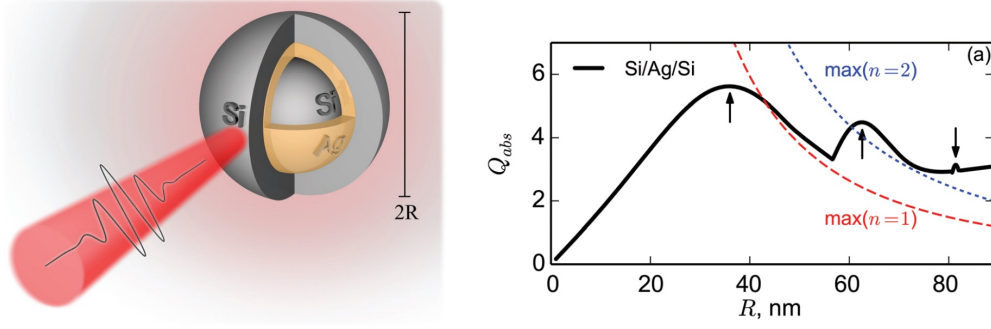


Figure 3.24: Superabsorption of light by multilayer nanospheres. (a) Schematic view of multilayer spherical nanoparticle studied for superabsorption of light, and (b) optimised values of absorption efficiency by a Ag/Si core/shell nanoparticle [80].

The superabsorption occurs when we overlap several resonances in the structure. We can reasonably expect that these resonances can be of different character, such as electric as in plasmonic or magnetic as in all-dielectric structures. In addition to overlapping the resonances, we need to ensure that these modes should be well absorbing. In general, the absorption of the particle in resonance depends on the resonant mode structure, and there are optimal values of material loss parameters that provide best absorption. In all-dielectric structures, absorption in dielectrics may be sufficient in order to provide efficient absorption, and presence of metals are not a necessary condition for creating a super-absorber. This is demonstrated in Fig. 3.23 by analysing the absorption properties of an all-dielectric multilayer nanowire with Si-AlAs-Si layers in which the superabsorption wavelength is tuned to $\lambda = 600\text{nm}$. The enhanced absorption is due to absorption of light in silicon, as AlAs is practically lossless in this range of frequency [174].

In addition to two-dimensional analysis, our further studies [80] on three dimensional (3D) configurations by employing a similar approach, reveal that achieving enhanced absorption of light is also possible with overlapping the resonance of different modes in multilayer spherical nanoparticles, as Fig. 3.24 demonstrates. Discussing about nanospheres is not in the scope of this thesis, however, the achieved results prove that the applicability of the developed techniques for controlling the behaviour of light, is not restricted to 2D studies.

In this chapter, I demonstrated the high capabilities of multilayer nanowires for engineering suppressed and enhanced conditions for scattering and absorption of light. This is demonstrated in both all-dielectric and hybrid configurations and at any given frequency by the use of experimental data to describe materials. It was shown that nearly 80 fold suppression of total scattering cross section is possible by using three or less number of coatings. The achieved results prove that increasing the number of layers in the multi-layer shell, leads to saturation of the minimal scattering cross-section. To achieve enhanced scattering and absorption, it was shown that even by choosing only appropriate size parameters' value with given materials, one can make the resonances of different

modes overlapped at any frequency in multilayer nanowires. I demonstrated the possibility of co-existence of enhanced and suppressed scattering simultaneously in one core-shell nanowire. The importance of employing experimental material data and high sensitivity of the resonance effects to the material parameters were discussed. It was shown that superabsorption effect can be achieved with multilayer nanowires even for the wavelengths in which none of the solid nanostructures with similar materials show considerable absorption. I calculated singular points of the energy flow, which allows us to explain the origin of the superabsorption effect in such structures.

I studied the high capability of single multilayer nanowires and controlling their optical properties. The high performance of the developed approach suggests its employment for studying more complicated structures. In the following chapter, the design of optimal systems with more than one nanowire is studied.

Multi-element Nanowire Systems

It was discussed in Chapter 2 that in multi-element systems the scattered field from one particle becomes an incident field on the other ones in addition to the original incident beam. Multiple scattering starts with having two elements, and by increasing the number of particles the volume of required calculations increases, making it a more complicated problem. Therefore, I start this chapter by discussing the electric and magnetic properties and near-field hotspots in cylindrical dimers [87] in Section 4.1. I compare dielectric and metallic dimers by using experimental data for all materials and consider both TM and TE polarisations of light. Then it is demonstrated that dielectric dimers allow us to achieve pure magnetic and electric hotspots in both polarisations in contrast to plasmonic structures. This offers new approaches for near-field engineering such as sensing, control of spontaneous emission, and enhanced Raman scattering.

Later in Section 4.2, by analysing a more complicated structure, a novel type of metamaterial-based optical shielding nanostructures is introduced made of a cluster of nanowires, which prevents the light from penetration and suppresses both the electric and magnetic fields [88]. Such a metashielding with well-separated nanowires, becomes possible by a careful design of the nanowires as well as their arrangement. I show that metashields preserve their functionality for almost any geometrical arrangements, which we call *metacages* for certain configurations. It is possible to design optical metacages with both plasmonic and dielectric materials, by using experimental material data, for either TE or TM polarisations. Then, optical properties of the introduced structures are studied in near and far-field, including their frequency selectivity, effect of the large gaps between the nanowires, and zero backward scattering. Finally, I verify the obtained results by the semi-analytical approach with direct numerical simulations, and demonstrate that the achieved results are also applicable for three-dimensional configurations.

4.1 Optical response of nano-dimers

In the last decade, nanoplasmonics has attracted a lot of attention due to its ability to generate strong near-field enhancement by using metallic nanoscale structures. Such elec-

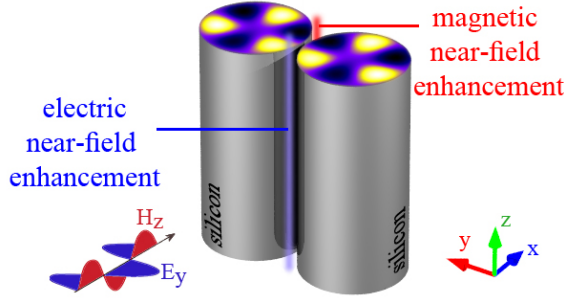


Figure 4.1: Schematic hotspots excitation in a silicon nanowire dimer.

tromagnetic field enhancement has been actively studied using clusters of nanoparticles created from different materials. Plasmonic nanoparticles with various geometries have been reported to control the behaviour of light in near-field region [175–187]. However, plasmonic structures suffer from strong dissipative losses in metallic components, even far from any resonances [95]. Recently, it was suggested that dielectric materials offer a competitive alternative to their plasmonic counterpart allowing us to reduce the dissipative losses [188]. At the same time, the ability to achieve such level of the near-field enhancement comparable with plasmonic nanostructures, is still a challenge [189–192]. To address this, in this section, optimal dimer configurations are analysed and designed to achieve the strongest near-field enhancement in the visible region by using realistic experimental data for materials [144, 170]. I demonstrate that by using dielectric materials, it is possible to create both electric and magnetic hotspots comparable with plasmonic structures in TE polarisation (magnetic field parallel to the axis of nanowires). Then, the possibility of achieving near-field-enhancement in TM polarisation is shown with dielectric nanowires, which is not possible by using metallic materials, and finally the pure magnetic and electric hotspots are introduced both together simultaneously by using dielectric cylindrical dimers.

4.1.1 Nanowire dimers

The comparative analysis of both dielectric and metallic dimers, provides us with an in-depth understanding of the optical response of such structures. For our purposes we choose silicon and silver as two commonly used dielectric and plasmonic materials, respectively. To simplify our analysis we focus on a symmetric dimer configuration and assume that nanowires are solid without shells, are made of the same material, with same diameter and also placed symmetrically around the origin [97]. A silicon nanowire dimer is schematically demonstrated in Fig. 4.1 with the formed magnetic and electric hotspots. Two-dimensional general arrangement of dimer’s elements (nanowires) is shown in Fig. 4.2. The incident planewave is illuminating in the x direction with either TE or TM polarisation.

In the first step we solve the boundary condition equations for individual wires sepa-

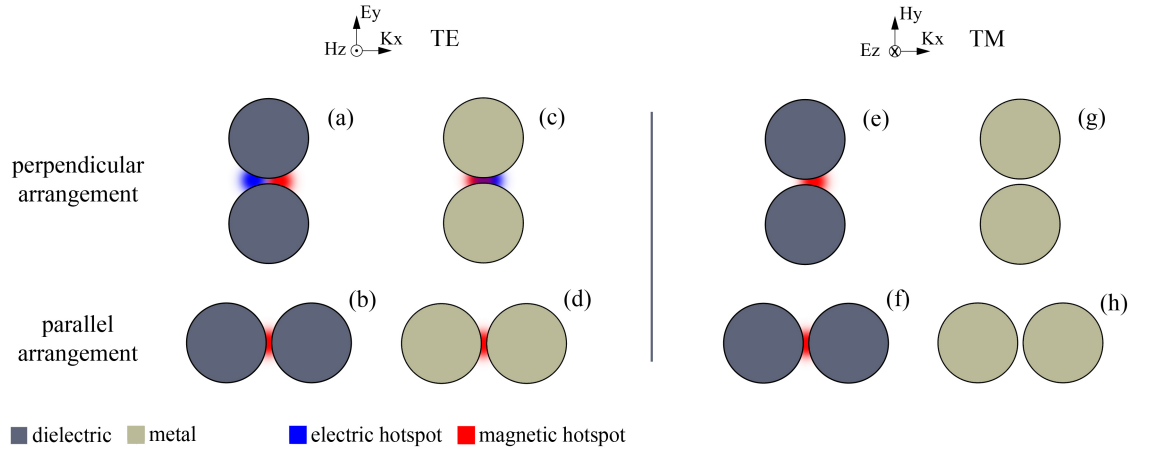


Figure 4.2: Schematic near-field hotspots excitation in dielectric and metallic dimers. Figures (a-d) and (e-h) demonstrate hotspots in TE and TM polarisations respectively. The dimers are shown in two perpendicular and parallel arrangements with respect to the direction of the propagation of the incident wave. Panel (a) demonstrates that for dielectric nanowires, it is possible to separate magnetic and electric hotspots. The small shift of hotspots' location from the centre of the gap is demonstrated in panels (a, e). The shift becomes smaller with almost overlapped magnetic and electric hotspots in the plasmonic case, as demonstrated in panel (c). Panels (a, c, e) show that the direction of the locational displacements of magnetic and electric hotspots are opposite in dielectric and plasmonic dimers. Note here, that such hotspots do not exist for TM polarisation in metallic nanowires.

rately and find the expansion coefficients, using the wave equations for single nanowires from Section 2.1 [89, 90]. The tangential fields, H_z and E_φ for TE polarisation and also E_z and H_φ for TM polarisation should be equal for every mode in both sides of the boundary of the nanowires and air. Solving these boundary value equations gives us ${}_s\tau_n^l$ and ${}_s\rho_n^l$ coefficients. In the second step we employ multiple scattering problem solution from Section 2.4, to consider the interaction between the nanowires. As the next step, we search for the optimised parameters to maximise the fields' amplitude in the middle of the dimer's gap to form enhanced hotspots using the genetic algorithm described in Section 2.5. We define a fitness function in the middle of the gap as

$$f(r, \lambda, d) = \max [FieldAmplitude(r, \lambda, d)], \quad (4.1)$$

where r , λ and d are the nanowires radius, the wavelength and the centre-to-centre distance, respectively, which also are the optimising parameters here. 'FieldAmplitude' is chosen as $|H_z|$ or $|E_{trans}|$ in TE and $|E_z|$ or $|H_{trans}|$ in TM polarisation. We restrict the wavelength range, started from $300nm$ to $900nm$ to cover the visible region. The radius is changing in a wide range from $10nm$ to $200nm$. We also confine the gap size ($d - 2r$) to be smaller than $50nm$ to stay away from diffraction effects. Also, to prevent the tunnelling effect in plasmonic dimers [193], we start the gap size from $3nm$.

We analyse two different directions of the dimer's axis, parallel and perpendicular to the direction of the incident planewave propagation. The optimisation is done for two

Table 4.1: Optimisation results for the electric and magnetic hotspots in the middle of the gap in dimers with their axis perpendicular to the direction of the incident planewave. The optimised field values are normalised to the corresponding $|H_0|$ or $|E_0|$ values. In all our calculations the first 30 modes have been taken into account.

Material	Si				Ag			
Polarisation parameter	TE $ H_z $	$ E_t $	TM $ E_z $	$ H_t $	TE $ H_z $	$ E_t $	TM $ E_z $	$ H_t $
λ (nm)	626.28	613.36	579.17	615.47	806.47	432.1	317.76	306.1
r (nm)	121.47	150.63	50.79	88.95	199.97	56.93	10.13	16.35
gap ($d - 2r$) (nm)	3	3	3	3	3	3	20	16.57
optimised value	8.05	17.84	2.19	9.63	9.31	20.41	0.93	1.01

Table 4.2: Optimisation results for the electric and magnetic hotspots in the middle of the gap in dimers with their axis parallel to the direction of the incident planewave. The optimised field values are normalised to the corresponding $|H_0|$ or $|E_0|$ values. In all our calculations the first 30 modes have been taken into account.

