Advanced Modeling of Solid-State and Nanomaterial Systems and Their Implications for the Development of Contemporary Medical Physics Devices and Technologies

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Contents

Abstract

The tremendous promise of solid-state and nanomaterials in medical physics is increasingly evident, given advances in hybrid sensor and imaging technologies, secure implantables, personalized nanomedicine, and implantable multiphoton nanomedicine systems. Such functionality relies on the sophisticated merging of diverse materials into coherent systems that optimally exploit the probing power of Multiple Internal Reflection (MIR), the nanoscale fields of Localized Surface Plasmon Resonance (LSPR), the encoding of Emission Lifetime Differences in Precise Imaging, and the modulation offered by nanoscale sensors and nanomaterials, in conjunction with novel power management strategies. Similarly, the potential utility of nanomaterials is being assessed for their ability to enhance radiotherapy by local atomic number modification and reactive oxygen generation, employing Monte Carlo models to realistically estimate the dose enhancement around the nanomaterials and ultimately reduce side-effects.

The 17 chapters detail the quantum and solid-state physics foundations relevant for the development of devices in the field of medical physics and the engineering tools necessary for the design and optimization of real systems, covering solid-state and nanostructured materials. A detailed discussion of the principles of solid-state physics in the most general case is presented, together with a description of Quantum Mechanics tailored particularly for confined systems. A solid description of the computational techniques used in advanced device modeling is included, together with the potential and challenges related to the use of artificial intelligence in data-driven materials modeling and the fabrication technologies for solid-state devices employed to realize proof-of-concept systems, offer complete support for Charge-Coupled Device (CCD) and Complementary Metal-Oxide-Semiconductor (CMOS) detector technology development in medical imaging.

Chapter - 1

Fundamentals of Solid-State Physics in Medical Technology

An understanding of the fundamentals of solid-state physics is essential for the development and engineering of advanced medical device technologies. Material properties and related physical phenomena directly determine the performance, efficacy, safety, and usability of many solid-state medical devices. This chapter provides a solid-state physics background that underpins and enables the advanced modeling of material systems for medical device engineering.

A focus on thermodynamics and statistical physics provides a valuable foundation for understanding solid-state phenomena. Thermodynamic systems with a high degree of order contain more available states than those with less order, leading to the minimal-energy principle. Systems strive to attain their equilibrium state, the most stable and well-defined representation of order for a given energy and substance. Macroscopic state variables such as pressure and temperature emerge from ensembles of atomic-scale arrangements, facilitating the study of large-scale phenomena using statistical considerations.

Atomic interactions drive the observed phases of matter: solid, liquid, gas, or plasma. Crystals emerge when an ensemble of atoms arranges into a highly ordered and repeated lattice structure [1]. Solid-state device operation relies on the availability of energy levels for different types of particles; therefore, the presence of a crystal structure strongly influences chemical and solid-state behavior. These insights frame the discussion of core solid-state principles that follow. Major solid-state topics relevant to medical technology, devices, and technologies including crystal structure; electronic band theory; semiconductor theory; dielectric, magnetic, and nanoscale properties; nanostructured devices; and device-enabling physical, chemical, and biological modeling are identified to demonstrate the applicability of solid-state physics to the field of medical technology [2].

Crystal structures and lattice dynamics

Crystal structures of solids basically are classified into two basic types:

crystalline and non-crystalline (amorphous) materials. Crystalline solids are those in which the constituent atoms are arranged in a periodic, three-dimensional pattern. In non-crystalline (amorphous) solids, on the other hand, the ordering of constituents is limited to short-range only. In nature, most of the solids occurring in minerals, rocks, and metals, in general, are crystalline in nature. Single crystals and polycrystalline solids have, in a sense, a three-dimensional order extending over a long range. A solid crystal, when examined carefully in optical microscopy, is composed of a number of individual crystals linked together along their faces and these are called as grains. Hence materials that have a crystalline structure made up of an aggregate of many small crystals are called polycrystalline materials. Each of these small individual crystals is called as a grain crystal. Crystalline solids are characterized by smooth facets, possession of symmetry, and sharp melting points.

A crystal lattice is a three-dimensional arrangement of data points or lattice points that denotes the periodic arrangement of the constituents. Each point is connected by three lines along x, y, and z axes. The smallest three-dimensional lattice that can be repeated over a long range in all three directions is called the unit cell of the lattice. The collection of all the unit cells in a given lattice defines it. A two-dimensional representation of a crystal lattice is called a 2D lattice. A 2D lattice can be characterized by five 2D lattices called Bravais lattices. In two dimensions, a crystal lattice has two translation symmetries as described along elemental lines above [3, 4, 5, 6].

Electronic band theory and charge transport

In electron band theory, the formation of energy bands in solids is analyzed, based on the arrival of a limit where the lattice repeats its unit cell in all regions of space. In these circumstances, the basis functions of each atom combine to form a set of functions, that describe a complete lattice vibration and the distribution of electrons around the atom. If the atoms are seen as positive charges in the lattice of ions, the potential energy can be written as a periodic function whose periodicity is the same as that of the lattice of nuclei. Within a band, electrons in the solid move with comparable energies in similar directions, and the ions act at the mean potential. The conservation of electrons is accounted for by taking a certain number of electrons per unit volume of the crystal, so that within a band of energy widths larger pockets are formed by other electrons.

In the particular case when the solid is a semiconductor, such as silicon or germanium, consider an incident electron beam of speed of the same order

of magnitude as that of the electrons in the solid. The electrons of the band being crossed by the incident beam and moving in the same directions arrive at the same point in the lattice at the same time; the scatter is smaller than that due to an external field, and detailed scattering may be neglected. With large models, a rapid parasitic electronic emission takes place, in the sense that a further increase of the incident density of electrons results in a current but negative to that of the incident beam. Under this condition the doping atoms act as 3d or 5d sites of opposite nature, where the mobility is determined by the band structure or by the dilatacy and does not have a strong dependence on the 2D or on the type of impurity atoms [7, 8, 9, 10].

Semiconductor physics principles

The performance of semiconductor detectors and sensors is influenced by fundamental semiconductor principles, with material parameters defining manufacturing and operation conditions.

Semiconductor physics concepts describe the depletion region of a reverse-biased diode, the injection of charge carriers into the space charge region of forward-biased diodes, the transient response of the junction and the FET to external stimuli, the dynamics of majority and minority carriers, and their participation in charge transport in opengate FETs and charge-coupled devices. These basic principles are widely used in the responses of semiconductors acting as detectors and sensors as well as for the description of solid-state devices that utilize doping, such as charged-coupled devices and field-effect transistors.

A pn junction depleted of free charge carriers extends into both crystals, exhibiting a large electric field perpendicular to the junction. The reverse-bias applied voltage forces the depletion regions to widen, reducing the junction current to the leakage level in the order of nanoamperes. The hole and electron concentrations can be modeled by the continuity equation for charge carriers in one dimension. In the case of a forward-biased pn junction, the time taken for majority carriers to diffuse through the space charge region is much shorter than the time constant associated with the diffusion [11, 12, 13, 14, 15].

Dielectric and magnetic properties

The study of dielectric materials and their functional behavior in the presence of an electric field are of great interest not only for applications in electromagnetics, but also in modern biomedical imaging and sensing. The dielectric permittivity of materials is strongly dependent on the nature of their lattice vibration. Further, efficient incorporation of magnetic materials and nanostructures into medical devices presents new opportunities, such as

improved sensitivity in biosensors, contrast enhancement in Magnetic Resonance Imaging (MRI), and new avenues for cancer therapy.

The performance of dielectric materials can be characterized by the complex dielectric permittivity $\varepsilon = \varepsilon' - i\varepsilon''$. The real part ε' is associated with dipole orientation under the applied electric field, while ε'' describes electric energy dissipation as heat, generally attributed to ohmic conduction, electrode polarization, or dipolar relaxation. Magnetic ordering is also a prominent physical phenomenon in many solid-state systems, and magnetic nanoparticles are becoming increasingly popular for enhancing MRI signal contrast and for hyperthermia applications [16, 17, 18, 19, 20].