Material	Si				Ag			
Polarisation parameter	TE $ H_z $	$ E_t $	TM $ E_z $	$ H_t $	TE $ H_z $	$ E_t $	TM $ E_z $	$ H_t $
λ	633.66	649.47	634.34	553.52	476.82	330.49	324.49	309.93
r	84.25	132.82	93.13	27.85	55.15	20.04	20.04	20.04
gap ($d - 2r$)	3	3	3	3.1	3	7.8	40	3.1
optimised value	6.16	1.95	2.62	8.45	7.67	1.64	0.88	0.99

different types of materials, dielectric (silicon) and metallic (silver) structures separately. Tables 4.1 and 4.2 illustrate the optimisation results for electric and magnetic hotspots in two cases of dimer orientation. The optimised values in the last row of Tables 4.1 and 4.2 are achieved by using the optimised radius, gap size, and the wavelength illustrated in the previous rows. The summary of the results is demonstrated schematically in Fig. 4.2 which also shows the position of the electric and magnetic hotspots in dielectric and metallic dimers separately.

Tables 4.1 and 4.2 reveal interesting facts about hotspots in cylindrical dimers. For TE polarisation, electric and magnetic hotspots are achievable with almost lossless dielectric dimers, comparable with plasmonic ones. The results also show that for TM polarisation, it is possible to obtain strong hotspots by dielectric dimers, which is not possible using plasmonic materials.

Moreover, by analysing the near-field profiles, which are schematically presented in Fig. 4.2, it is revealed that the hotspots are not exactly in the middle of the gap in perpendicular arrangement. In particular, Fig. 4.2(a) shows that in dielectric dimers, the location of the magnetic hotspot is shifted toward the x direction, in respect to the middle of the gap, the same as Fig. 4.2(e). The electric hotspot in this dimer is shifted in the opposite direction. It is interesting to note, that the shifts of the location of the hotspots in plasmonic dimers are reversed, as can be seen from Figure 4.2(c). However, the amount of these shifts in plasmonic dimers are smaller and the two hotspots have overlapped fields in the middle.

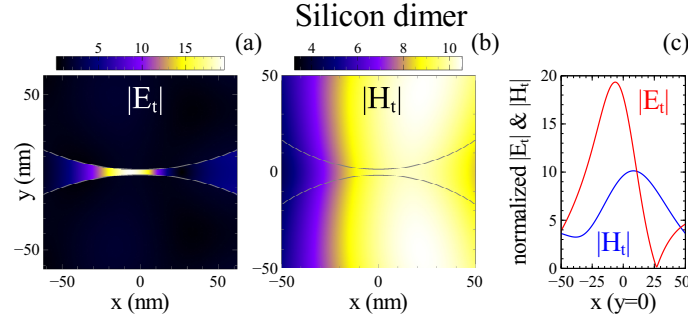


Figure 4.3: The field profile of two different silicon dimers optimised for their (a) electric and (b) magnetic hotspots, based on the results in the second and fourth columns of Table 4.1 respectively. Figure (c) shows the fields' distribution along the x axis, and the location of the hotspots in the structures of figures (a) and (b). The incident planewave is illuminating in x direction and the fields' value are normalised with respect to the absolute value of the incident fields.

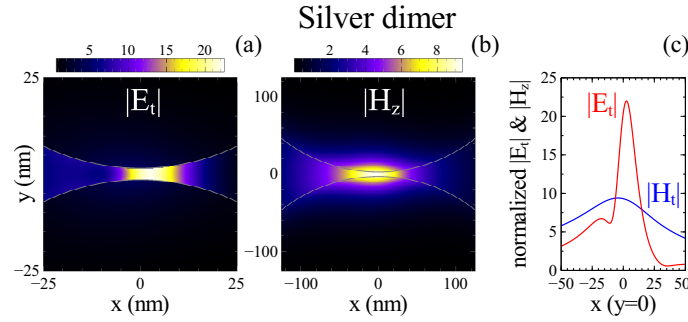


Figure 4.4: The field profile of two different silver dimers optimised for their (a) electric and (b) magnetic hotspots, based on the results in the sixth and fifth columns of Table 4.1, respectively. Figure (c) shows the fields' distribution along the x is, and the location of the hotspots in the structures of figures (a) and (b). The incident planewave is illuminating in x direction and the fields' value are normalised with respect to the absolute value of the incident fields.

Now we analyse the hotspots and their local shifts in both dielectric and plasmonic dimers, presented in Figs. 4.2(a,c,e). All three figures indicate that the local shift of magnetic and electric hotspots are opposite for dielectric and plasmonic dimers independent of the polarisation. To have more in depth interpretation of Fig. 4.2(a), the field profile of two different dimers are plotted with optimised electric and magnetic hotspots with TE and TM polarisations in Figs. 4.3(a) and (b), respectively. The parameters are can be found in the Table 4.1 in the second and fourth columns, respectively. In the dielectric dimer, the magnetic field intends to remain mainly inside the dimer elements, however, Fig. 4.3(b) shows that the magnetic field has a considerable field amplitude in the gap region.

Figures. 4.3(a) and (b) demonstrate that the maximum of the absolute value of the fields is more than the optimised results in the Table 4.1. The reason is that Table 4.1 presented the optimised values in the middle of the gap. In Fig. 4.3(c) the exact location of the hotspots and the field distribution around it are shown, along the line perpendicular to the dimer's axis passing through the centre of the gap. Similar results are shown

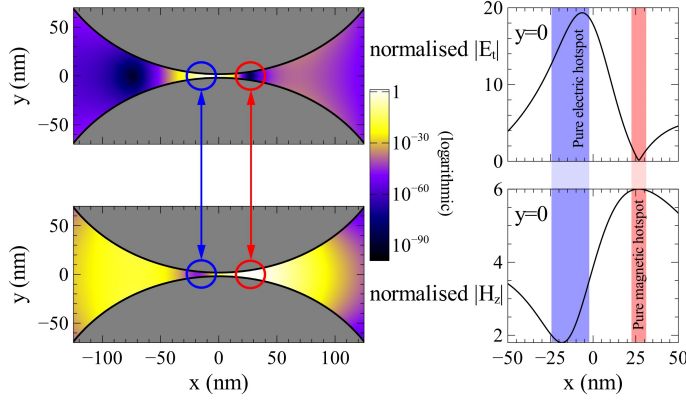


Figure 4.5: The electric and magnetic field profiles of the silicon dimer shown in Fig. 4.3(a) optimised for its electric hotspot based on the results in column two of Table 4.1. The figure compares the locations of the hotspots and demonstrates their electric and magnetic purity. The fields' amplitude values are normalised to those of the incident wave.

for plasmonic dimers in Fig. 4.4. Figures 4.4(a) and (b) show the electric and magnetic hotspots for two different silver dimers, based on the results in columns six and five of the Table 4.1, respectively. Comparison between Figs. 4.3(c) and 4.4(c) reveals that the amounts of the local shifts of the hot spots from the centre of the gap are much less in plasmonic dimers compare to dielectric ones. The magnetic and electric hotspots are almost overlapped in the middle of the gap in plasmonic dimers as it is demonstrated in Fig. 4.2(c).

4.1.2 Hotspots' origin

The results shown in Figs. 4.3(c) and 4.4(c) reveal another interesting fact that the electric field becomes near zero in a region close to the electric hotspot, making two maximised and minimised electric field strength points close to each other. This becomes more interesting in the case of dielectric dimers, where this zero electric field point, overlaps the magnetic hotspot. This means that the magnetic hotspot in dielectric cylindrical dimers, is *pure magnetic*. Figure 4.5 compares the electric and magnetic field profiles in the dimer shown in Fig. 4.3(a) which also demonstrates a similar pure electric hotspot with near zero magnetic field. To have a deeper insight to the origin of how these hotspots are formed, I present modes decomposition of the dimer and analyse the dominant mode contribution to the formation of the corresponding hotspots, which are created by interference of different overlapping harmonics.

First, I note that the behaviour of the harmonics in a dimer is quite different from a similar single particle. To explain the behaviour of different modes, we analyse the dimer shown in Fig. 4.5 [same as Fig. 4.3(a)] as an example of dielectric dimers. We plot the spectrum of the dimer's extinction cross section for different modes in Fig. 4.6, by changing the gap size in the range of very close (3nm gap) to very far (single wire limit) elements.

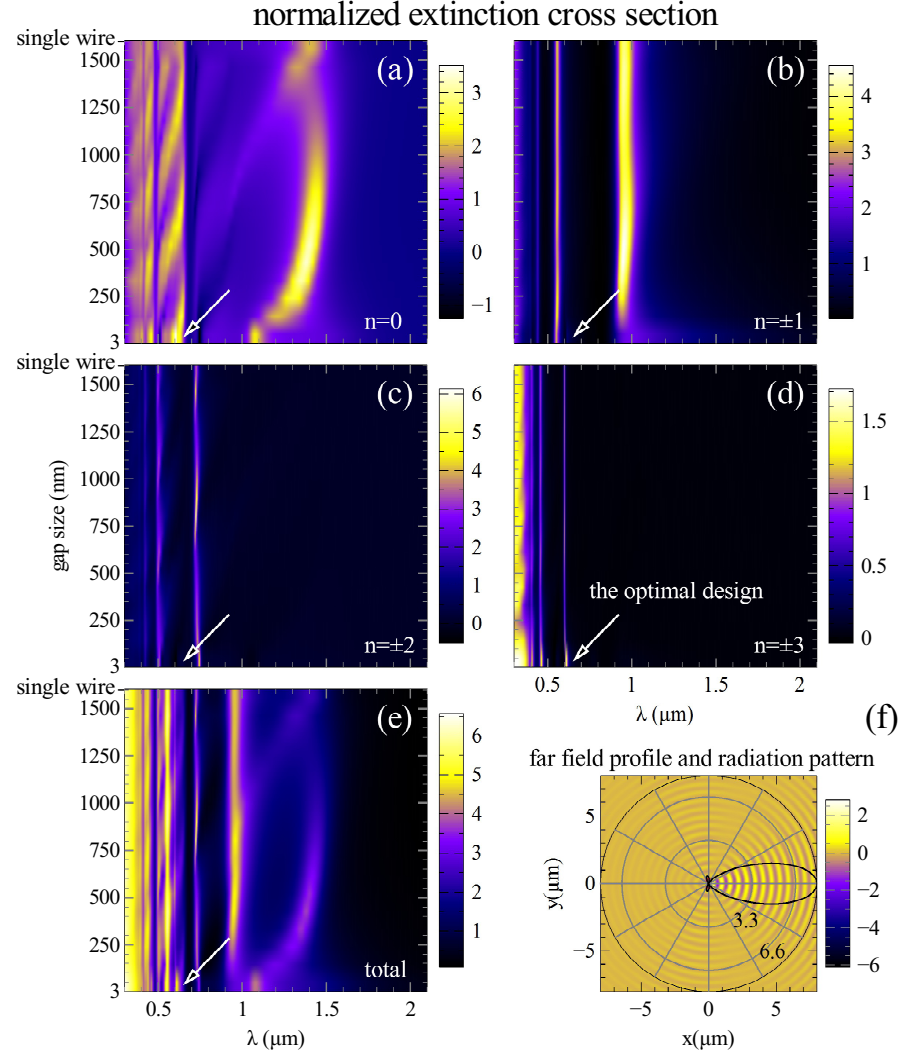


Figure 4.6: The spectrum of the normalised extinction cross section (NECS) of the silicon dimer specified in the second column of Table 4.1, starting from very far (a single wire in the last curves) to very close dimer elements (from 1503nm to 3nm gap size). The value of NECS of a single nanowire is multiplied by two to be comparable with those from the dimer. Figures (a-e) show the NECS spectrum for the first four harmonics and also the total field respectively. There is a blue-shift in ECS of magnetic dipole spectrum by shifting the nanowires closer to each other. The higher order modes do not experience considerable spectral variations by changing the gap size. The oscillation of the amplitude of the NECS resonances with the gap size indicates the presence of the diffraction effect. The white arrows show the optimised design in 613nm and the gap size equal to 3nm . Figure(f) demonstrates more far-field properties of the structure by showing the scattered field profile and the radiation pattern. The small red circles in the middle, indicate the nanowires.

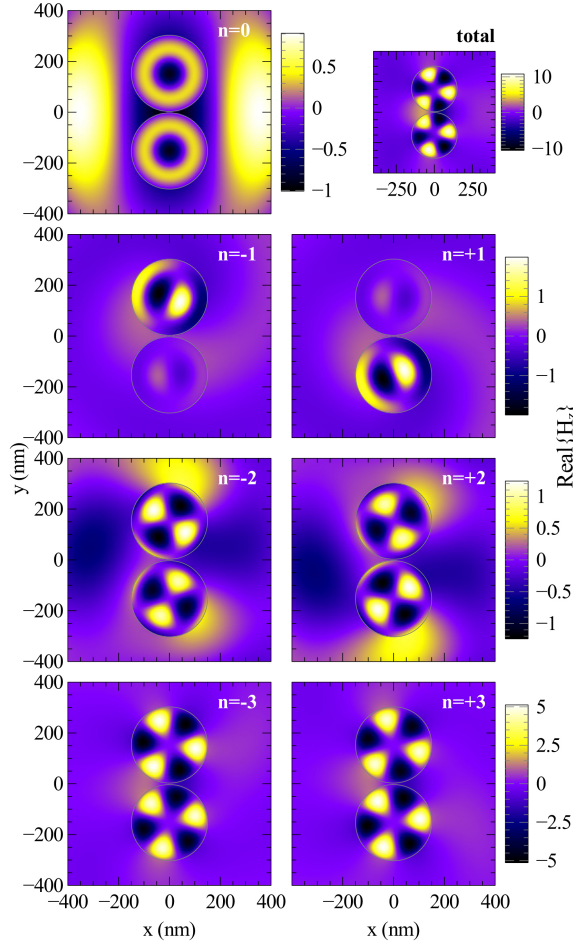


Figure 4.7: The real part of the magnetic field H_z , normalised to $|H_0|$ in the silicon dimer described in the second column of Table 4.1 ($\lambda = 613.36nm$). The field amplitude for modes $n > 3$ becomes negligible. The expansion coefficient ${}_m\rho_n^l$ of one cylinder is equal to ${}_m\rho_{-n}^l$ of the other one. The structure is the same as the one in Fig. 4.3(a), but the magnetic field is plotted instead of the electric one which is much weaker than magnetic field inside the structure. In this structure, the dominant mode is $n = \pm 3$, in both far- (see Fig. 4.6) and near-field regions, while for instance, for the dimer described in the column four of the same table, the quadrupole harmonic is dominant.