Relevance to medical device engineering

Linking material properties with practical metrics quantifies direct relevance to medical device performance

The physical, optical, magnetic, and chemical properties of solid-state and nanomaterials determine the response of medical devices under external stimuli. Quantitative modeling of these properties clarifies their impact on device operation, and aids in engineering reliability and lifetime. Two important aspects are emphasized:

1) Identification of a reduced set of metrics directly connected to properties
2) Correlation of property variation with these metrics

Six principal categories of response are considered:

1) Effect of physical and dielectric properties on high-frequency response of detectors and sensors
2) Connection between carrier transport and charge collection speed of medical imaging detectors
3) Link between thermal properties of nanomaterials and conditions for reliable operation
4) Relation between magnetic properties and contrast quality of magnetic resonance imaging
5) Control of chemical functionalization and dependence on surface-to-volume ratio by biocompatibility and selectivity
6) Influence of emission spectrum tuning in quantum dots on efficiency and safety of optical imaging agents. All cases highlight the importance of physics-based properties [21, 22, 23, 24].

Chapter - 2

Quantum Mechanics in Solid-State and Nanomaterials

Core quantum mechanics principles and effects shape solid-state nanomaterials and systems containing them at small scales, where the range of electrons, excitons, and phonons approaches the limiting behaviors described by quantum mechanics rather than classical physics. Systems of smaller sizes show increasing deviations from classical mechanics a feature exploited in sensors and imaging devices based on solid-state quantum-confined systems. Accurate modeling of solid-state nanomaterials for device applications requires appropriately aligned quantum mechanical principles, methods, and technologies. When quantum mechanics principles are correctly considered, the response of the devices can be related to important characteristics, such as signal-to-noise ratio, resolution, and efficiency.

Consideration of quantum mechanics begins with the Schrödinger equation, which describes the wave function's space (or time) dependence. For charge carriers in potential wells, the problem is typically presented with boundary conditions that force the wave function to vanish outside a finite region supporting a discrete energy spectrum. Quantum wells, wires, and dots differ by the confinement direction. Quantum wells are widely used in detectors based on electron-hole pair recombination in semiconductors and direct bandgap-type compounds. Quantum effects are also prominent in the response of two-dimensional GaAs quantum wells and dots beyond simple confinement-energy shifts. Tunneling across barriers can have both beneficial and detrimental effects on device performance. Spin physics essentially a one-particle effect has recently been applied in a novel sensing approach based on spin transport and spin-polarized bolometric response [25, 26, 27, 28].

Schrödinger equation in confined systems

When derivation of the Schrödinger equation was defined, it considered three-dimensional free particle motion, which means that the particle is in a system that has no potential energy. However, in confined systems, where something like a potential energy wall contains the particle and prevents it from moving toward a determined direction, i.e., a quasi two-dimensional

system, partial derivative phenomena emerge. Depending on the type of confinement generated by the potential energy, the solution of the Schrödinger Equation may remain one-dimensional, which means that the spatial coordinate perpendicular to the confinement direction does not vary anymore.

The solutions of the Schrödinger Equation, in general, are determined by a region of space that does not have a potential energy wall, and therefore there is gain of energy levels. Direction confinement generates energy level quantization, which may directly or indirectly indicates any type of solid-state device, thus influencing the operation and also the detection processes. The devices may be constructed with materials that have larger or smaller phases of quantization emitting in larger or smaller regions of the spectrum that, when detected, for example, in the optical structure, determine the solution(s) [29, 30, 31, 32].

Quantum wells, wires, and dots

Quantum confinement plays a significant role in reducing the dimensionality of solid-state systems as compared to bulk materials. are classic examples of such systems, corresponding to the quantum-mechanical description of charge carriers confined in real-space along one, two, or three dimensions. These dimensional reductions lead to dramatic and often constructive changes in the materials and their properties and broad classes of applications in different areas of medical imaging.

Consider a semiconductor whose electronic structures and related properties evolve as the space confining dimension is reduced progressively. In three dimensions, the Boltzmann transport equation describes the charge transport properties through a quantum-mechanical diffusion approximation. In two dimensions, the inherent discreteness of energy levels arises from quantum confinement, with quantized Landau levels forming under carrier transport in a magnetic field. The second-derivative tensor (or, in isotropic systems, the effective mass) relates spatial changes in the scattering processes to the charge motion. Nevertheless, the Density of States (DOS) diverges and causes efficiency degradation in optoelectronic devices.

In one-dimensional quantum wires, electrons move semiclassically along the wire with spatially modulated effective mass due to band nonparabolicity, while scattering by surface roughness and defects occurs in the transverse directions. The confinement potential also leads to concentration of the electrons in the thin region in close proximity to the surface of the channel, with scattering rates higher than in bulk material due to the short channel

length. Models incorporating these elements have been shown capable of reproducing quantitatively experimental data on InP, InAs, and other narrow bandgap materials. The successful validation of the prediction of SiC as a dramatic improvement over conventional escape routes indicates how these quantum effects can be exploited to achieve better-functioning detectors, particularly in the operation of noncryogenic systems [33, 34, 35, 36].

Tunneling phenomena in nanostructures

To fully exploit tunneling in devices, it is important to understand the underlying physical mechanisms. Fowler-Nordheim (FN) tunneling is observed at metal-insulator-semiconductor junctions, where charges penetrate a triangular-shaped potential barrier due to the large width of the barrier in the transport direction. The tunneling current density can be expressed as

$$J_{FN} = \frac{c}{\theta^2} e^{-\theta},$$

where θ is a dimensionless parameter equal to

$$\theta = \frac{(EB)^{3/2}}{E_{F}}$$

(assuming a constant work function) and c is a constant depending on the permittivity of the oxide, the barrier height, and the thickness of the oxide layer. The average FN current density during the tunneling process is controlled by the oxide thickness and the type of semiconductor, which determines the thermal generation of carriers. FN tunneling can be limited as the distance from the gate to the drain or channel decreases, making other tunneling processes more significant.

Resonant tunneling occurs when charge carriers traverse a very thin barrier between two regions with a large density of states. The tunneling current density can be expressed as

$$J_{RT} = \frac{q^2}{(2\pi \hbar)^{3}}\int \frac{g_{1}(E)g_{2}(E)}{1 + C(E)}dE,$$

where $g_{1,2}(E)$ represent the densitiy of states in the first and second regions of the tunneling, respectively. Resonant tunneling through a thin barrier is a fast process and therefore constitutes a bottleneck if the areal density is not large.

Leakage current may seriously affect devices, thermal sources at the contacts modify the gain and response of optical modulators, excessive leakage currents limit the bandwidth of detectors, etc. Noise increases when the leakage current flow is on the order of the detected signal. Noise arising

from leakage can be estimated as

$$I_{n} = \sqrt{\delta t \left(2eI_{leak} + I_{leak}^{2}/I_{p}\right)},$$

where δt is the measurement time, I_{leak} is the leakage current, and I_{p} is the photoinduced current.

Spin physics and quantum coherence

Understanding spin relaxation processes and coherence times in solid-state systems is critical for the development of spin-based sensors, imaging devices, and quantum-information platforms. Various spin-polarized optical methods can probe spin dynamics on ultra-short time scales down to a few picoseconds. Measurements on paramagnetic defects, diamagnetic centers, and ferromagnets reveal important spin properties in materials currently being explored for imaging agents. Several solid-state systems exhibit long spin-coherence times in the microsecond range. Techniques such as Optically Detected Magnetic Resonance (ODMR) investigate the formation of coherent spin states and spin-wave propagation [37, 38, 39, 40].

The ability to manipulate and detect spins on ultra-short time scales enables the direct observation of microwave magnetization dynamics and the visualization of precession of spin-polarized carriers. These methods can characterize the spin properties of magnetic nanostructures and improve the performance of high-frequency spintronic devices, RF generators, and emitters [41]. Quantum imaging techniques enable the detection of optically generated spin populations, spin-up and spin-down components, and the determination of spin-relaxation times. Atomic-scale imaging of ferromagnetic structures and the investigation of carrier-induced ferromagnetism via pulsed opto-magnetic techniques is also possible [42].

Applications in medical imaging detectors

Correlations between quantum effects in solid-state and nanostructured materials, and the performance of scattering-type nanocrystal detectors for ionizing radiation, are highlighted. The discussion encompasses improvements in energy resolution and temporal response, along with reduction of excess noise, by leveraging quantum dots in a pin-diodes configuration, and through the implementation of a surface-derive structure. Third generation of quantum dots used in scintillation consider besides energy resolution and temporal response also intrinsic scintillation efficiency, because light yield is still a crucial feature for practical application. Superlattice nanowires are considered as a promising alternative for the

realization of quantum-confined detectors sensitive to visible radiation for integrated imaging applications. The potential of ferromagnetic resonance imaging by employing solid-state two-dimensional electron gases, and its possible integration in proximity to already available nuclear magnetic resonance tomographic systems, are also investigated.

Quantum effects play a relevant role in nanostructured and quantum solid-state materials. In the specific case of detectors for medical physics and imaging applications, they can be beneficial or deleterious depending on the nature of the radiation and on the corresponding detection principle. Furthermore, the control or proper exploitation of such effects goes beyond the mere accuracy of model predictions. Such prediction accuracy is essential for material screening. Attempts to correlate quantum effects with transport phenomena in detector signals are supported by experimental results; the objective is to identify possible implications for noise performance of radiation detectors [43, 44, 45, 46, 47].

Chapter - 3

Computational Modeling Techniques for Solid-State Systems

Advances in theoretical solid-state physics are linked to the increased computation power available in recent decades and the introduction of new numerical methods. As expected, already developed techniques based on the resolution of the Schrödinger equation by Density Functional Theory (DFT), charge transport modeling with the Monte Carlo method, Molecular Dynamics (MD) simulations, and the Finite Element Method (FEM) are well documented and extensively applied in the literature for material screening and special case studies. However, its efficiency remains proportional to the number of atoms in the system. Beyond such methods, multiscale modeling strategies integrating quantum, atomistic, and continuum physics descriptions have been implemented in physics research. Appropriately coupling quantum-mechanical, semi-empirical, atomistic, and continuum descriptions of the system is fundamental to efficiently treat experimental semi-empirical and analytical results developed for specific regimes or cases.

Established methods are presented with a detailed analysis of the Density Functional Theory (DFT) formalism, typically the first step for solid-state prediction of electronic properties and band gaps, defect properties, and doping trends. Charge transport modeling is examined, focusing on Monte Carlo simulations of radiation transport through a variety of materials and Semiconductors, for which transport can be modeled as photoionization with charge collection modeled as either drift or diffusion. The finite element method for modeling electromagnetic fields is underpinned with details for structural and thermal simulations. The chapter also indicates emerging techniques such as MD combined to DFT for defect dynamics modeling and multiscale strategies integrating these techniques. In addition, an example of DFT-MD-MC simulation applied to a two-step sequential artificial diamond growth is presented [48, 49, 50, 51].

Density Functional Theory (DFT)

The is a computational technique based on quantum mechanics widely

used in solid-state physics and chemistry for modeling electrons in a many-body system under the Born-Oppenheimer approximation. The electronic energy is obtained as a functional of electron density by solving the Kohn-Sham equations. DFT has proven a powerful tool for materials screening, for example in exploring defect energetics; however, the accurate description of the band gaps of insulators and semiconductors remains a challenge, especially for user-implemented codes relying on semilocal exchange-correlation functionals. Furthermore, local test sets have demonstrated that despite routinely matching experimental values of formation energy and defect level positions within the gap, DFT's suitability for defect level screening in a wider context, accurately predicting the relative stability of competing defect candidates, also warrants further investigation. Non-local and hybrid functionals that include a fraction of Hartree-Fock exact exchange have been shown to correct the gaps for technologically important oxides. DFT coupled with the appropriate approach such as the Clusters Approach or Scissors Operator Method has provided reliable gaps for several oxide semiconductors used in radiation-detection applications. Consequently, materials-savvy searches based on user-friendly DFT implementations and publicly available databases are often preferred, and the methodology has been employed to screen the properties of several semiconductor nanocomposites for biosensing applications.

DFT has become a workhorse of quantum-mechanical structure prediction in the condensed phase and has provided accurate energies and structures for thousands of crystalline solids, oligomers, clusters, and molecular liquids. Methods of molecular DFT have achieved similar status for condensed-phase systems containing many solvent molecules along with potentially bio-logically active solute. With the advent of non-local exchange-correlation functionals, DFT of van der Waals complexes has grown in importance. Nevertheless, the accurate description of the band gaps of insulators and semiconductors remains a challenge. Local test sets can nevertheless identify cases where the DFT description of the band gap may risk or limit the utility of DFT in defects and impurities modeling within a wider range [52, 53, 54, 55].

Molecular dynamics simulations

Molecular Dynamics (MD) simulations provide atomic- and molecular-level insight into phenomena that occur on timescales ranging from the pico to microsecond. It consists of solving Newton’s equations of motion for a system of a large number of atoms, thereby generating a set of trajectories that

describe their motion in time. In MD, the forces that act on each atom are calculated atomistically from a potential that takes account of the interactions between all the atoms. Such calculations are based on interatomic force fields, or more physically accurate empirical potentials, that express the potential energy of the system as a function of the positions of its atoms; the gradient of this potential is then used to determine the forces on the atoms.

The range of timescales over which MD is applicable is determined by the simulation time step. For classical MD simulations, steps of about 1 fs must be used to ensure numerical stability. MD simulations have, however, been successfully applied to several problems in condensed matter physics. These include the study of the time evolution of temperature upon laser excitation; the investigation of the reduced-temperature vs. time relationship; the determination of the self-diffusion coefficient of simple metals at melting; and the study of sintering processes in ceramic materials [56, 57, 58, 59].

Finite Element Modeling (FEM)

Allows the prediction of physical fields originating from electrical and thermal sources, and also from mechanical loading, making this method suitable for a wide range of applications in solid-state systems. In the following sections, the application of FEM to the modeling of solid-state devices relies on the same strategy: defining a bulk material in the region of interest, describing how boundary conditions and sources modify that bulk response, and solving the governing equations with an adequate set of algorithms and numerical techniques. Devices operating in the linear regime of the governing physical equations can be accurately modeled using FEM.

FEM is applied to study the structural response of a solid-state system either to external mechanical forces or to an internal thermal source. For these studies, the solid-state system is treated as a macroscopic block in which that response is computed within the multi-domain part of the package, where either displacements or temperature respond to the applied loads. The input parameters needed for modeling surface displacements are Young's modulus, Poisson's ratio, and an exponential function relating stress to strain, while, for thermal studies, the specific heat, density, and thermal conductivity of the material are sufficient descriptors. In the case of electrostatics, the governing equation is solved with the help of the device descriptors relative to its charge transport mechanism [60, 61, 62, 63].

Monte Carlo radiation transport models

A stochastic approach to modeling radiation transport is employed in

cases where isotropic scattering, mixed discrete-continuous particle interaction processes and the consequence of small but non-negligible interaction probabilities must be taken into account. For this purpose, a Monte Carlo method is particularly suited since it accurately implements random sampling of interaction probabilities and physical process simulations, is computationally inexpensive to apply, and is very flexible in terms of geometry and physical models.

Models of medical physics devices make significant use of the Monte Carlo method, in the modeling of radiation transport within the interaction volume of detectors. Since detector response is needed, in a very wide range of radiation types, energies and angles of incidence, and media of transport, from which the phase space of secondary emitted particles must be tracked, the solution of the task is compatible with the Monte Carlo approach. The simulated response may be achieved in an inverse fashion using a simple ray-tracing algorithm, tracking the probability of interaction as a kernel of the probability of radiation transport through a layered structure.

The stochastic solution to the transport equation employs a volume distribution of the cross-section σ. For a radiation beam impinging on a biological material of density ρ, as a first-order approximation, the phase density of secondary particles Σ becomes the real density times the transmission factor of the mixed tissue, $\Sigma \sim \rho(1-e-\Sigma x)$, where $\Sigma=\sigma\rho$ is the interaction cross-section per unit mass and x is the thickness of the tissue. The correction to the multiplicative factor in the probability density of secondary particle detection reflects the volume density of the interaction process, but is totally implicit in the coded form [64, 65, 66, 67].

Multiscale modeling strategies

Device-oriented problems often require the consideration of multiple physical effects occurring at vastly different scales. For instance, a medical imaging detector relies on the scattered radiation intensity, which is dictated by radiobiological considerations, the transport of the incoming radiation, attenuation by the sensor volume and absorption in the detection material, charge transport within the active volume and readout electronics, and how these paths overlap. A correct assessment of the detector efficiency therefore mandates the coupling of, at least, four independent models:

1) A radiobiological model
2) A Monte Carlo radiation transport model

3) A Monte Carlo or deterministic model of electron transport, and
4) A Monte Carlo or deterministic model of charge transport within the sensor and read-out electronics

Similar multiscale modeling procedures can be devised for a broad variety of device-oriented problems.

Multiscale models should combine quantum, atomistic, and continuum modeling techniques via an appropriate coupling strategy. Coupling the models at different level of details requires special care, as material properties, such as thermal conductivity, may differ appreciably between scales. One of the simplest strategies to enforce the coupling is based on a set of heuristic rules. For instance, when modeling thermal transport, the atomistic model is first used, and the atomistic temperature is passed to the continuum models as a boundary condition. Subsequently, once the continuum models are solved, the temperature gradient across the atomistic region is extracted and passed as a boundary condition to the atomistic model for the next time step. Closeness in the structure of the involved systems helps ensure that the material responds consistently across the different models. So far, the discussed coupling strategy has been validated for electron and thermal transport across systems where the lattice structure is preserved [68, 69, 33, 70].