The NECS can be calculated by having the expansion coefficients ${}_m\rho_n^{air}$ and ${}_m\rho_n^{air}$ of the nanowire one and two, respectively, from Section 2.4. Figure 4.6 demonstrates the spectrum of the NECS of the first four modes plus the total NECS using the modes from $n = -30$ to $n = +30$. This figure shows that the spectral distribution of corresponding resonances of various modes remain almost the same with increasing the gap size. Such revivals are associated with the diffractive coupling between the particles [187]. The optimal conditions for the enhanced hotspot are indicated by white arrows on Fig. 4.6 and are associated the resonant near-field excitation of the octupole mode, which does not exhibit such revival features with the increasing gap size. It indicates the peculiarity of this mode in the formation of the near-field hotspot. Another interesting feature is a strong blue shift of the collective magnetic dipole spectrum with decreasing the gap size

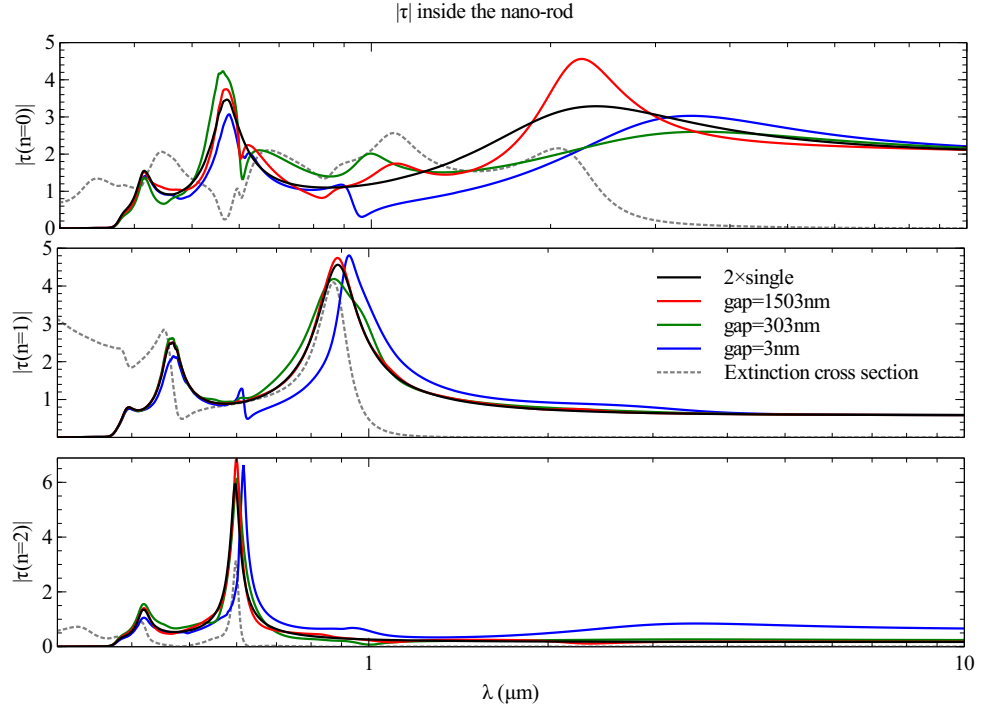


Figure 4.8: Comparison of the spectrum of τ_n^1 (inside the nanowires) for different gap sizes and a single nanowire.

while the other harmonics do not experience critical changes up to quite small separation.

The variation of the NECS resonance amplitudes by changing the gap size is associated with the refraction effect in the case of having the gap size comparable with the wavelength. This is affected by the spectral shifts in magnetic dipole mode and consequently the total ECS. The far-field radiation pattern and the scattered field profile are also demonstrated in Fig. 4.6(f) indicating forward directional scattering properties of the dimer. The demonstrated far-field pattern radial values are normalised to those of a single nanowire, indicating the directivity gain in respect to a single nanowire with the same specification.

Second, in Fig. 4.7 the real part of the magnetic field profile of the first four harmonics is shown in the same silicon dimer. The amplitude of the higher modes become smaller in comparison with the shown modes. The dimer's axis is perpendicular to the direction of the propagation and both nanowires are excited in phase. As a result of this symmetry, the expansion coefficients $m\rho_n^l$ of one cylinder are equal to $m\rho_{-n}^l$, which confirms the theory that the cylinders are practically indistinguishable.

Figure 4.7 demonstrates how the superposition of the different modes forms the total field profile with no symmetry with respect to the centre of the gap in x direction, resulting in magnetic bright and dark spots shifted from the centre of the gap. In other words, destructive and constructive effects of different harmonics of the scattered and incident fields, make it possible to engineer the magnetic hot and cold spots in two sides of the

gap. The map of the electric field modes' distribution also shows similar results but in the opposite direction. Consequently, by overlapping the electric and magnetic hotspots on the other field's dark area, both pure magnetic and pure electric hotspots are formed as is demonstrated in Fig 4.5.

I note that the above investigated silicon dimer is optimised for the electric near field enhancement, based on the descriptions in column two of Table 4.1, which indicates that the behaviour of the resulting magnetic hotspot is not necessarily optimal. This generally applies to the introduced designs in both Tables 4.1 and 4.2. To have a better understanding of the near-field behaviour of the dimer, the expansion coefficient τ_n^1 is plotted in Fig. 4.8 for $n=0, 1$ and 2 . The values are compared in different ranges of gap size. This figure shows the behaviour of light inside the dimer elements and how the resonances of modes become independent of the gap size by increasing the mode number, similar to Fig. 4.6 and in a wider spectral range.

All the results in this section are achieved using the first 30 harmonics. The presented optimised designs, offer new approaches for near-field engineering for variety of applications.

4.2 Metacages

Nanophotonics is finding its way toward modern applications. In communication and signal processing, the electronic signal transmission between the integrated circuit elements is expected to be replaced by optical signals [194, 195]. This would require scaling down laser sources [196] and light detectors [197], for efficient on-chip integration. This is why creating an optical isolation between different components is an extremely important task for eliminating unwanted interferences.

In medicine, new techniques for drug delivery based on optical control of shielded nanostructures attract a growing interest. It became possible to achieve near-complete drug release from hollow gold nano-shells by illuminating them with laser pulses [198, 199] or by microwave radiation of magnetic core-shell nanocarriers [200]. Cubic gold nanocages can be used for controlled drug release, based on photothermal effects and absorption of near-infrared light [201–203], while the organometallic cages can hide photosensitisers to facilitate their delivery to cancer cells [204]. The vesicles covered by gold nanoparticles are unusually stable to high temperatures, chromatographic purification, and high salt concentrations - the conditions which are too harsh for ordinary self-assembled vesicles to survive [205].

The shielding of objects from the optical radiation should also benefit many other research areas. For example, such functionality was predicted with metamaterials [206, 207], graphene sheets [208] and epsilon-near-zero or epsilon-very-large materials [209].

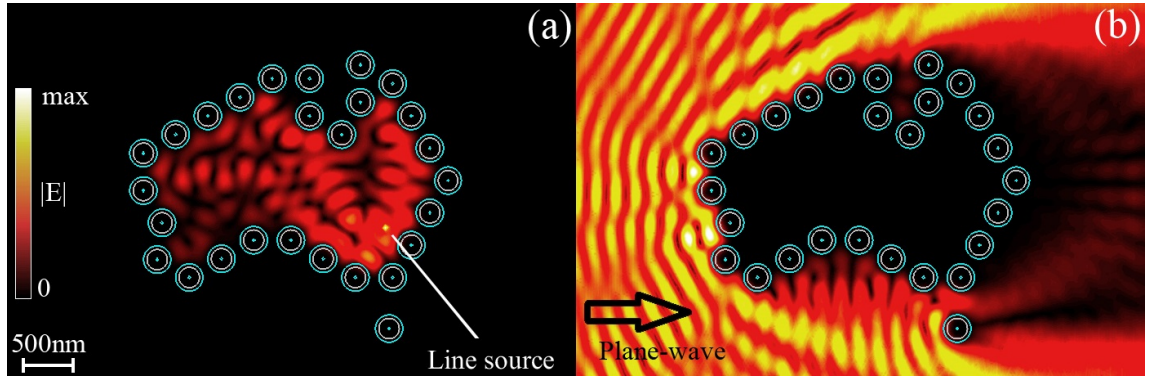


Figure 4.9: Demonstration of metacage functionalities for an arbitrary shape (here is an outline of Australia) made of multilayer nanowires: (a) radiation of a point source placed inside the metacage is contained within the structure. (b) A volume inside the metacage is screened from an incident plane wave. Three-layer Si-Ag-Si nanowires are used to form the metacage. The amplitude of the electric field is plotted at $\lambda = 378\text{nm}$, using the commercial software CST Microwave Studio. The design parameters are found by an analytical approach, and are summarised in Table 4.3.

However, the proposed shielding structures have various limitations, i.e. they can cover either only small subwavelength objects, or only specific geometries, they may require inhomogeneous and/or magnetic materials, and some of the designs do not work in the optical frequency range.

Various thin absorbing structures have been studied for different frequency ranges, ranging from visible [168, 210] and infrared [211–213] to THz [214] and GHz [215]. Perfect symmetric absorbing structures [216, 217], with zero reflection and transmission from either side, have recently attracted considerable attention in THz [218, 219] and GHz [220] frequency ranges.

Here, a novel approach is introduced for designing ultra-thin optical shielding nanostructures (which we call them ‘metacages’), with symmetric functionality across the visible and infrared range, and in both nano- and micrometre scales [88]. We study metashielding structures made of long nanowires composed of realistic materials, enclosing relatively large volumes, which *can operate with a considerable space between the nanowires*. In this section, we do not aim to design perfect absorbers (that can also create fully shielded structures) but instead we design metacages with large gaps between their constituent elements. This condition can be useful for integrated optics since it allows to make shielded spaces of arbitrary shapes. In biological applications, such metacages can be employed to protect live micro-organisms and cells from electromagnetic radiation, while keeping them alive inside the shielded volume in lab-on-a-chip structures by enabling the access of liquids and gases from outside. These nanostructures can operate independently of their shape, being designed effectively in a wide spectral range.

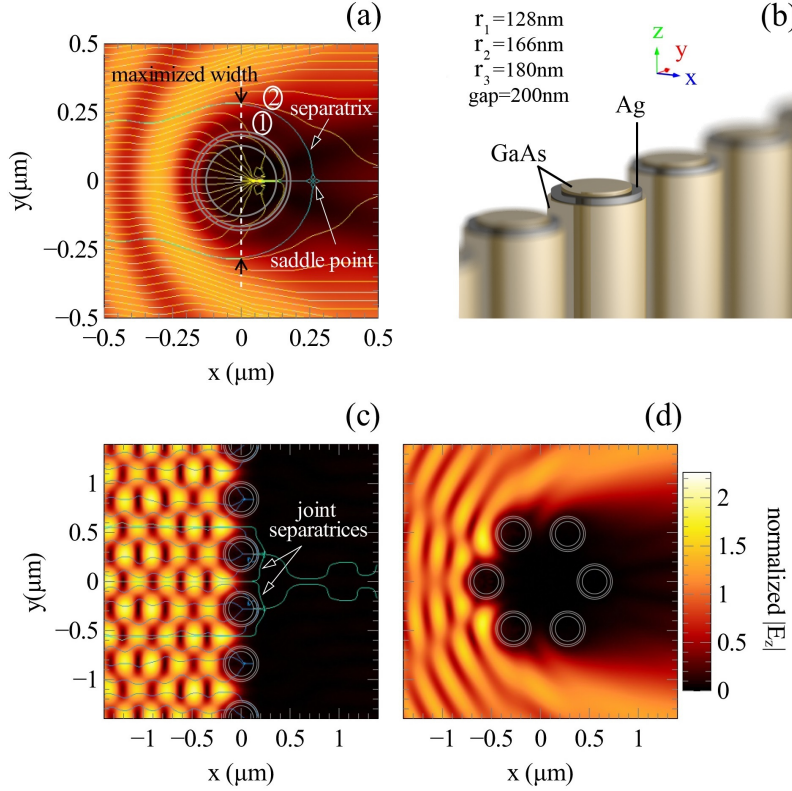


Figure 4.10: Design of metacages. (a) Wave interaction with a single nanowire, colour map shows the field profile, thin lines show the Poynting vectors. Separatrices of the energy flow divide the space into two parts, with energy flowing into the nanowire or going around it. (b) Schematics of the array of multilayer nanowires. (c) A one-dimensional chain of nanowires, which blocks the light propagation. (d) Enclosed volume shielded by nanowires, which can have an almost arbitrary shape (see, e.g., Fig. 4.9). Design parameters are summarised in Table 4.3.