Chapter - 4

Nanomaterials: Structure, Properties and Synthesis

Nanomaterials are typically classified according to dimensions along the three axes of space. A distinction is made between zero-dimensional, one-dimensional, two-dimensional, and three-dimensional systems. Compared to their bulk counterparts, nanomaterials are characterized by an increased proportion of surface atoms, thus generating a higher surface-to-volume ratio. The consequences of these nanomaterials for chemical reactivity, diffusion, and functionalization have been systematically studied, and such effects can significantly affect the suitability of these materials as sensing devices, imaging agents, or drug delivery systems. The effect of size on mechanical properties has been summarized, highlighting the increase in stiffness, tensile strength, and hardness, as well as the large thermal conductivity of carbon nanotubes. Numerous methods of chemical functionalization exist, allowing the introduction of specific groups at the surface of nanomaterials, providing accurately defined reactive sites and exploring bioconjugation chemistries for targeting a particular biological structure. The impact of nanomaterial-induced cytotoxicity, immune response, and biodegradation on their biomedical applications is also analyzed, framing future research attempts within a concise discussion of the current regulatory guidelines.

Nanomaterials exhibit unique optical, electronic, and delivery properties that can facilitate medical imaging and therapy. In medical imaging, they are essentially used to provide contrast enhancement for the detected signal, either through direct generation of a signal (quantum dots) or as chemical agents that increase the contrast of the signal coming from specific tissues. Contrast-material performance is affected by several physical processes, which are determined by the physical conditions and the biological environment of the nanomaterials. Because of the possible broad applications in these imaging technologies, nanomedicine is growing rapidly. Emerging nanotechnology continues to produce new classes of imaging modalities, either combining existing contrast agents or proposing novel detection processes. The modeling of these contrasting agents allows quantifying the expected signal enhancement and further directing experimental work toward obtaining the best possible imaging [71, 72, 73, 74].

Classification of nanomaterials

Nanoscale systems comprise materials whose size approaches nanometers (1-100 nm), with properties determined by the interplay of bulk properties and strong surface effects due to the small size and large surface/volume ratio. Nanomaterials are classified based on particle dimensionality. Zero-dimensional (0D) materials are characterized by all dimensions on the nanoscale and display unique quantum phenomena. One-dimensional (1D) nanostructures exhibit two dimensions in the nanoscale range and allow efficient carrier transport along their length. Two-dimensional (2D) materials possess a thickness in the nanometer range while extending laterally over much larger distances.

The large surface-to-volume ratio of nanomaterials enhances their chemical reactivity, promotes diffusion kinetics, and enables chemical functionalization, making them particularly suitable as imaging agents or for sensing applications. Nanosystems with very high surface-to-volume ratios, such as hollow nanostructures, facilitate the transport of low-molecular-weight species and support a high degree of chemical functionalization for organ-targeting mechanisms or drug loading. The special mechanical and thermal properties of nanocrystals (high stiffness, strength, thermal conductivity) also enable the development of more reliable nanocomposite devices. On the other hand, proper high-throughput and quality-controlled manufacturing approaches should keep production costs low and ensure reproducible biocompatibility [75, 76, 77, 78, 79].

Surface-to-volume ratio effects

Owing to their minuscule size, nanomaterials possess an increased surface-to-volume ratio, consequently featuring larger surface area per weighed unit than bulk counterparts. A high surface-to-volume ratio is a characteristic property of nanomaterials and leads to different physico-chemical properties than bulk systems. The higher reactivity seen in nanomaterials compared to their coarser counterparts emerges from the inherent characteristics of their surface, which is the only interface for the majority of their constituents. The greater the surface area per unit mass, the more active sites available for interaction. This enhanced reactivity is directly reflected in electrochemical or catalytic processes, which can occur at significantly lower concentrations than in bulk or micro-regimes. The acceleration of fluorescent decay kinetics in quantum dots, which can be interpreted as an increase in radiative and/or non-radiative transition rate constants, is also a bearable consequence of the heightened available surface area.

Beyond such accelerated reaction rates, shortening of the molecular diffusion distance between a surface and the reactants can be significant. The rate of molecular interactions can be increased by an adequate functionalization of the nanomaterial surface by thereby inducing a sort of "tailor-made" nanomaterial to ensure optimal alignment of the sensing molecules at the surface, while still controlling their distance from the surface in a selectively defined way. All these aspects are particularly relevant in the case of nanoparticle-based biosensors. Furthermore, the high surface-to-volume ratio suggests the potential to significantly increase the biocompatibility and biodistribution properties of nanomaterials with suitable surface modification. The chemical reactions that take place on the nanomaterials' surface strongly depend on the chemical stability of the surface during the reaction. For this reason, surface functionalization is often required in order to achieve the desired level of surface stability without giving up the advantages provided by the small sizes. Surface stability corresponds to consideration of the possible interactions of the nanomaterials with the body fluids *in vivo* [80, 81, 82, 83].

Mechanical and thermal properties

Nanomaterials exhibit a unique set of mechanical and thermal properties stemming from their reduced dimensions and large surface-to-volume ratio. These characteristics differentiate them from their bulk counterparts and, in several cases, explain the observed superior performance in devices incorporating nanostructures.

The small size of nanomaterials combined with a high surface-to-volume ratio results in enhanced reactivity and a different diffusion behavior when compared to bulk materials. A change in physical properties is also expected, as for example the Young's modulus of silicate nanoparticles tends to be two orders of magnitude greater than the value found for the bulk. The extent of these modifications depends on the interplay between size and surface effects. In turn, the nature of the structural material may also influence the scaling of mechanical properties with particle size, with oxides and metals following a different behavior [84, 85, 86, 87, 88, 84, 85, 86, 87].

Chemical functionalization

The two-dimensional surface of nanomaterials is in many cases highly reactive and readily undergoes spontaneous processes such as oxidation. This reactivity can contribute to adverse biological effects or undesirable aggregation but can also lead to chemical reaction with targeted analytes or

other biomolecules, facilitating detection in biosensing applications. Precise control of these chemical reactions, often referred to as functionalization, is therefore essential for numerous applications in medicine, biomedicine, and nanomedicine. The surface of nanomaterials can be chemically functionalized using a wide range of strategies that enable grafting of biocompatible or targeting molecules and control of the resulting interface.

Organic and inorganic groups are typically grafted to the surfaces of nanomaterials using classical covalent, self-assembly, or noncovalent methods. Classical surface modification protocols rely on the presence of specific surface atoms, groups, or bonds on the nanomaterials and exploit well-established homogeneous or heterogeneous grafting reactions. Precise grafting of a wide range of species to the surfaces of organic and inorganic nanomaterials can be achieved under well-defined conditions by Self-Assembled Monolayer (SAM) methods, in which a variety of biomolecules spontaneously adsorb onto the nanomaterial surface from solution. Biological functionalization introduces biochemical specificity to the surface of the nanomaterials, enhances their biocompatibility, and allows formation of hybrid inorganic-biomolecular structures. These modifications elicit either desirable tissue and cellular levels of accumulation (through passive distribution or active being surface-engineered) or undesirable biodistribution (to organs of clearance), and these characteristics must be considered when assessing biocompatibility or the effectiveness of the nanomaterials as imaging or therapeutic agents.

Biomedical compatibility considerations

Function and safety aspects of nanomaterials incorporated into medical products are scrutinized by following a series of protocols defined to prevent material residues in organs during and after interactions with the organism. Iron oxide and gold nanoparticles are frequently employed in imaging and therapy, respectively, as well as bismuth compounds due to lower toxicity than other heavier materials. Safety assessments aim to render the use of nanomaterials safer; still, novel solutions that enhance the qualities of existing products and those with fundamentally new principles still require thorough studies before their applications in humans. While medical nanotoxicology prepares for the use of nanomaterials, their behavior as enhanced contrast agents and as components to amplify therapy efficiency is explored; although beneficial for patients, regulatory agencies reflect and demand the fulfillment of testing protocols more detailed than for traditional materials.

The actions of nanostructures in living organisms are addressed at two levels: their presence and possible accumulation in organs, and their action as

therapeutic agents by the generation of reactive oxygen species in tissues. Even without harmful residues, the use of heavy metals is limited, and to avoid their accumulation in organs such as the liver and kidneys, bismuth-based solutions show great promise as imaging contrast agents with lower toxicity; by virtue of the same property, other high-Z materials are also tested, particularly for radiotherapy dose enhancement, but still require careful screening. The increase of cytotoxicity of gold and iron oxide nanoparticles with decreasing size follows the size-dependent increase of the surface area and hence of the interaction with biomolecules. Empirical models and databases provide important guidance in these studies, while approaches based on the physical model of cytotoxicity enable more physics-related prediction capabilities [89, 90, 91, 92].

Chapter - 5

Semiconductor Materials for Radiation Detection

Four semiconductor materials are considered: silicon, germanium, and two CdTe and GaAs compounds. A general description of their radiation-detector suitability is presented, followed by a closer examination of the factors affecting the charge-collection process in solid-state detectors, in particular the trade-offs involved in optimizing the collection mechanism and minimizing the noise sources that ultimately define the device resolution. Silicon-based detectors occupy a privileged place as the most widely employed devices; their successful integration with readout electronics delivers a compact solution for CMS. Germanium devices achieve better energy resolution, although their use is frequently limited by cooling requirements. Compound semiconductors, on the other hand, due to their high atomic number, may offer better contrast in gamma cameras or experience an increased attenuation for X-ray imaging if the signal-to-noise ratio can be preserved while reducing the thickness of the piece. Finally, CdZnTe combines some favorable properties in particular a large band-gap yet still presents serious challenges for the energy collection process.

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Silicon-based detectors

play an important role in the detection of radioactive radiation, both for measurement and for medical imaging. By means of a Semiconductor (Si), the phenomenon of charge collection is used for the detection of created charges in the Si volume, where interaction takes place. However, the excess noise ultimately limits and stabilizes the signal. Findings from modeling and simulation can be used to identify noise sources and establish methods for their reduction. When the correlation coefficient between the energy deposited in the detector and the reconstructed signal is improved, the effect results in an improved noise.

Silicon-based detectors operate through the collection of charges generated in the bulk, due to the passage of ionizing radiation. For any ionizing event that produces charge carriers, noise is present as an underlined concern in the signal acquisition. Fluctuations during the collection process can be classified into: Poisson, electronic, 1/f and thermal you need this in passive! The main applications are in X-ray and proton detection. Structured detectors and their integration with readout electronics, for charge collection and signal processing, can be grouped into three categories: pixel, strip, and wire chambers" [97, 98, 99, 100].

Germanium detectors

The main mechanisms at play in germanium detectors are similar to those described for silicon, with some relevant differences dictated by the higher atomic number of germanium. Its main advantage lies in the better energy resolution that can be achieved, owing primarily to the lower thermal noise level that arises from the necessary cooling of the detectors. This degree of cooling, however, is an important drawback of germanium detectors, limiting their acceptance in many applications. In the case of CMS, for example, most of the systems are based on silicon, which, being a cheaper and more widely used material in the semiconductor industry, is available in large volumes at a relatively low cost. The cooling required for germanium detectors, especially for medical applications, has therefore to be justified in terms of improved resolution rather than in terms of the miniaturization of the achieved system.

Germanium operates in a similar manner to silicon in terms of charge carrier transport. The transport mechanisms are also analogous, but the charge density is considerably higher in germanium than in silicon. For any radiation intensity such as that from a hot source, therefore, the number of detected events will be greater for a germanium detector with the same volume as the

silicon detector. In this sense, detectors made of germanium have an obvious advantage in the detection of gamma radiation with energies around 1 keV. These detectors have reduced applied voltages and lower transport times, and in the case of nuclear medicine, the half-life of the radioemitter used for the gamma camera is usually of the order of 1 m, which results in high detection rates. The only disadvantages of germanium are that the optical phonon trapping density is very high compared to silicon and that intrinsic impurities such as gold or copper introduce deep levels that can cause local trapping of the charge carriers [101, 102, 103, 104].

Compound semiconductors (CdTe, GaAs)

Considerations for high-Z materials, charge collection efficiency, and device thickness guide the selection of compound semiconductors in radiation detectors. Although dense, high-Z single crystals such as CdTe and HgI2 provide benefits regarding interaction probability, charge transport often requires charge transport optimization. Integration allows significant reduction of beryllium filters in gamma cameras based on aligned GaAs nanowires, while heterojunctions between low- and high-Z materials enable signal amplification.

Compound semiconductor materials are increasingly used in gamma and X-ray detection, where their high atomic number compensates for the relatively lower interaction density in comparison to silicon. Given the high energy of the arriving radiation, dramatic reduction of the time of interaction is expected and experimentally verified. Nevertheless, the charge extraction capabilities must be carefully considered: while in a thick crystal the charge collection occurs under the full drift action of the electric field, in a thin crystal the trapping and recombination processes compete during the charge transport. If the conversion takes place in a region where the electric field is low, the extraction process can become very inefficient, resulting in low detection efficiency.

Other aspects of these materials must also be taken into account. The technological difficulties related to the growth of CdZnTe crystals lead to the use of CdTe in commercial detectors. Not only is the crystal small but also the manufacture of the electrodes in well-defined positions is a problem almost always inefficiently solved. Moreover, the diode cannot be cooled and often needs to be directly coupled with cryogenic systems. Finally, the material presents surface quality problems affecting the efficiency of the detection systems that use an incident X-ray of low energy. On the other hand, GaAs is also considered, mainly in the form of wire arrays or QWs shrunk to be

integrated with the readout electronic systems. The argument behind this choice is the reduction of the thickness of the beryllium filter in gamma cameras: the use of aligned nanowires allows decreasing its width and can give an enhance of the detection for high-energy gamma rays. Heterojunctions between low- and high-Z materials are also envisaged for signal amplification [105, 106, 107, 108, 109].

Charge collection mechanisms

The collection of charges generated by radiation in semiconductor detectors may occur according to two different mechanisms Exploiting the high efficiency of ionization charge collection, considering that the signal generated by an ionization event in a solid-state detector is essentially the consequence of Coulomb interaction of the electron and hole drifting in opposite directions in the potential barried at the junction. The primary mechanism is based on drift motion of the ionisation-induced charge in the internal electric field across the junction, independent of whether the charge carriers are majoring or minority carriers.

Drift motion becomes inefficient when ionization is produced close to the depletion region edges because the charges remain in the region of high recombination probability, or when it occurs outside the extraction electric field, particularly for holes in n-type detectors when operating by hole collecting. In such cases the second mechanism, based on diffusion, has to be taken into consideration. Consequently, the ratio of the distance from the doping junction to the ionization event to the Cathode-Anode distance governs the relative importance of the two mechanisms [110, 111, 112, 113, 111, 112, 113].

Noise and resolution optimization

In the context of CMS radiations sources, the following factors should be kept in mind. Random electronic noise - the fluctuation of the electric current, which inevitably accompanies the functioning of every radiodetector used in radiation measurement, reduces the optimal signal-to-noise ratio. Other types of noise (thermal noise, flicker noise, avalanche noise, etc.) and interference detection (influence of the connection wires, sources of electromagnetic oscillation) adversely affect the signal-to-noise ratio. For this important reason, it is very desirable to reduce the surfacing area of the detector chip as much as possible, which automatically leads to increasing the dimension of the electrical and electronic component of the beam.

Small volume radio-detectors based on silicon thin membranes for CMS can considerably diminish the electronic noise owing to reduction of the

surfacing area. The noise can be further lowered medium's mixing between several detection chips on a system board with a very small surfacing area according to the scheme "system in a chip". Diphenyl cyclosiloxane doped by cadmium have been introduced into silicon membranes as active media in order to move to radiation detection in the energy band of 3-5 μm. Thermoelectrical cooling has been suggested for heat removing or for the increase of energy resolution of radiodetectors in the band of 1.55 μm. Multithin film detectors with temperature operating down to about liquid nitrogen and their noise have been investigated. Tuning the threshold of temperature around this point one can minimize the total noise of the system and hence the upper bound of the detectable single photon flux.

Chapter - 6

Nanostructured Materials in Diagnostic Imaging

Nanostructured materials enable targeting, enhancing diagnostic imaging signals and precision. Imaging agents based on quantum dots exhibit versatile bandgap tuning and feature biocompatibility concerns. Nanoparticles improve contrast by size-dependent diversity, while plasmonic structures enhance signals through localized surface plasmon resonance. Optimization for x-ray attenuation exploits material composition and density. Mechanistic modeling quantifies these amplification pathways.