4.2.1 Scattering and absorption of light by an array of nanowires

Using well-spaced nanowires as building blocks of metacages is not only a proper choice to provide a considerable physical space to connect the sides, but also offers flexible design capabilities. Two examples of the analysed structures are demonstrated in Figs. 4.9(a,b) with shielding achieved for a structure with the shape of Australia. Such shields work for any angle of incidence of light, and for any position of the source inside or outside the structure. In what follows, we consider long and identical nanowires with the same gap size between the adjacent elements, and analyse the metacages as two-dimensional structures. Experimental data to describe materials and plasmonic small-size effect have been also considered.

I start with analysing a single, three-layer nanowire made of gallium-arsenide [170] and silver [144], as shown in Fig. 4.10(a) (the choice of materials along with the material parameters used in the simulations is discussed in the following sections). Figure 4.10(a) represents the cross section of the three-layer nanowire. The power flow is shown along

with the calculated saddle point and the separatrices [172, 173]. The separatrices indicate the boundary of two regions marked in Fig. 4.10(a): (1) a region in which energy flow streamlines pass through the nanowire, leading to absorption and scattering of light, and (2) a region where the energy flows around the structure without being absorbed.

Our main idea is to form metacages with large gaps between the elements, but still scattering and absorbing most of the light by making an array of nanowires, as demonstrated schematically in Fig. 4.10(b). *Overlapping the separatrices of individual nanowires eliminates the energy flow that is not affected by the nanoparticles* [region 2 of Fig. 4.10(a)]. Such an array of nanowires can block the electromagnetic waves propagating through the structure. In general, not all this energy is scattered or absorbed by the nanowires, and this causes some power leakage. This effect can be quantified, and a careful design of nanowire structures allows to maximise the absorption and to decrease considerably the energy penetrating through the shield.

The joint separatrices and the formation of a shielding structure is demonstrated in Fig. 4.10(c). This figure shows the functionality of a *shielding meta-wall* in the middle of an array made of twelve nanowires separated by gaps which are larger than their radius. Once the separatrices are overlapped, by keeping the gap size below a certain threshold value, the shielding array operates independently of its shape. As an example, Fig. 4.10(d) shows a closed array of similar nanowires with the similar gap as in Fig. 4.10(c). This is a simple form of a metacage which does not allow electric and magnetic fields to penetrate inside.

The separatrices of the energy flow responsible for the optimal separation of nanowires can be easily calculated by finding the saddle points. To do so, we use the fact that there is no energy flowing through these singular points. In cylindrical coordinates for TM polarised waves, the Poynting vector characterising the energy flow, is $\mathbb{P}_{av} = \frac{1}{2} \text{Re}\{E \times H^*\}$, being expressed as

$$\mathbb{P}_{av} = \frac{1}{2} \left[-\hat{a}_r (E_z^{\text{Re}} H_\varphi^{\text{Re}} + E_z^{\text{Im}} H_\varphi^{\text{Im}}) + \hat{a}_\varphi (E_z^{\text{Re}} H_r^{\text{Re}} + E_z^{\text{Im}} H_r^{\text{Im}}) \right], \quad (4.2)$$

where $\hat{a}_r$ and $\hat{a}_\varphi$ are the unit vectors in r and φ directions, the superscripts ‘Re’ and ‘Im’ indicate the real and imaginary parts, and the fields are functions of r and φ . Solving the equation $\mathbb{P}_{av} = 0$ gives us the locations of the saddle points. For the nanowire shown in Fig. 4.10(a) we find $x_{\text{saddle}} = 262.5 \text{ nm}$. However, in the twelve-element array shown in Fig. 4.10(c), the saddle point shifts to $x_{\text{saddle}} = 237.2 \text{ nm}$ for two nanowires in the middle of the array, due to the multiple scattering and interaction between the nanowires. Once we obtain the saddle points, we choose points close to it ($\pm 1 \text{ nm}$ in x and y directions in our study) and calculate the energy flow using Eq. (4.2), to plot the separatrices, as shown in Fig. 4.10.

An interesting peculiarity of metacages made of multilayer nanowires is their capability

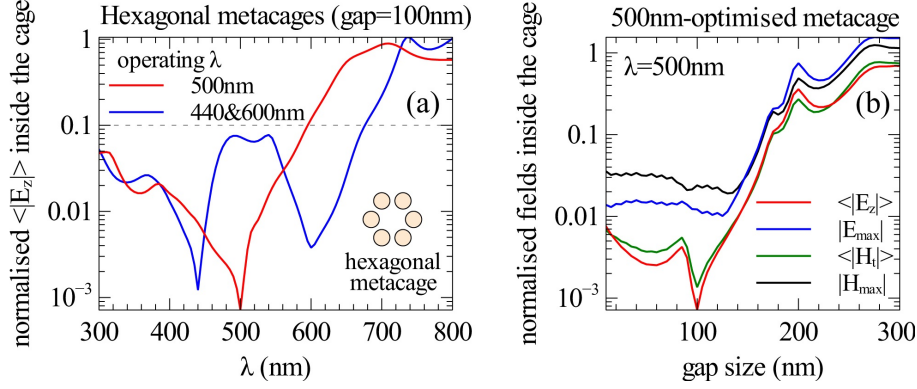


Figure 4.11: (a) Two different hexagonal metacages designed for operation at three different wavelengths (TM polarisation) by optimising the radii of the layers. An average value of the field amplitude inside metacages, remains under 0.1 of the incident wave amplitude across a considerable spectral range. Metacages are made of GaAs-Ag-GaAs multilayer nanowires with radii $r_{1-3} = 72, 165, 200\text{nm}$ and $r_{1-3} = 60, 124, 187\text{nm}$ for the red and blue curves respectively. (b) Variation of the fields' amplitude inside the metacage of figure (a) (red curve) vs. the gap size.

to be designed for frequencies across a wide spectral range. Figure 4.11 demonstrates how modifying the size parameters of the GaAs-Ag-GaAs nanowires in a hexagonal metacage, makes it possible to achieve shielding for the visible range with a high flexibility of selecting the central operating frequency. In this figure, two metacages are compared with the same gap size of 100nm . The cage designed for the wavelength of 500nm has stronger field suppression than the cage designed for 440nm , but it has smaller relative spacing between the nanowires with respect to the nanowires' outer radius. The results show that it is also possible to design metacages for two different wavelengths simultaneously. Figure 4.11(a) shows such a cage, optimised to operate at 440nm and 600nm . The metacages shown in Fig. 4.11(a) suppress the fields in a wide spectral range, so that the average electric field inside the cage stays below 0.1 of the incident wave amplitude.

4.2.2 The role of spacing between the nanowires

The maximum spacing allowed between the nanowires, is not directly proportional to the maximum spacing between separatrices of *individual* nanowires shown in Fig. 4.10(a) by a dashed line. This is caused by the interaction between nanowires that we account for in the multiple scattering method. In order to increase the spacing, we perform the numerical optimisation and find that the optimal period of the array is less than the maximised width between the separatrices for an individual nanowire. Such an optimisation can be done for any desired operation wavelength and for a given set of materials. To demonstrate the dependence of optical shielding on the distance between the nanowires, we analyse two different metacages corresponding to Figs. 4.10 and 4.11 (the red curve). Figure 4.12 shows dependence of the average and maximum field amplitudes inside the cage as functions of the spacing between the rods. We see that both metacages perform well up to relatively

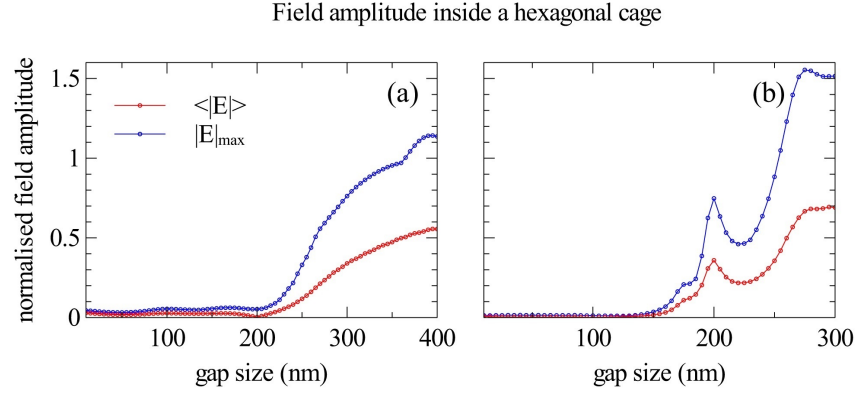


Figure 4.12: Dependence of the maximum and average field amplitudes inside metacages on the size of the gap between the cylinders. (a) for the structure described in Fig. 4.10, while (b) is for the structure shown in Fig. 4.11 (the red curve).

large sizes of the gaps between the nanowires. From these two examples we see that as “a rule of thumb”, metacages work well when the spacing between the cylinders is equal to their radius or smaller.

If we increase the gap between the nanowires so that the separatrices of the adjacent nanowires split, the electromagnetic energy will penetrate into the structure. On the other hand, by decreasing the gap, we suppress the field inside the metacage further and increase the bandwidth of its operation. With a small gap ($5 - 20nm$) between the nanowires, it is possible to achieve wideband shielding, up to hundreds of nanometres, depending on the materials used. For example, by using GaAs nanowires, a considerable shielding bandwidth is achievable from very short wavelengths ($\lambda < 300nm$) up to around $\lambda = 450nm$. With such a close spacing, the bandwidth follows the absorption of the material used in the nanowires construction and the spectrum of the imaginary part of the dielectric constant. Our study shows that shielding bandwidths up to $\lambda = 370nm$ and $\lambda = 600nm$ is possible by using Si and Ge nanowires, respectively.

Despite the improvement of the shielding quality for closer placed nanowire, this suppresses the physical connection between the inside and outside of the metacage. A compromise between the larger gap size and the fields’ suppression can be achieved by designing metashields (see Fig. 4.11). We can ensure the uniformity of the electromagnetic field suppression inside the cage by keeping both the maximum and average fields’ amplitude close to each other during the optimisation process.

4.2.3 Robustness against fabrication inaccuracies

Typically, proposed designs are quite challenging to fabricate with the current available fabrication facilities, and one should always expect presence of some imperfections and inaccuracies, e.g. in thicknesses of the layers of cylinders. There is a range of parameters

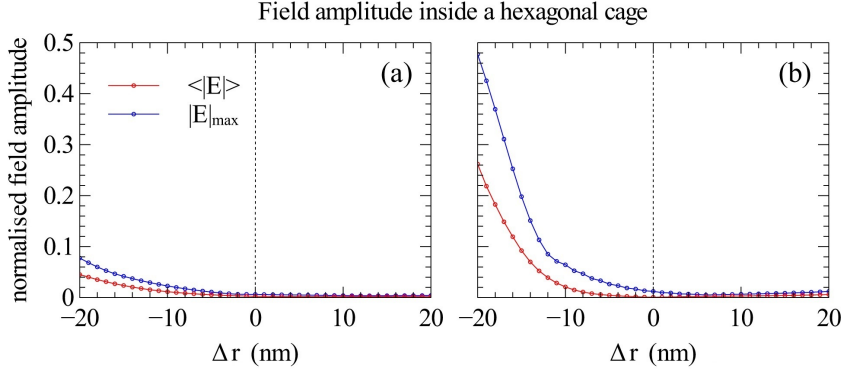


Figure 4.13: The sensitivity of two different metacages to the total radius accuracy. (a) for the structure described in Fig. 4.10, and (b) for the structure in Fig. 4.11 (the red curve).

of the structure that can be distorted in experiments, and as an example, here the effects of imperfections of the fabrication of the outer layer are evaluated. We perform the calculations of the two structures considered in previous section and vary the outer radius, with Δr being a deviation from the optimised condition. The results are shown in Fig. 4.13. We see that in both cases the structures are stable against size variations in a substantial parameter range.

We also observe that the increase of the outer shell size does not lead to the degradation of the performance of the cage. This may be caused by the fact that we vary the size of the nanoparticles but keep the distance between cylinder's centres fixed, so this would reduce the size of the gap between the cylinders as we increase their radius. This reduction of the gap size can explain the low field amplitude inside the structure as we increase the radius.

4.2.4 Choice of materials for optical metacages

There is no general recipe for choosing materials for constructing optimal metacages, since not only material dissipation rates, but also the size parameters and scattering between various nanowires can influence the performance of cages. Such multiple scattering can effectively induce more absorption inside each element even with lower dissipation rates. As an example, gold has more dissipative losses than silver in the visible part of the spectrum, and both imaginary parts of the dielectric constant of these two metals are shown in Fig. 4.14(b). Thus, intuitively, gold should produce a better metacage in visible spectral region. To demonstrate that this is not exactly the case, we replace silver by gold in the structure shown in Fig. 4.10 (where average and maximum fields inside the shielded region are $\langle |E| \rangle = 0.0056$ and $|E|_{max} = 0.055$, respectively, at $\lambda_{opt} = 453$ - see Table 4.3). We find that the structure with gold still shields, but it performs worse with $\langle |E| \rangle = 0.075$ and $|E|_{max} = 0.14$ inside the cage, as the corresponding field distribution is shown in Fig. 4.15(b). This is partly expected, since all the size parameters of the structure are optimised for silver. To make a fair comparison, I ran the optimisation

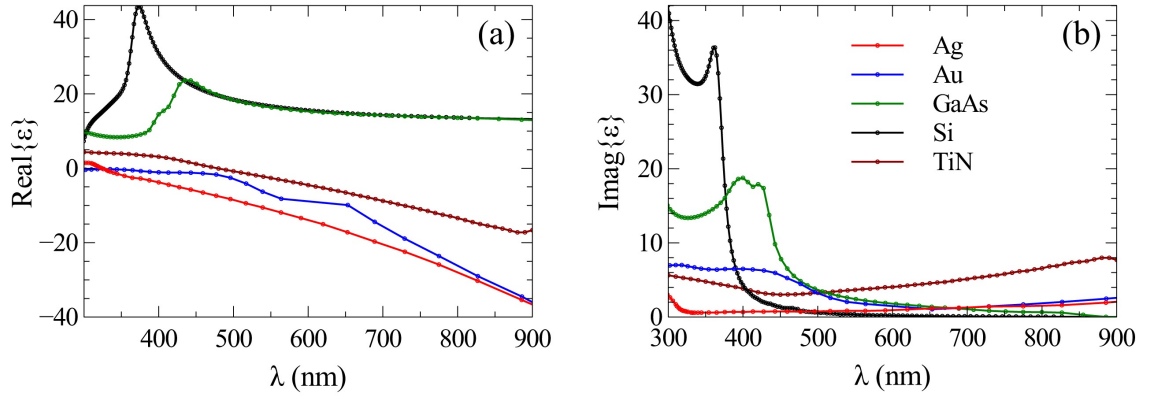


Figure 4.14: (a) Real and (b) imaginary parts of dielectric constant of the used materials (silver and gold [144], gallium arsenide and silicon [170] and titanium nitride [221]).