Recent advances in medicine have shifted toward enhanced diagnostic techniques by reducing patient risk and improving detection capability. In this context, the incorporation of nanotechnology by using nanomaterials in a specific application has shown great promise. Particular interest is given to nanostructured materials acting as imaging agents. Nanoparticles designed with different sizes, shapes, and compositions are being implemented for biomedical imaging with either intrinsic or extrinsic properties. Intrinsic contrast agents, based on Magnetic Resonance (MR) imaging, are usually considered, according to the properties of nanomaterials synthesized. These materials can be regarded as molecular drugs that include magnetism capability and chemical reactivity. Besides that, X-ray imaging techniques, like Computed Tomography (CT), employ nanoparticles as extrinsic agents. Here, the capability of improving the X-ray contrast agent is determined basically by the size of the nanomaterials. Plasmonic materials intended as CT agents and for optical imaging modify the contrast through localized surface plasmon resonance. For biologically compatible materials, radiation therapy may be a way of application. In this respect, gold nanoparticles are being investigated as radiosensitizers.

The rationale underlying these applications stems from the physical phenomena occurring at the nanometer scale. When the size of the particles decreases to the nanometric range, the ratio of the surface area to the volume increases considerably. Due to this enhancement, many physical properties of the nanostructured materials change when compared to their bulk

counterparts. Such changes often confer them higher reactivity, smaller diffusion lengths, and distinct catalytic activity that enable unique detections in biological systems [114, 115, 116, 117].

Quantum dot imaging agents

Biocompatible Quantum Dots (QDs) possess size-dependent optical properties, biocompatibility of the core, high quantum yield, and significant radiative transition cross-section. Nevertheless, the gap in their regulatory approval remains a technical and commercial challenge. Their anticipated use as tunable imaging agents for multimodal medical imaging has encouraged considerable investment. A layer of biocompatible material is deposited on top of the core to improve biocompatibility and reduce toxicity. Surface chemistry variation permits control of the QD charge state, enabling tuning of their emission or absorption wavelength, or further conjugation with organic molecules for contrast enhancement in X-ray or ultrasound imaging.

QDs act as near-infrared photon emitters and are bioconjugated to specific proteins targeting cancer cells. The polymer coating provides biocompatibility and control of QD aggregation during and after cell internalization. Emission spectra from conjugated and free QDs overlap in spectral ranges unused by biological media. QDs are probed to determine conjugation-induced modification of the emission spectrum, which is essential for confirming targeting and predicting imaging quality. Previous studies indicate that a suitable combination of core material and polymer coating ensure prevention of ion release and significant toxicity [118, 119, 120, 121].

Nanoparticle contrast enhancers

Signal enhancement is a key strategy in the development of imaging agents. Several considerations must be simultaneously addressed to achieve a gain in imaging quality (temporal or spatial resolution, contrast, or signal-to-noise ratio) during use in a specific imaging technique or mode of operation. In the context of imaging agents based on RIT, the agent needs to meet the experimental requirements of biocompatibility, low immunogenicity, stability over time, and fast clearance from the organism, among others. Indeed, once administered, RIT agents do not need to linger in the organism for prolonged periods in order to provide the desired clinical information. For contrast-enhancing nanoparticles intended to be used in *in vivo* imaging applications, the size of the particles is a determining factor, with average diameters in the range of 10-100 nm being optimal. Nanoparticles with diameters larger than those typically encountered for biological structures tend to induce high levels of background noise in images.

Examples of these considerations include the design of quantum dot imaging agents for fluorescence imaging (where biocompatibility can be achieved with a proper surface functionalization), the preparation of nanoparticle-based CT contrast enhancers with the required X-ray attenuation characteristics, the fabrication of MRI contrast agents capable of drastically modifying the T 1 signal, and the use of plasmonic nanostructures amplifying the surface-enhanced Raman scattering (SERS) effect, being highly desirable targets for specific signal enhancement.

Nanoparticles based on metallic elements or oxides with a high atomic number (high-Z nanoparticles) are especially promising as RIT contrast-enhancing agents for Computerized Tomography (CT) and as contrast agents for Magnetic Resonance Imaging (MRI). In these cases, size optimization is usually more critical than achieving the lowest possible toxicity or the maximal possible modifycation of the imaging signal. Indeed, metal labels (e.g., Au, Pb, etc.) provide the greatest contrast enhancement for X-ray techniques, whereas Fe 3 O 4 and other paramagnetic materials are the most suitable candidates for MRI. The signal of metal-based contrast agents also tends to improve with their administration.

Plasmonic nanostructures

are systems in which Optical Light Absorption leads to a Localized Surface Plasmon Resonance (LSPR). This resonance Localizes the light-matter interaction around the nanostructures' surface, provides an enhancement of the local-light intensity, and thereby dramatically amplifies the signal of fluorescence- or Raman-tagged molecules near the nanostructure. Moreover, the plasmonic coupling of incident light with the atomic and/or molecular adsorbates of the nanostructure produces improved Imaging Contrast Capability of commonly used techniques.

Different types of Plasmonic Nanostructures are being fabricated to address the requirements of each application. Additionally, these materials can be used as contrast agents for Magnetic Resonance Imaging (MRI) or for Electron Spin Resonance (ESR) Imaging. More recently, Metal Nanoparticles have also been proposed for Dosimetry Enhancement Applications in Radiotherapy.

Materials can be engineered to achieve a suitable attenuation coefficient value for the desired X-ray energy range, providing the basis for more efficient X-ray Imaging by lowering the X-ray dose administered for the same Image Quality. Quantifying the Relationship between the Material Composition and

Density with the Attenuation Coefficients at Different Energy Levels allows for the identification of Materials with high Composition Density but low Atomic Number Adequately Tuned for X-ray Imaging Applications. Such Materials reduce the Shielding of Nanoparticles with Low Atomic Number Elements while Allowing the Creation of Compounds with High Atomic Number for Better Resolutions in Medical XRays.

X-ray attenuation engineering

X-ray dose efficiency in absorption-based imaging is influenced by the attenuating agent's atomic number (Z) and density. Engineering material composition and arrangement can optimize signal enhancement while respecting safety limits. Functionalized gold nanoparticles have emerged as promising X-ray sensitizers. Their affordability and versatile optical properties facilitate their integration into various imaging systems. Recent evidence also indicates that using high-Z nanostructured materials other than gold may yield sufficient image contrast. Nanostructured alloys like bimetallic or hollow spherical particles seem to combine signal-quality benefits with improved biodistribution properties and handling safety.

To predict the imaging performance attained with a particular material, it is important to establish a correlation between composition, shape, and X-ray attenuation properties. Attenuation coefficients, defined at any given X-ray energy for all elements, can readily be compiled from the literature. For the case of metallic compounds and alloys, present results for Z^4-based mixing rules accounting for the mean atomic number in conventional attenuation-coefficient formulations can be applied to estimate complete sets of coefficients for any specific composition or structure. Furthermore, experimental validation confirms that deviations from the prediction can be kept within a few percent for bimetallic and shell-core nanoparticles formed by two neighbouring isotopes [122, 123, 124, 125].

Modeling signal amplification mechanisms

Signal amplification is a powerful imaging strategy that aims to enhance the signals collected by different detection techniques. In this context, nanomaterials can serve as a means of signal amplification through various processes. Quantifying such signal amplification mechanisms is fundamental for the integration of the nanostructured material into operational systems. For every process proposed to contribute to the signal amplification, a model quantifying the contribution of the amplification path with respect to the signal accumulated by the detection technique should be developed.

A complete analysis of the factors affecting imaging quality should be performed to ensure the viability of the detection system. The analysis should consider the entire signal amplification cycle, from the origin of the signal during the interaction of the primary signal with the sample to the signal capture by the imaging system. This comprehensive approach will enable the identification of the most promising pathways for signal amplification by nanomaterials while taking into consideration potential noise sources and complementary pathways that can degrade the imaging quality [126, 127, 128, 129].

Chapter - 7

Solid-State Dosimetry Systems

Advanced modeling is increasingly used to support the development of a growing range of medical physics technologies. Recent work has focused on solid-state physics principles and on more complicated solid-state systems, including nanomaterials. The principles underlying solid-state dosimetry systems are summarized. Water-cooled Thermoluminescent Dosimeters (TLDs), Optically Stimulated Luminescence (OSL) dosimeters based on aluminium oxide, MOSFET devices, and diamond detectors are considered in detail. The complementary nature of these systems is emphasized. Special attention is given to modelling approaches for quantifying uncertainty in calibration protocols.

Thermoluminescent Dosimeters (TLDs) incorporate materials with well-characterized luminescent traps. Ionizing radiation induces the formation of charge carriers that can be trapped and later released during heating, resulting in a light pulse with an integral proportional to the dose received. The main steps involved from charge trapping and heating to light emission, readout and data reduction are considered. Particular attention is devoted to modeling the uncertainties associated with radiation dose assessment.