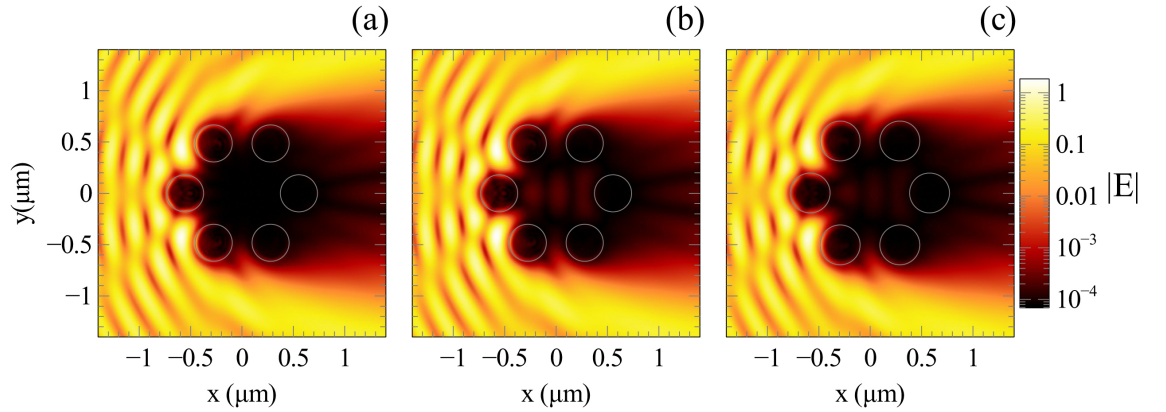


Figure 4.15: Comparison of field profiles of metacages with different materials: (a) the metacage with a silver layer optimised at $\lambda = 453\text{nm}$ as discussed in Fig. 4.10, (b) the same metacage operating in the same wavelength with replacing silver by gold, and (c) a metacage with the gold layer and re-optimised radii at the same wavelength. Studies show better shielding by the silver layer, despite of the spectral behaviour of imaginary part of dielectric constants in two materials (see Fig. 4.14).

process again to find the optimal size parameters for the structure with gold to operate at the same wavelength of 453nm . The field distribution in the obtained structure is shown in Fig. 4.15 and I found, however, that the field suppression is still less efficient for the structure with gold than for the original structure ($\langle |E| \rangle = 0.045$ and $|E|_{\text{max}} = 0.1$, with radii of the shells 129 , 187 and 198nm). In the next step I ran the optimisation in order to find the best possible regime within the wavelength range between 300 and 900nm , and we found that at 475nm the structure with gold can show an excellent optical insulation, comparable to silver performance at the wavelength of 453nm (the results are summarised in Table 4.3).

Table 4.3 summarises the design parameters of the discussed metacages. The results are based on hexagonal structures, which necessitates defining the effective area. To do

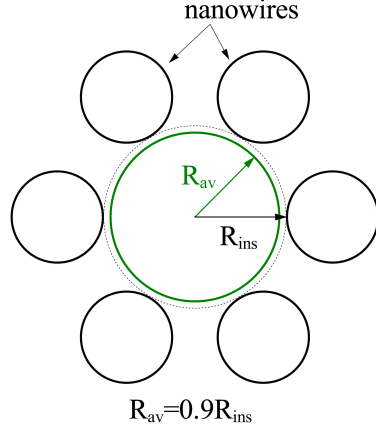


Figure 4.16: The definition of the shielded space inside a metacage shown by the green circle.

Table 4.3: The design parameters of various metacages made of multilayer nanowires with different materials. The average and maximum fields' values indicate $|H|$ and $|E|$ for TE and TM polarisations respectively, inside a hexagonal cage, with external incident plane wave. The fields' value as well as normalised scattering and absorption cross sections (NSCS & NACS) are calculated using the first 30 harmonics (see Section 2.4).

Pol.	$\lambda(\text{nm})$	$r(\text{nm})$	gap(nm)	Configuration	Ave.	Max.	NSCS	NACS	Figure
TM	378	11,102,137	100	Si-Ag-Si	4.2e-4	4.5e-3	6.68	2.46	4.9
TM	453	128,166,180	200	GaAs-Ag-GaAs	5.6e-3	5.5e-2	7.01	4.08	4.10
TM	500	72,165,200	100	GaAs-Ag-GaAs	7.2e-4	1.2e-2	8.30	1.21	4.11 (red)
TM	440	60,124,187	100	GaAs-Ag-GaAs	1.2e-3	2.3e-3	6.79	0.73	4.11 (blue)
TM	449	138,148,158	100	GaAs-TiN-GaAs	1.0e-2	2.7e-2	5.58	3.06	4.17
TE	648	74,163,188	100	Si-Ag-Si	1.10E-03	5.60E-03	5.81	1.07	4.18(a) & 4.20(a,b)
TE	333	78,200	100	GaAs-Ag	8.70E-03	2.10E-02	9.71	4.46	4.18(b)
TM	445	193	100	GaAs	2.50E-03	6.20E-03	7.42	2.71	—
TM	378	102,137	100	Ag-Si	5.90E-04	4.50E-03	6.68	2.46	—
TM	475	73,180,193	200	GaAs-Au-GaAs	5.40E-03	5.70E-02	6.89	4.23	—
TM	300	137,145,195	8	GaAs-TiN-GaAs	1.40E-07	3.80E-07	9.42	3.4	4.20(c)

this in the hexagonal metacage, we start with the inscribed circle of the radius R_{ins} that fits into the metacage (see Fig. 4.16). Since the structure supports resonances, one can expect large EM field enhancement on cylinder surfaces, therefore, we limit the radius of the area that we average over to $R_{av} = 0.9R_{ins}$.

Further studies show that the design of metacages with an acceptable performance is also possible with two-layer or even solid nanowires (see Table 4.3). The benefit of three-layer structures discussed in this letter is their high degree of varying parameters, either for specific wavelengths or for optimisation of other performance parameters, such as the gap size.

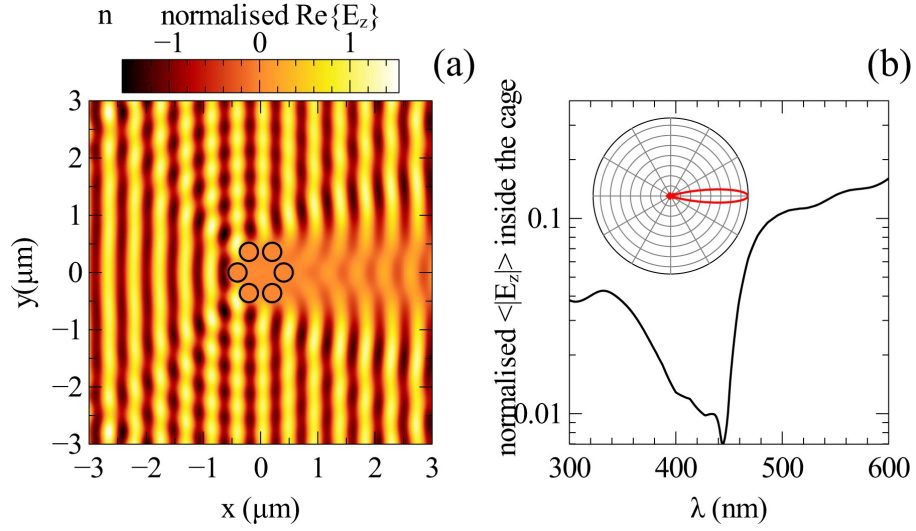


Figure 4.17: (a) Real part of the field shows the absence of the backward reflection (the incident plane-wave is propagating in x direction). (b) Metacage keeps the shielding functionality. The inset shows the far-field scattering pattern; metacage is made of gallium arsenide and titanium nitride [221] and the design parameters are listed in the last row of Table 4.3.

4.2.5 Backward scattering cancellation, polarisation and incidence angle independence

In addition to discussed shielding functionality, arbitrary shapes, physical connection between the two sides, and frequency selectivity, metacages can also be designed to show other interesting properties simultaneously. Figure 4.17 demonstrates the shielding functionality and far-field scattering pattern of a metacage which is designed with substantially decreased backward scattering (described in Table 4.3). Such suppressed backward and enhanced forward scattering is useful for many applications such as biophotonics and imaging.

Cylindrical geometries for normal incidence typically are designed to operate for a given polarisation only. I investigated various shielding examples operating in TM polarisation. However, by employing the introduced approach, we can also design metacages that can efficiently block electromagnetic waves in TE polarisation where the electric field is perpendicular to the nanowires. By the same shielding mechanism as that for TM polarisation, Fig. 4.18 shows magnetic field structure for the case of TE polarised wave incident on two different metacages, and they show excellent shielding performance. The parameters of these metacages are shown in Table 4.3.

Another feature of optical metacages which they preserve in all the designs, is their robustness against the angle of incidence. The simulations are performed for various incident angles in the plane perpendicular to the wires, done for the arbitrarily shaped metacage of Fig. 4.9. The results are shown in Fig 4.19 and demonstrate that the functionality of the metacage is efficiently preserved for any incident angle (a-c), including the case of the

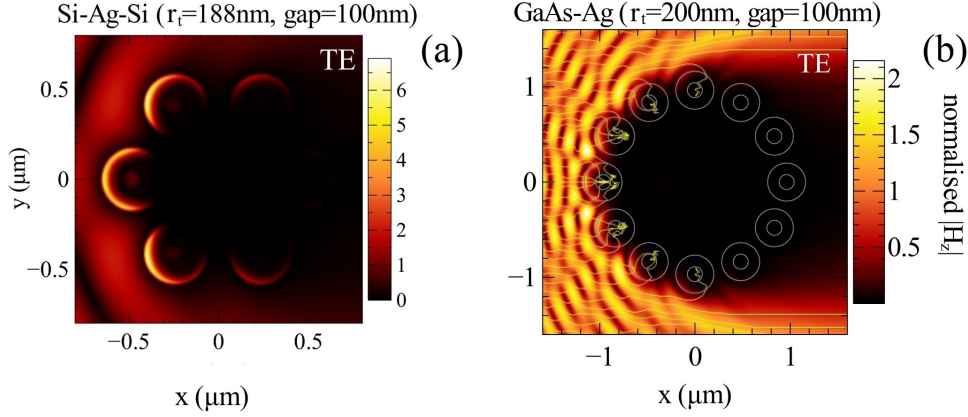


Figure 4.18: Magnetic field amplitude distribution in two metacages for TE polarised illumination; (a) three layer and (b) two layer nanowires, with parameters shown in Table 4.3.

line source excitation placed at arbitrary points inside (d,e) or outside the cage (f-h).

Here, I remind that apart from studying, analysing and controlling of scattering and absorption by nanowires, one of the main goals of this thesis, is developing a solution that is not basically restricted to two-dimensional (2D) problems. As was mentioned in Chapters 1 and 2, assuming long nanowires and 2D analysis, by simplifying scattering problems facilitates the development of novel solutions and designs, and this will be of more interest if we can expand the solutions to 3D structures. In this thesis, 2D nanowires were chosen to study light-matter interaction and discussing 3D structures is out of the scope of this study. However, to demonstrate that the discussed results and the developed approach are also applicable on 3D problems, some of the 2D studied metacages are briefly analysed, as examples of multi-element interfering systems, in 3D platform. I demonstrate that the discussed solutions are basically valid even by taking the third dimension into account.

For instance, here we study the metacage of Fig. 4.18(a) as an example of metacages introduced in TE polarisation (described in Table 4.3), in a simple 3D configuration by confined length of the nanowires and even in a bigger cage rather than Fig. 4.18(a). Figure 4.20(a,b) demonstrates that apart from in-plane variation of the angle of incidence, it is also possible that the wave can be incident from an out of plane angle, when the direction of propagation does not form a normal to the wires. This figure demonstrates the shielding properties of a metacage made of finite length of $1 \mu m$ long nanowires excited by an electric line source, which creates a wide angular spectrum of incident waves. Therefore, the functionality of this metacage, remains independent of the out of plane angle of incidence, in addition to the discussed in-plane angle independence, forming a 3D functioning cage. I note that Fig. 4.20 uses logarithmic scale and this exaggerates the power leakage inside the cage.

In another 3D simulation, the metacage introduced in the last row of Table 4.3, has

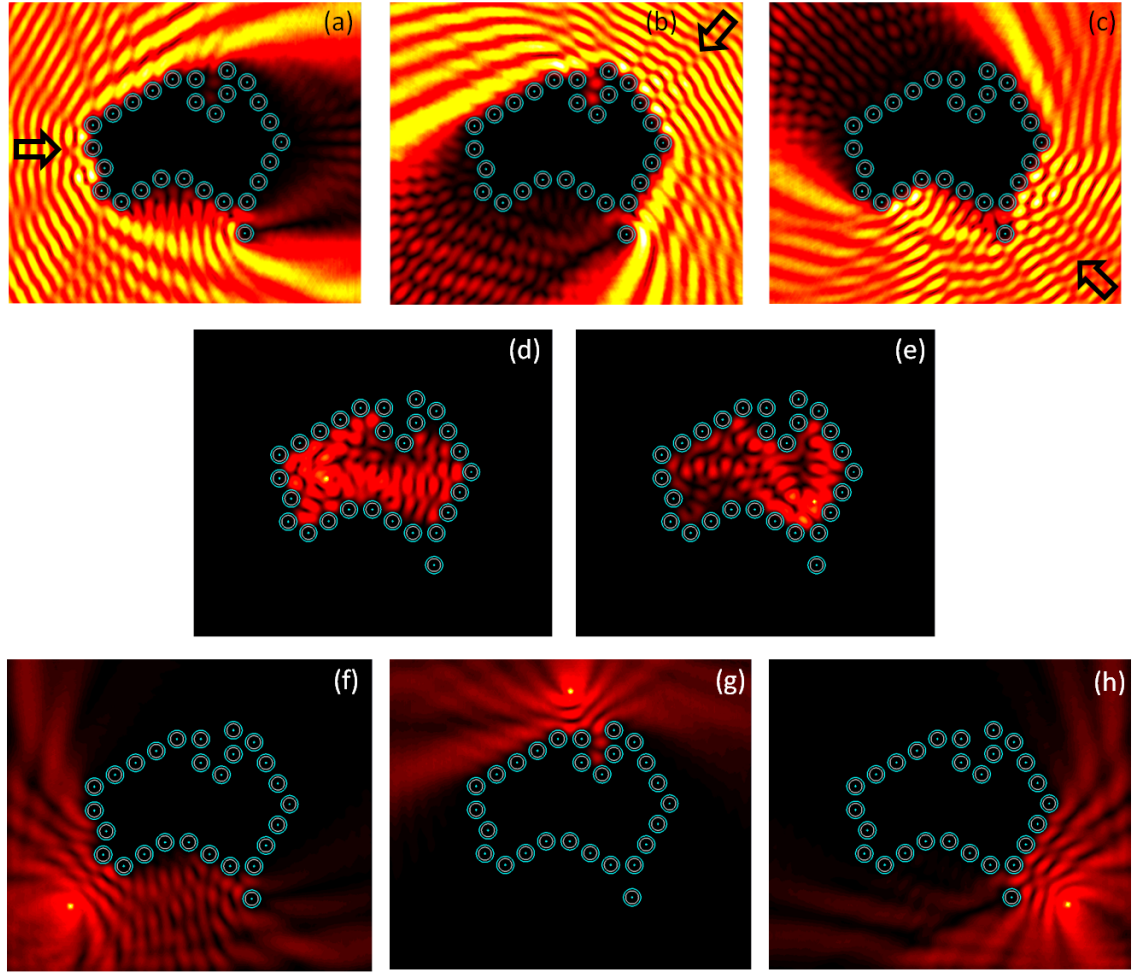


Figure 4.19: The cage with an arbitrary shape (from Fig. 4.9) and plane-wave/line-source incidence from different angles (inside/outside).

been chosen to study on a glass substrate. Figure 4.20(c) demonstrates distribution of the electric field perpendicular to the surface of the glass (TM polarisation). The logarithmic scale of the plot indicates negligible amount of energy inside the cage.

Excellent three dimensional functionality of metacages based on the achieved results with 2D approach and even by presence of substrates, confirms the applicability of the presented 2D study of nanowires for 3D structures. The presented results in this section and the 3D approach mentioned in Chapter 3 are different functioning examples of single and multiple-elements structures in 3D, meeting one of the important goals of this thesis.

In this chapter I studied light interaction with multi-element nanowire systems. Multi-pole expansion and multiple scattering solutions employed in the smart genetic algorithm lead us to develop optimal designs with multilayer nanowires. Dielectric and metallic dimers were studied with their axis parallel or perpendicular to the direction of the incident wave propagation in different polarisations. Both electric and magnetic hotspots were investigated and different harmonics and their behaviour were analysed with making

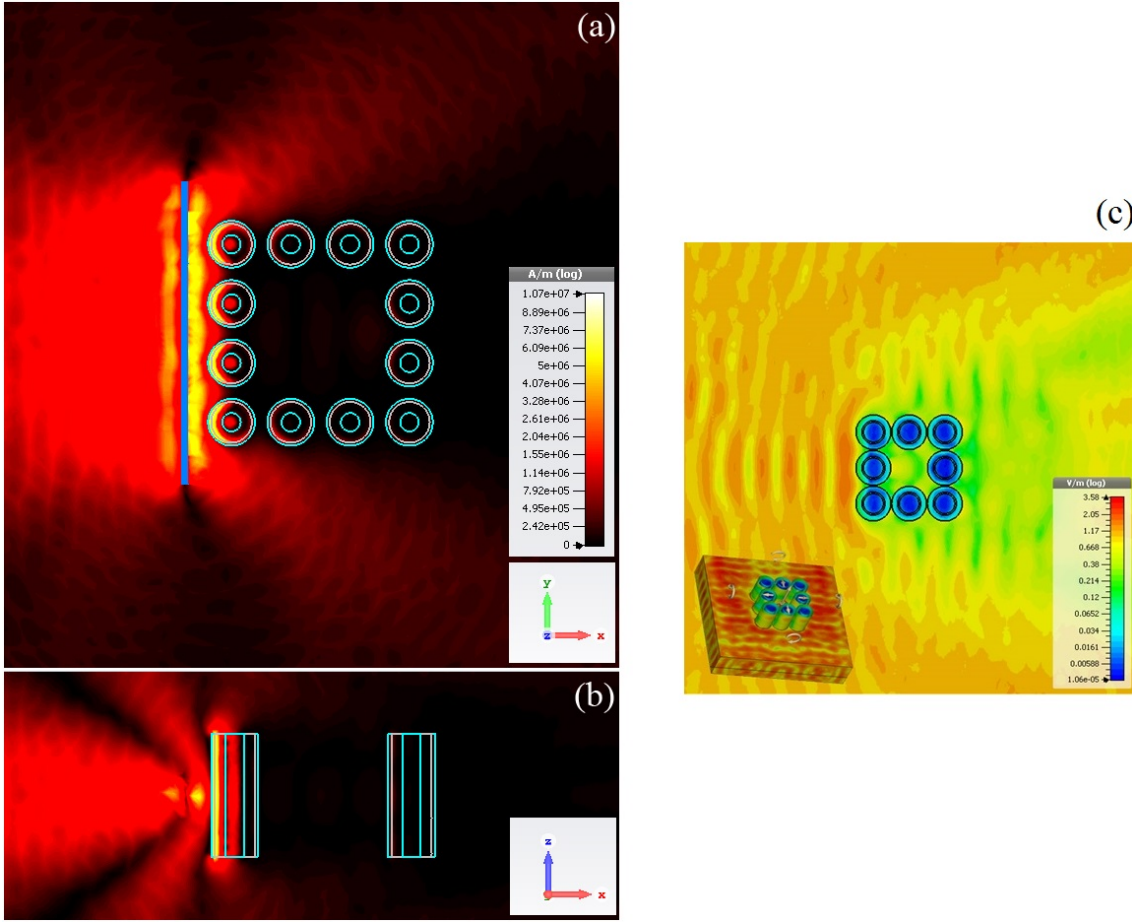


Figure 4.20: (a,b): Magnetic field (H_z) distribution for a finite length metacage [based on Fig. 4.18(a)] illuminated by waves created by a line source. (a) top-view and (b) side-view. A line source creates waves with angles of incidence in the range $\pm 70^\circ$. Vertical blue line in (a) shows source position. The metacage is made based on Si-Ag-Si nanowires for TE polarisation with parameters shown in Table 4.3. (c) Electric field (E_z) distribution by a TM planewave illuminating from left, on a metacage with finite length wires on a glass substrate, based on the last row of Table 4.3. All the plots are in log-scale to exaggerate the power leakage inside the cage.

the dimer elements closer, starting from a single nanowire. I also analysed the displacement of the hotspots from the centre of the gap. It was shown that for electric/magnetic hotspots in dielectric dimers, there is a point on the other side of the gap with zero amplitude of the same field (electric/magnetic), which overlaps the hotspot of the other field (magnetic/electric). This leads to formation of both pure magnetic and electric hotspots in opposite sides of the gap, suitable for sensitive sensing applications.

By having more complicated structures with more nanowires, I introduced a novel approach for designing optical shielding structures based on arrays of nanowires. Optimised metacages for both TE and TM polarisations were analysed with both hybrid and non-metallic configurations based on realistic material data. Also, the results were confirmed by numerical simulations based on a finite-element method and demonstrated that the introduced meta-shielding structures can maintain their functionality for an arbitrary

shape due to the suppression of transmission by overlapping the energy flow separatrices. I discussed a design of metacages for any selected wavelength in a wide spectral range, and analysed an interplay between gap size and efficiency of the fields' suppression. Metacages' robustness against experimental inaccuracies as well as canceling backward scattering and their angle independence were discussed, and some 3D examples of the obtained results were presented. Metashields have potential application in various fields of study such as shielding different nano-component in integrated optics. Metacages also can be employed to protect live organs from harmful radiation while they allow liquids and gases to pass through their structure for feeding and studying them. Creating noiseless sensing platforms is another suggested application for metacages.

Nonlinearity in Multilayer Nanowires

In the previous chapters, linear properties of single/multi-layer nanowires were discussed in detail for various applications. I demonstrated that by using multilayer nanowires one can achieve significant local field enhancement either due to the band-gap effects, or due to presence of metals and excitation of localised plasmons. Optical nonlinearity also benefits from long interaction lengths. Therefore, the geometry of multilayer nanowires, their unique optical properties and the possibility of their fabrication out of various materials, provide an excellent platform for tightly focusing high intensities of light in a long interacting area.

By the use of very high intensities comparable to inter-atomic electric fields, the polarisation of constructive electric dipoles of the material (discussed in Chapter 1) respond nonlinearly to the incident external electric field. As a result, two or three photons with the fundamental frequency can be converted into a single photon at twice or triple the fundamental frequency respectively, producing higher order harmonics. Doubling the frequency of light or tripling it, are called second and third harmonic generation respectively (SHG and THG) and are describable using susceptibility tensors. Characterisation of harmonics generation in nonlinear nanowires [222] and their various applications such as light-emitting diodes and lasers [223], photodetectors [38] and waveguides [194] have been vastly studied [224, 225]. However, investigating the behaviour of light in the fundamental frequency remains significantly important in nonlinear systems, both for fundamental study of nonlinear light interaction, and also for various applications, for instance, in ultra-fast all-optical modulation and switching [226, 227]. All-optical switching in fundamental frequency, where a light control signal, switches another output beam, is an important concept of optical logic gates.

Considering local field enhancement by multilayer nanowires can be a highly efficient solution for designing nonlinear systems in fundamental frequency. This suggests strongly enhanced nonlinear effects, such as bistability and switching, which is the subject of my study in this chapter.

I study scattering of light by cylindrical multi-layer structures containing Kerr-type nonlinear materials. To analyse nonlinear properties in nanowires, direct numerical simulations such as finite difference time domain approach (FDTD) are possible [228]. However, as is demonstrated in this chapter, FDTD is very time consuming and often does not allow exploration of the full parameter space. Therefore, develop a new semi-analytical method is developed for solving nonlinear problems by reducing the original two-dimensional system by a one-dimensional nonlinear Helmholtz equation.

In the developed solution [84] to study nonlinear nanowires, practical and realistic considerations are taken into account. For instance, previous works have demonstrated that it is possible to analyse cylindrical structures using various approximations, for example, for perfectly conducting metals [229], for homogeneous structures [230–232] or for weak nonlinearities [233, 234]. In this chapter, a precise, robust, semi-analytical method is developed for studying two-dimensional and circular multilayer nanowires, which can contain, in general, lossy dielectric and metallic layers. This method is applied for scattering by a core/shell metal/dielectric nanowire, and it is shown that this approach allows us to perform nonlinear control of scattering cross-section, which in resonant regime demonstrates optical bistability. I compare this method to an FDTD approach, and find that the new approach is accurate, 10^5 times faster, and more numerically robust than FDTD. This approach can be applied to study nonlinear properties of various nanowire structures.

5.1 Rewriting linear equations

We study TM polarised light scattering on a multi-layer cylindrical structure, which may contain both dielectric and metallic layers, see Fig. 5.1 (similar approach applies for TE polarisation). Propagation of the time harmonic electromagnetic waves is governed by the Helmholtz equation for the magnetic field $\nabla^2 H_{||} + k^2 H_{||} = 0$ where $k^2 = \varepsilon(\mathbf{r})k_0^2$, where $H_{||}$ is the magnetic field component along the cylinder axis, $k_0 = \omega/c$ is the free space wavenumber, k is the wavenumber in medium, $\varepsilon(\mathbf{r})$ is the inhomogeneous dielectric permittivity of the multi-layer cylinder and c is the speed of light. In cylindrical coordinates (r, ϕ, z) , for the cylinder aligned along z axis this equation can be explicitly written as

$$\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial H_z}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 H_z}{\partial \phi^2} + k^2 H_z = 0. \quad (5.1)$$

We consider self-action effects [235], when the dielectric permittivity acquires Kerr-type intensity-dependent correction and it can be written as $\varepsilon_{NL}(r, \phi) = \varepsilon_L(r) + \Delta\varepsilon(|E(r, \phi)|^2)$. In the current study we neglect higher harmonic generation, thus Eq. (5.1) together with the Ampere's law, which allows us to express the electric field via magnetic field, form a closed set of partial differential equations (PDEs).