In Optically Stimulated Luminescence (OSL) dosimetry, the traps are released under optical stimulation instead of thermal excitation. The phenomenon is discussed, along with the factors affecting trapping and stimulation, fading, readout protocols, and uncertainty quantification. Metal-oxide-semiconductor field-effect-transistor (MOSFET) detectors are based on the structure used in modern integrated circuits. The operational principles are summarized, including the factors affecting dose response.

Diamond detectors exploit the wide bandgap and highly useful electrical properties of synthetic diamond. The mechanisms behind charge transport in these systems are reviewed, together with their advantages and disadvantages for medical applications. Possible calibration protocols are presented, with an emphasis on uncertainty assessment, and the complementary nature of the systems considered is highlighted [130, 131, 132, 133, 134].

Thermoluminescent Dosimeters (TLDs)

Thermoluminescent Dosimeters (TLDs) employ thermoluminescence from traps to estimate absorbed doses with high spatial resolution. Accurate readout requires focused heating, appropriate stimulation temperature, and calibration against absorbed dose. The TLD readout technique is determined by the underlying crystal lattice structure.

TL behavior relies on the availability of thermally stable traps that can store radiation-induced electrons. These traps must have activation energies enabling electron release into the conduction band by a single-heating cycle at high temperatures (300-600°C) and maintaining a negligible probability of filling during readout. The TL peaks are interpreted as resulting from successive, non-interacting, thermal releases into the conduction band. The release of the trapped electrons is temperature sensitive, so careful control of the heating cycle and rate is required for accurate estimates of the absorbed dose.

The absorbed dose is inferred from the release of the electrons during the readout process. The readout determines which part of the TL glow curve is generated. The shape is sensitive to the details of the readout cycle. Differences in the shape and intensity of the TL glow curves arise from ionizing radiation interaction with the crystal lattice. Fishbone dynamics can be used for modeling uncertainty in the TL detection process using appropriate statistical methods [135, 136, 137, 138].

Optically Stimulated Luminescence (OSL)

After the stimulation of Luminescence centers through specific wavelengths of light, the electron in traps are excited back to the ground state of the conduction band. It recombine with holes in the valence band and initiate the radiative or non radiative transitions which ultimately produce heating in the material.

The phenomena of OSL fading is mainly due to the fault handing of the scintillator materials in laboratory methods and also due to dislocation densities. The left over outgoing light after stimulation is difficulties, it cause merging of stimulation band and the broad emission band. Due to these factors the OSL dosimetry readings deviated from the actual readings.

The Optical Stimulated Devices are prepared by adopting the top down approaches. Devices like semiconductor and insulator always allows the tagging at the Metal Oxide and Semiconductor on the Channel. The Optical

Stimulation of the device introduce the colour centres which has normal trapping levels and also Quasi-Atomic energy levels in the forbidden Band Gap which helps in optical probing [139, 140, 141, 142, 143].

MOSFET-based dosimeters

Metal-oxide-semiconductor field-effect-transistor (MOSFET) dosimeters rely on measurement shifts in the threshold voltage of MOSFETs subjected to ionizing radiation doses. The simplest structure of a MOSFET consists of a very thin (20-200 nm) n+ polysilicon layer (source and drain), doped n-bulks and a very thin oxide layer (180 nm). In practical sensors, only the area covered by the oxide layer is sensitive to radiation damage, which reduces the bulk dose response when additional oxide layers are added. Studies have also shown that the SiO2 dielectric layer can partially shield the sensitive region from the main dosimetrically important radiation deposited in solid materials, limiting the readout signal.

The radiation response of MOSFET detectors is directly related to oxide-trap production, leading to a negative shift in the device threshold voltage. The increase in the concentration of trapped charge reduces the vertical electric field inside the oxide region of the MOSFET, leading to a reduced value of the current flowing in the channel and a decreasing sensitivity at higher doses. The decrease in the current flowing through the MOSFETs and the observed saturation of the sensor response at high doses are attributed to both saturation and recombination of charge carriers in the conduction band of the oxide layer.

Diamond detectors

Diamond radiation detectors are solid-state dosimetry devices exploiting the large bandgap of diamond to minimize dark current and damage effects. Because of their wide bandgap, diamond detectors possess negligible leakage currents, allowing for large bias voltages without efficient thermal excitation of charge carriers. This property results in good detection limits, making these devices suitable for radiation dose monitoring at very low levels. The significant atomic number of carbon, coupled with the low atomic number of hydrogen, also makes diamond detectors advantageous for detecting thermal neutrons when coupled to a boron layer.

A diamond detector comprises two closely spaced symmetrical electrodes fabricated on opposite sides of the detector chip. Under typical operating conditions, the applied bias voltage induces an electrostatic field across the diamond volume. As the radiation passes through the detector, the created ion pairs drift toward the electrodes, thus producing the detection signal. The basic

dosimetric properties of diamond detectors are shaped by the electrostatic field inside the volume, which drives the electron and hole ionization pairs toward the electrodes. The charge collection process is efficient, depending on the radiation energy and the electrode distance.

Carbon diamonds are promising due to their high radiation hardness and resistance to high temperatures, hot plasma, pressure, and chemical attack. The solid-state detection principle utilizes the formation of electronic tracks either in a tantalum-doped synthetic diamond or in the implanted region of a boron-doped diamond. These detectors are also promising for internal dosimetry of \(\alpha\) particles or heavy ions to power scientific instrumentation dedicated to the detection of highly ionizing particles.

Calibration and uncertainty modeling

Accurate calibration of medical devices is essential to ensure compliance with safety guidelines and to provide reliable results. Most calibration routines rely on physical relations between the quantity being measured and the detector output. In some cases, when these relationships are not well established or when it is impossible to obtain standardized samples, the calibration involves determining a set of calibration curves. The proper calibration of established standards is essential, since it controls the entire dosimetric chain. The information is introduced in the detector run by means of calibration curves for a proper measurement. A statistical treatment can then indicate the uncertainty of the measurement that results.

Following the fundamental principles of metrology, all the above aspects combine to generate a proper description of the uncertainty for the measurement process. In general, a measurement can be considered as the result obtained from applying a function of several variables. The uncertainty characterization in this case can be treated via an extended First-Order Taylor Series expansion around the mean value of the input parameters. The method is also known as the law of propagation of uncertainty (LPU). As the name implies, the method considers only the first derivatives of the function with respect to each variable at the mean values in the uncertainty budget [144, 145, 146, 147].

Chapter - 8

Advanced Modeling of Radiation-Matter Interactions

8.1 Photon interaction cross-sections: Compile attenuation coefficients for relevant energies and materials.

8.2 Electron transport modeling: Model scattering, energy loss, and range via Monte Carlo or deterministic methods.

8.3 Secondary particle generation: Track characteristic radiation, sputtering, and activation considerations.

8.4 Energy deposition algorithms: Compare track-structure vs condensed-history approaches for dosimetry accuracy.

8.5 Radiobiological modeling frameworks: Integrate physical dose with biological effect models and uncertainty analysis.

Appropriate modeling of radiation-matter interactions is essential for accurate predictions of response in various physical and medical applications. Attenuation coefficients for photon interactions covering a wide energy range are presented. The modeling of electron transport is discussed, with focus on primary scattering processes, energy loss mechanisms, and range prediction. The generation of secondary emitting particles (e.g. photoelectrons, Auger electrons, Bragg peak protons, characteristic X-rays, and radiative and non-radiative recoils) is covered, together with their subsequent interactions and determination of activation residues, which should be considered for realistic calibration of novel radiation detection systems. Energy depositions by photons and electrons can be modeled with different levels of accuracy, depending on the requirements; track-structure algorithms can achieve high precision but at increased computation times, whereas condensed-history methods represent a faster approach more appropriate for routine studies. Finally, the physics-based description of physical doses is combined with mathematical or machine learning formulations of biological models to simulate radiobiological responses. Aligned with clinical priorities, a predictive capability quantifying treatment effects to be expected from different combinations of nanomaterials and radiation modalities is also presented [148, 149, 150, 151].

Photon interaction cross-sections

Extensive sets of photon interaction cross-sections are crucial in many fields of radiation physics, especially for radiation dosimetry and biological response studies. Along with doses, the predictive capability of a radiobiological model strongly depends on the quality of the employed interaction cross-section data, and a limited availability of consistent and complete datasets may adversely affect the reliable assessment of radiation risk. Consequently, the present database is a synopsis of relevant photon interaction cross-sections, specifically mass energy-attenuation coefficients for 50 compounds covering the energy range from 0.1 to 100 MeV and half- and mean-free-path estimates.