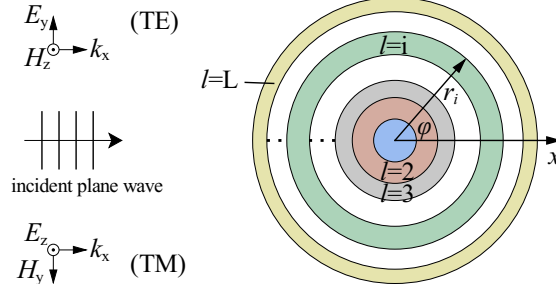


Figure 5.1: Schematics of the problem: TM polarised plane wave is scattered on a multi-layer cylindrical structure.

Considering the positive and negative modes degeneracy in a single nanowire, the decomposition of fields into cylindrical harmonics from Section 2.1, can be rewritten as:

$$\mathbf{H}_z(r, \varphi) = \hat{\mathbf{a}}_z H_0 \sum_{n=0}^{+\infty} N(n) i^n \left[\tau_l^n J_n(\bar{r}) + \rho_l^n H_n^{(1)}(\bar{r}) \right] \cos(n\varphi) = \hat{\mathbf{a}}_z H_0 \sum_{n=0}^{+\infty} N(n) H_z^n(r) \cos(n\varphi), \quad (5.2)$$

$$\mathbf{E}_\varphi(r, \varphi) = \hat{\mathbf{a}}_\varphi E_0 \sum_{n=0}^{+\infty} \frac{N(n) i^{n+1}}{\sqrt{\varepsilon(r, \lambda)}} \left[\tau_l^n J_n'(\bar{r}) + \rho_l^n H_n^{(1)'}(\bar{r}) \right] \cos(n\varphi) = \hat{\mathbf{a}}_\varphi E_0 \sum_{n=0}^{+\infty} N(n) E_\varphi^n(r) \cos(n\varphi), \quad (5.3)$$

$$\mathbf{E}_r(r, \varphi) = \hat{\mathbf{a}}_r E_0 \sum_{n=0}^{+\infty} \frac{n N(n) i^{n+1}}{\sqrt{k_0 r \varepsilon(r, \lambda)}} \left[\tau_l^n J_n(\bar{r}) + \rho_l^n H_n^{(1)}(\bar{r}) \right] \sin(n\varphi) = \hat{\mathbf{a}}_r E_0 \sum_{n=0}^{+\infty} N(n) E_r^n(r) \sin(n\varphi), \quad (5.4)$$

where $k(r) = k_0 \sqrt{\varepsilon(r, \lambda)}$, $\bar{r} = rk(r)$, $E_0 = \eta_0 H_0$, $\eta_0 = \sqrt{\mu_0/\varepsilon_0}$ is the free space impedance. Coefficient $N(n) = 1$ for $n = 0$ and for all other modes $N(n) = 2$ due to the symmetric relation of the Bessel functions between positive and negative indices.

5.2 Nonlinear scattering by multilayer nanowires

Now we assume that some of the layers are nonlinear, and the nonlinear correction to the dielectric permittivity is a function of the intensity of the electric field at the corresponding point in space:

$$\Delta\varepsilon(r, \varphi) = \alpha |E_{total}(r, \varphi)|^2, \quad (5.5)$$

in where α is the nonlinear coefficient that determines the correction in the dielectric constant. Calculating α is possible by having nonlinear refractive index coefficient ' n_2 ' using $n_{NL}(\omega, |E|^2) = n_L(\omega) + n_2 |E|^2$, in which $n_{NL}(\omega, |E|^2)$ and $n_L(\omega)$ are total and linear refractive index respectively [4]. However, in this chapter, the total variation of dielectric constant remains a variable to study nonlinearity in multilayer nanowires. We use the symmetry of the problem, and write nonlinear correction to the dielectric permittivity

$\Delta\varepsilon(r, \varphi)$ in the form of Fourier cosine series as

$$\Delta\varepsilon(r, \varphi) = \delta\varepsilon^0(r) + \sum_{m=1}^{+\infty} \delta\varepsilon^m(r) \cos(m\varphi). \quad (5.6)$$

The coefficients of the Fourier cosine series can be explicitly calculated as

$$\delta\varepsilon^m(r) = \frac{N(m)}{\pi} \int_0^\pi \alpha |E_{total}(r, \varphi)|^2 \cos(m\varphi) d\varphi, \quad (5.7)$$

where $|E_{total}|^2 = |\vec{E}_\varphi|^2 + |\vec{E}_r|^2$. I note that the intensity of the electric field can be represented as follows:

$$|E_{total}|^2 = |\vec{E}_\varphi|^2 + |\vec{E}_r|^2 = (E_\varphi^R)^2 + (E_\varphi^I)^2 + (E_r^R)^2 + (E_r^I)^2, \quad (5.8)$$

where R and I indicate real and imaginary parts, respectively. For $(E_\varphi^R)^2$ and $(E_\varphi^I)^2$, using Eq. (5.3), we write

$$(E_\varphi^{R,I})^2 = E_0^2 \sum_{i=0}^{\infty} \sum_{j=0}^{\infty} N(i)N(j) E_\varphi^{i,R,I} E_\varphi^{j,R,I} \cos(i\varphi) \cos(j\varphi), \quad (5.9)$$

and similarly, using Eq. (5.4),

$$(E_r^{R,I})^2 = E_0^2 \sum_{i=0}^{\infty} \sum_{j=0}^{\infty} N(i)N(j) E_r^{i,R,I} E_r^{j,R,I} \sin(i\varphi) \sin(j\varphi). \quad (5.10)$$

Using trigonometric identities $\cos(x)\cos(y) = [\cos(x+y) + \cos(x-y)]/2$ and $\sin(x)\sin(y) = [\cos(x-y) - \cos(x+y)]/2$, we can represent electric field components as follows

$$(E_\varphi^{R,I})^2 = E_0^2 \sum_{i=0}^{\infty} D_{E_\varphi}^{i,R,I}(r) \cos(i\varphi), \quad (5.11)$$

$$(E_r^{R,I})^2 = E_0^2 \sum_{i=0}^{\infty} D_{E_r}^{i,R,I}(r) \cos(i\varphi), \quad (5.12)$$

where

$$D_{E_\varphi}^{i,R,I}(r) = \frac{1}{2} \sum_{j=0}^{\infty} \left(N(i-j)N(j) E_\varphi^{i-j,R,I} E_\varphi^{j,R,I} + \frac{2N(i+j)N(j)}{3-N(i)} E_\varphi^{i+j,R,I} E_\varphi^{j,R,I} \right), \quad (5.13)$$

$$D_{E_r}^{i,R,I}(r) = \frac{1}{2} \sum_{j=0}^{\infty} \left(-N(i-j)N(j) E_r^{i-j,R,I} E_r^{j,R,I} + \frac{2N(i+j)N(j)}{3-N(i)} E_r^{i+j,R,I} E_r^{j,R,I} \right). \quad (5.14)$$

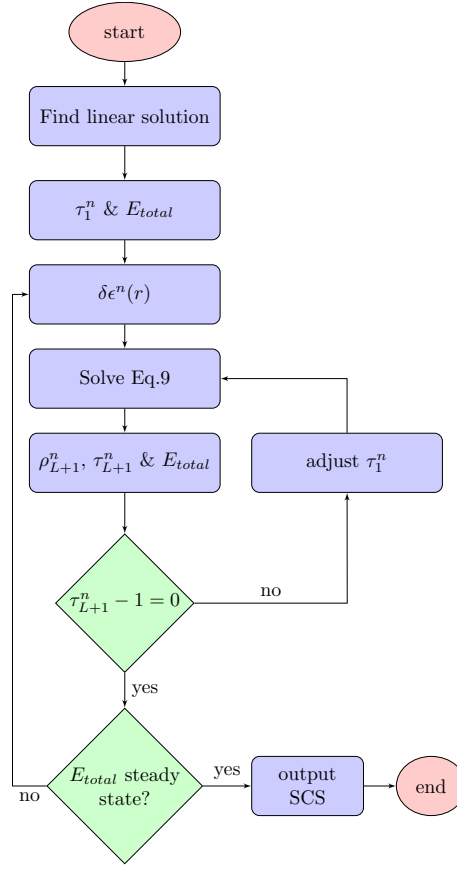


Figure 5.2: Flowchart of the iterative algorithm used for the solution of nonlinear problem.

As a result, we obtain the explicit expressions for the coefficients of the Fourier cosine series in the form

$$\delta\epsilon^m(r) = \alpha E_0^2 (D_{E_\varphi}^{m,R} + D_{E_\varphi}^{m,I} + D_{E_r}^{m,R} + D_{E_r}^{m,I}). \quad (5.15)$$

Now we substitute field and dielectric permittivity decompositions into Eq. (5.1) and obtain

$$\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial H_z^n}{\partial r} \right) + \left[k_0^2 (\epsilon_L + \delta\epsilon^0) - \frac{n^2}{r^2} \right] H_z^n + \frac{k_0^2 S_{H_z}^n}{N(n)} = 0, \quad (5.16)$$

where

$$S_{H_z}^n(r) = \frac{N(n)}{\pi} \int_0^\pi (\Delta\epsilon(r, \varphi) - \delta\epsilon^0(r)) H_z(r, \varphi) \cos(n\varphi) d\varphi. \quad (5.17)$$

Equation (5.16) is an ordinary differential equation (ODE), and along with Eq. (5.6) it forms a closed set of nonlinear equations. To solve the complete set of equations, an iterative method is used, and the algorithm is outlined in the diagram shown in Fig. 5.2. As a first iteration, we find solution of the problem in the linear limit using mode decomposition method. Then, we use the values of the mode amplitudes in the innermost

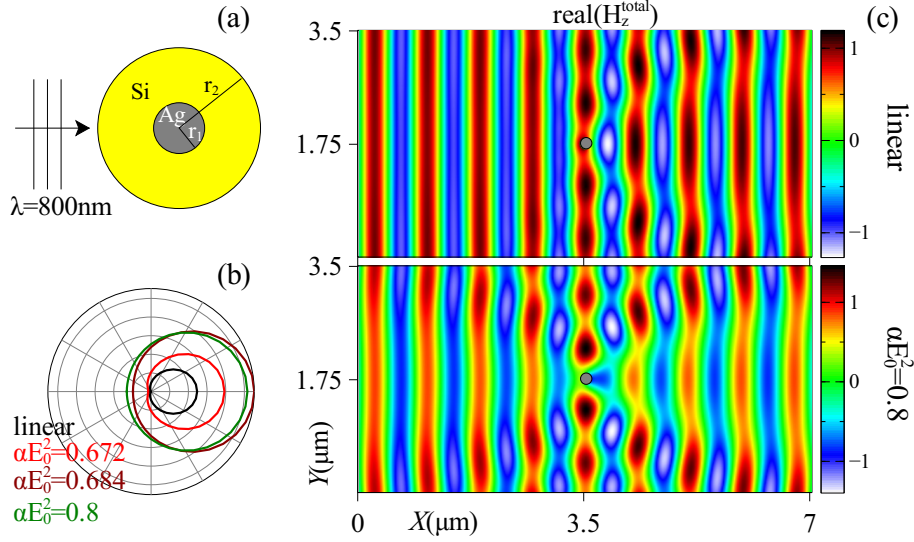


Figure 5.3: (a) The core-shell structure and the incident plane wave, $r_1 = 18nm$ and $r_2 = 73nm$. (b) Far field radiation pattern for linear and nonlinear cases, (c) Field profile outside the structure in two linear and nonlinear regimes. The gray circle in the middle indicates the structure.

cylinder (τ_1^n) as initial condition for the next iteration. In nonlinear layers, we calculate $\delta\epsilon$ using the field profile found on a previous iteration step. As a result of each iteration we find $H_z^n(r)$, $E_\phi^n(r)$ and $E_r^n(r)$ in the whole structure. Outside the structure, the incoming wave should be a plane wave, therefore our target function that we want to find zero of is $F(\tau_1^n) = \sum_n |\tau_{L+1}^n - 1|$. Since in our structure the number of modes is small, we are able to use a simplified approach to minimise this function. In particular, we find zero of auxiliary functions $F_n = \tau_{L+1}^n - 1$, and do several iterations over all n to achieve desired accuracy of the condition $F(\tau_1^n) = 0$.

Note!

In nonlinear layers, Eq. (5.16) can be solved by two simultaneous iterations: (i) breaking down the power variation range into smaller steps to maintain the stability of the approach. The step size should be dynamically defined to make it possible to be smaller in case of instability. And (ii) iterations in every power step, using Runge-Kutta method. This is while, in linear layers we still use the mode expansion method.

Once the Eq. (5.16) is solved, and the magnetic field is found, we need to calculate electric field in the structure, since it defines nonlinear correction to the dielectric permittivity. Electric field is found using Maxwell's equations.

Direct use of the nonlinear correction to the dielectric permittivity given by Eq. (5.6) in simulations leads to numerical instabilities, therefore we would like to introduce the nonlinearity in the system gradually. To do this, we have an additional iteration loop, and

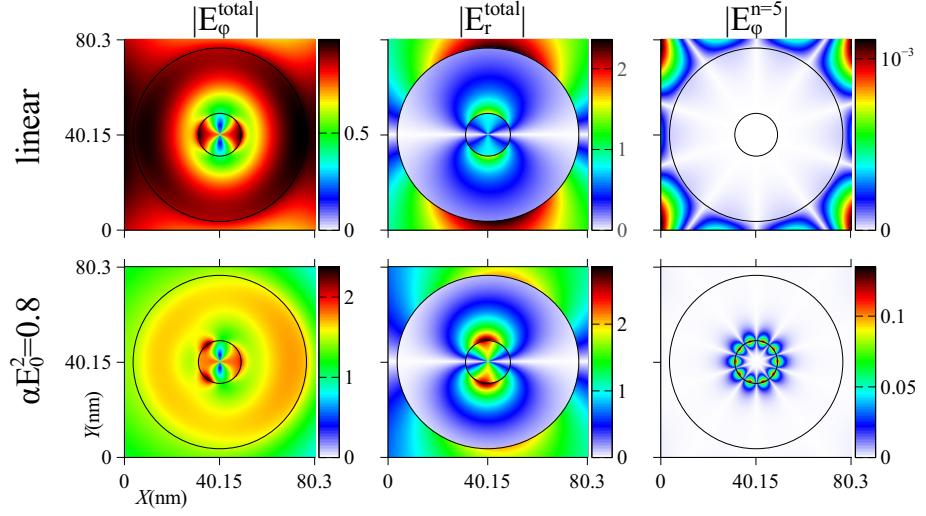


Figure 5.4: Field profile inside the structure for $\lambda = 800nm$; both linear and nonlinear regimes using the first eight excited modes. Total value of E_φ and E_r are plotted separately to demonstrate how they change in the boundaries. E_φ in mode $n = 5$ is also plotted as an example of how higher modes are excited in the structure in nonlinear regime.

in each step the nonlinear correction to the dielectric permittivity is taken in the form

$$\delta\varepsilon^n(r) = (1 - \beta)\delta\varepsilon_{prev}^n(r) + \beta\delta\varepsilon_{new}^n(r), \quad (5.18)$$

where $\delta\varepsilon_{prev}^n(r)$ is the correction to the dielectric constant at previous iteration step, and $\delta\varepsilon_{new}^n(r)$ is the correction to the dielectric constant calculated using the field from the current iteration step, β is a small parameter that controls convergence, which should be found empirically. In our simulations, we found that $\beta = 0.1$ is sufficient to ensure convergence. Clearly, when the iteration loop converges, $\delta\varepsilon^n(r) = \delta\varepsilon_{prev}^n(r) = \delta\varepsilon_{new}^n(r)$, and the fields that we find represent self-consistent solution of the original set of nonlinear equations.

5.3 Nonlinear control of superscattering

As an example of application of this method, we study nonlinear properties of a plasmonic core-shell nanowire which was introduced in Section 3.1.3. As was discussed, this nanowire can exhibit either enhanced or suppressed scattering at different frequencies [83]. The structure is made of a silver core and a silicon shell with $18nm$ and $73nm$ radii, respectively, as is shown in Fig. 5.3(a). We assume that the dielectric shell is nonlinear. In these simulations we consider the strength of nonlinear response above that available in natural materials, and this is to demonstrate the superior stability of our method [84].

Figures 5.3(b) and (c) show the far field radiation pattern and the field profile around the structure for low and high incident powers at $\lambda = 800nm$. Figure 5.4 compares the

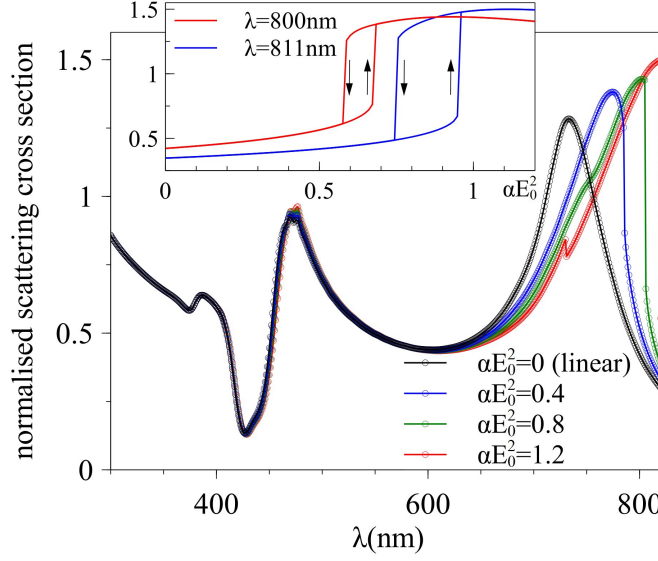


Figure 5.5: Change of the SCS spectrum with the increase of the incident field amplitude E_0 . The numbers on the curves indicate the value of αE_0^2 . The inset shows dependence of the SCS on the incident power at 800nm and 811nm.

field profile inside the structure in both linear and nonlinear regimes and shows how higher order modes are strongly excited in nonlinear regime.

Figure 5.3(b) demonstrates an abrupt change in the far-field radiation pattern at a certain threshold value of the incident power, and this is a result of the bistable response of the structure at high power levels. The mechanism of the bistability is similar to that in many nonlinear resonant systems. In particular, the increase of the power leads to the change of the dielectric constant of nonlinear materials and this, in turn, shifts the resonance frequency of the structure. For a chosen frequency, which is offset from the resonance, this may produce a multi-stable response, as we observe in our structure. Figure 5.5 shows SCS spectrum for different incident power levels and how the shift of the SCS resonance causes multi-stable response for the wavelengths above the resonance. Figure 5.6 shows the hysteresis loop properties and the values of threshold incident powers for different wavelengths. Figure 5.6 also shows, that for $\lambda = 811nm$ the width of the hysteresis loop reaches its maximum, and corresponding hysteresis is presented in the inset of Fig. 5.5.

In the invisibility region where scattering cross-section is suppressed, the electric field amplitudes are substantially reduced and we do not observe any noticeable nonlinear effects even for high levels of input power. Finally, to verify the accuracy of our method, we perform FDTD simulations of the structure. The simulations use two critical points technique [236] in two-dimensional domain with $dx = dy = 0.4 nm$ and 450×450 simulation points in which $dt = 0.99dx/\sqrt{2}c$. The comparison of the results is shown in Fig. 5.7. We see excellent agreement between semi-analytical method and full numerical simulations. The results of the FDTD are presented for a narrower range of the incident power levels

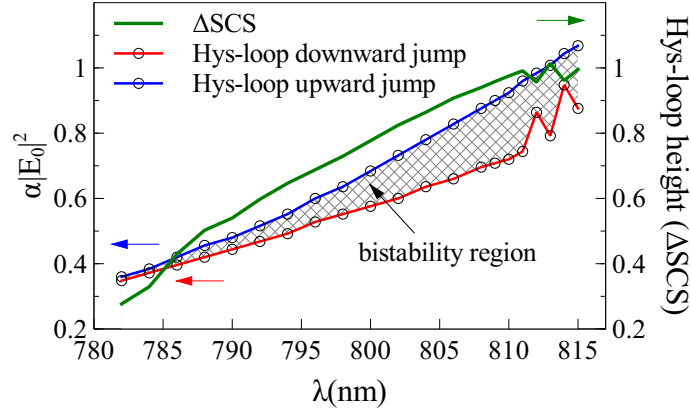


Figure 5.6: Dependency of hysteresis loop properties on wavelength of the incident plane wave. The difference between increasing and decreasing edges indicates the width of the loop. The hysteresis loop is plotted for two wavelengths in inset of Fig. 5.5

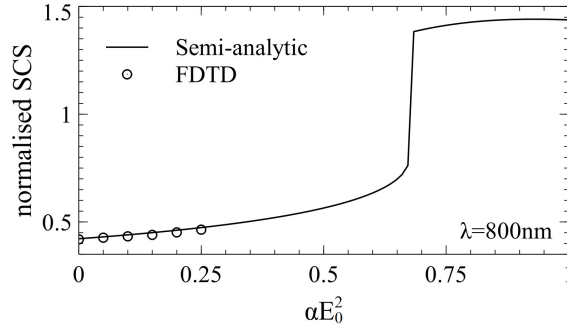


Figure 5.7: Scattering cross-section of the core-shell nanowire as a function of incident power at $\lambda = 800 \text{ nm}$. Solid line shows results of the semi-analytical method, while circles show results of the FDTD simulations.

as the FDTD becomes unstable at higher powers. With $\alpha E_0^2 = 0.25$ the FDTD takes approximately 6 hours and 15 minutes to reach the steady state. The introduced novel semi-analytical method using the same computational system decreases the required time to less than 0.2 sec, which makes it more than 10^5 times faster than the FDTD.

In this chapter, I developed a semi-analytical method for studying light-matter interaction in nonlinear multi-layer cylindrical nanostructures. By comparing the results with those of the FDTD simulations, it was shown that semi-analytical method is accurate and numerically stable. This method was applied to a core-shell plasmonic nanowire, which may exhibit both suppressed or enhanced scattering, and showed that the nonlinear effects are more pronounced in the enhanced scattering regime.

Conclusion and Outlook

In spite of the considerable progress in nanophotonics in recent years, all-optical signal processing still has a long way to become commercially available. More breakthrough ideas and technologies still are to be developed to make PICs a reality in our everyday life, and developing these novel solutions requires new platforms with more capabilities. High performance platforms without the current limitations to let us analyse optical nanostructures from different points of view.

To address this and to introduce a powerful approach different from typical methods, I developed novel techniques for designing nanostructures. In my thesis, an approach based on analytical and semi-analytical solutions and a smart optimisation algorithm were introduced. By choosing long nanowires and studying them in a two-dimensional platform, more flexible designing of nanowire systems becomes possible for various applications. My developed code in C++ by benefiting the fast and exact analytical solutions, investigates thousands of structures to form an optimal design for any mathematically definable functionality. With several examples, I described how the mathematical analysis of nanowire systems is employed in the optimisation algorithm, making an efficient link between analytical physics and computer science. This strategy can basically lead a randomly suggested model in the beginning of the optimisation process to become an optimally functioning design, generally in couple of seconds/minutes.

Analysing the excited harmonics separately by considering realistic and experimental data, provides us with information about underlying physics of light interaction and facilitates managing the behaviour of light. By controlling of scattering and absorption of light, I developed some novel designs to obtain optimal effects in nanowire systems. For instance, invisibility cloaking and superscattering were discussed in two opposite sides of scattering control. The same technique of overlapping the resonances of different harmonics used for superscattering effect, was demonstrated for overlapping absorption resonances, resulting in superabsorption. These extreme effects were discussed with different materials, in both all-dielectric and hybrid configurations. In more complicated problems by having more than one nanowire, I demonstrated that by a careful control of light behaviour, it becomes possible to achieve simultaneously existing, separate and pure, magnetic and

electric hotspots in nano-dimer systems. Optical meta-shielding effect by more complicated structures was also introduced, which proves the high capability of the developed approach. Our results show that metacages, in addition to blocking optical waves from penetration through their construction, have extraordinary properties, such as providing considerable physical access for gases and liquids from both sides, frequency selectivity, wide/narrow-band operation, zero backward scattering and shape independence with a wide range of material choice.

Beyond linear regime, in the last chapter, I discussed nonlinearity in multilayer nanowires and our novel semi-analytical recipe. This approach is more than 10^5 times faster than FDTD in analysing nonlinear systems. As one of the future plans, employing this fast and robust nonlinear approach in the developed optimisation algorithm, can result in optimal nonlinear structures which opens new doors for designing efficient nonlinear systems for various applications.

Analysing two-dimensional structures, eases developing solutions by removing the complications of the third dimension. However, I demonstrated different 3D examples of single and multi-element systems, which prove the applicability of the developed designs for 3D structures. This shows that our 2D obtained optimal results can be transferred to 3D configurations such as nano-spheres and limited length nanowires, even with presence of substrates.

The achieved results prove the high capability of my developed approach for designing optical systems, by providing more details from a different angle compared to direct experiments and numerical simulations. However, the lack of a comprehensive 3D analytical study of complex systems in nanophotonics yet remains. To fill this gap, the presented work in this thesis can be expanded to 3D platforms. Such a comprehensive semi-analytical and realistic study of optimal material composites by taking the effect of substrates into account, can significantly improve the current solutions for optical systems. Developing such extensive and super-fast 3D analytical approaches will cover topics from fundamental studies of simplified models to complex nonlinear systems composed of various multilayer nanoparticles. Consequently, we will be able to precisely engineer the light-matter interaction by optimally tuning their properties in three-dimensional space for a wide range of applications.

In this thesis, I introduced several techniques to control the behaviour of light, such as overlapping the peaks and valleys of different scattering or absorption harmonics, forming separate electric and magnetic hotspots, overlapping separatrices to stop wave propagation, solving nonlinear problems by transforming PDEs to ODEs and several numerical techniques for smart genetic algorithms. These are only some examples of great capabilities of the developed approach and more techniques can be developed in this platform for various applications. This shows that employing fast, exact, and robust analytical and semi-analytical solutions without meshing problems, and within a smart optimisation

process can open new doors to design high performance optical nanostructures for future PICs.

Nanophotonics and PICs are on their way to revolutionise human life-style. Electronic industry in spite of making a huge step forward in technology, has reached to its limits and is not enough for the quickly growing demand for faster data analysis and storage. As a consequence, the current electronic technology will be replaced by the best known possible solution, photonic integrated circuits. Replacing copper connections with optical links between the components in modern electronic integrated circuits has been already started. By making more progress in nanophotonics, a big revolution in data processing, medicine and biology, and energy generation and storage is on its way to become a reality.

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