Mass extinction coefficients have been compiled for all elements, together with mean and half-free path values and a separate generalized data set for C, H, N, O, and S at kT energies. An empirical formulation for the half-free paths in C, H, N, O, and S mixtures is also included. For TLD and OSL media, coefficients of gonadal dose conversion by X-ray and photon radiation have been assembled, supported by a survey of X-ray photon yellow filters. play important roles in areas such as the optimization of the design of X-ray imaging and diagnostic studies, the energy determination of X-ray spectra, and the evaluation of filter performance in yellow X-ray filters [152, 153, 154, 155].

Electron transport modeling

Electron transport in solid materials is a complex process that includes scattering, energy loss, and interaction with other charged particles. At low energies (<50 keV), where elastic scattering dominates the energy loss of electrons, direct Monte Carlo simulations can be performed. Conversely, at higher energies, where ionization processes dominate and a large number of secondary electrons is produced over small distances, the transport can be modeled using two coupled approaches: a condensed-history description of electron motion limited to a detailed modeling of energy-loss deposition of the primary electron and a proper track-structure description for the transport of the subsequent secondary electrons.

In the condensed-history approach, the motion of electrons before an ionizing collision is treated in a deterministic manner using a transport equation, and the electron track is divided into segments during which the effect of ionizing collisions is neglected. The corresponding electron flux density is then obtained by solving the stable form of the transport equation. The deposition of energy by heavy charged particles is considered under the

range-energy concept. Conversely, the cascading effect of secondary electrons is simulated by modeling the track structure of the secondary and lower-energy electrons [156, 157, 158, 159, 160].

Secondary particle generation

In Monte Carlo simulations of photon transport in matter, the generation of secondary particles is a critical aspect that must be carefully managed to ensure the accuracy of the results, both from a physical and computational standpoint. When a photon traverses matter, it can undergo various interactions, including scattering and absorption. In scattering, the photon transfers some of its energy to the medium and continues in a different direction; as a result, the bulk of the energy is preserved in the medium and is generally not of concern for radiation transport studies. With absorption, part or all of the energy of the photon may be transformed into secondary particles (electrons, positrons, and gamma photons).

A secondary photon can be produced in two different ways. Firstly, after photoelectric absorption, the excited atom may return to the ground state by either emitting a photon with an energy loss corresponding to the difference in energy levels, or by nonradiative mechanisms, thereby transferring the excess energy to the neighboring atoms. In the former case, characteristic radiation is emitted, while in the latter case, the energy may simply be dissipated as heat. Secondly, Compton scattering generates secondary photons with energies lower than that of the incident photon.

Because secondary particles carry information about the local conditions, careless modeling may compromise the accuracy of main particle transport. Electrons and positrons are usually generated in higher-energy photon transport for energies above the binding energy of the material. When a secondary particle is produced, it is necessary to follow its transport until the energy is dissipated in the matter. Interestingly, the total energy carried out from the photon beam that generates secondary particles should be taken into account when studying the profile of the radiation field [161, 162, 163, 164].

Energy deposition algorithms

Algorithmic approaches to energy deposition in matter take two broad forms, analogous to Monte Carlo simulation of radiation transport and deterministic methods. Monte Carlo algorithms track the evolution of the full history of secondary particles emitted from an energy deposition event, giving rise to a track structure of delta-ray processes, electronic excitations, ionization, and other effects. The main advantages of such track-structure

techniques are their accuracy and detail, which provide opportunities to study local mechanisms of biological response in radiobiology, nanotoxicology, and other areas of research. The deposition of energy by such detailed procedures is equivalent to the energy *S* loss that a particle beam, moving along the track of the secondary particle or particle system, would have experienced had it traversed the same volume. Energy deposition is obtained by summing the energy deposits of the individual processes or by summing all the energy deposition *S* losses scored by the particles along their self-generated tracks.

Determining the energy deposited in a volume element due to the dense concentration of secondary particles is much easier when central-limit processes associated with the energy transfer from primary radiation through multiple elementary interactions to the matter are exploited. In such condensed-history techniques, it suffices to know the expected values of the deposited energy per unit path length in different regions of the phantoms or materials. For each energy deposition event, the expected value of the energy deposited in an elementary volume is determined using a set of partition coefficients corresponding to its energy range. This technique is very efficient for dosimetry applications because it avoids the overhead of a full transport simulation yet retains high accuracy. Modelling energy deposition remains crucial for dosimetry calculations [161, 165, 166, 167].

Radiobiological modeling frameworks

Physical dose modeling can be integrated with radiobiological effect considerations in two ways. One approach consists of use the physical Monte Carlo code to simulate the dose distribution deposited in the exposed organs or tissues. Then, considering the Specific Absorbed Dose (SAD) for each area/tissue sample, the IDEAS module predicts the cell Survival Fraction (SFR) using the Linear-Quadratic (LQ) formalism with clinically determined parameters for different types of radiotherapy. The considered LQ equation can be written as [168, 169, 170, 171].

SFR = e^(-α·D + -β·D^2).

In this relation, D is the SAD (in Gy) and α and β are specific parameters for the organization, hypoxia and radio-sensitivity of the tumor. For the validation of the framework, the constructed IDEAS module was used to predict SFR during a clinical study of a patient with head and neck cancer submitted to radiotherapy. Another approach, here referred to as INCLI (INtegration of CLINical data with radiation mIcrodosimetry) is based in the microdosimetric-kinetic model. In this approach, the physical transport of

radiation in matter is managed by a dedicated Monte Carlo code, while the biological effect modeling, related to the LQ formalism, is emulated by dedicated modules.

The INCLI (Integration of Clinical data with radiation microdosimetry) methodology offers a basis to relate clinical radiosensitivity of tumor tissues with pre-clinical studies at the micro or nano levels. In this approach, the transport of radiation might consider the track structure of the radiation and-RD might be evaluated through any radiation-biological model, considering, for instance, the linear-quadratic model.

Chapter - 9

Nanomaterials in Radiation Therapy Enhancement

Various strategies for enhancing the effectiveness of radiotherapy have been explored, including the addition of exogenous compounds such as chemical agents, radiosensitizers, and high-Z inorganic materials. Among these, gold nanoparticles have been the most extensively studied, primarily due to the possibility of utilizing their properties as X-ray contrast agents, although practical use remains challenging because of their biodistribution *in vivo*. More recently, interest has shifted toward the use of other heavy metal, halide, and oxide nanomaterials, highlighting the effects of atomic number (Z), chemical composition, and biological compatibility on the sensitivity of tumor areas to neutrons or photons [172, 173, 174, 175].

Nanostructures can also serve as reservoirs of Reactive Oxygen Species (ROS) and radiosensitizers, which undergo deterioration during radiotherapy, and the spatial distribution of these nanomaterials throughout the body can be tuned to condition the desired treatment area. For platinum-based compounds, which are currently in clinical use, the biological response depends strongly not only on concentration but also on the species, shape, size, and accompanying elements. Latest developments in nanomedicine have included attempts to couple several enhancement strategies into a hybrid approach.

Monte Carlo simulations have proven useful for estimating the heats of chambers generated in the vicinity of nanomaterials, determining radiation transfer by multi-scale methods, and modeling effects associated with specific biological pathways. These developments have facilitated a more accurate representation of possible mechanisms and effects in large-scale radiotherapy enhancement studies by integrating upon independently proposed amplification mechanisms. However, multiple translational challenges remain that must be carefully evaluated before clinical trials.

Gold nanoparticles in radiotherapy

Gold Nanoparticles (GNPs) have drawn considerable attention from the medical physics community for their potential role in radiation therapy of malignant diseases such as cancer. It has been established that, when properly

delivered to tumors, GNPs can enhance the effect of X-ray and charged particle therapy. Two distinct mechanisms contribute to this enhancement:

a) The high atomic number Z of gold increases the absorption cross-section for photons via the photoelectric effect, and

b) This large-Z element can catalyze the production of Reactive Oxygen Species (ROS) upon irradiation, which can induce tissue damage.

Quantitative assessment of gold-based dose enhancement has been conducted using Monte Carlo particle transport codes, which offer a flexible and powerful framework for investigating biological targets exposed to ionizing radiation in the presence of GNPs of variable size and concentration [176, 177, 178, 179].

Despite their promise, clinical translation of Au NPs remains a major challenge, linked primarily to context-specific biodistribution and clearance limitations. Dose enhancement approaches based on high-Z nanoparticles other than gold are emerging as a complement to GNP strategies. Because some of these materials are less toxic or easier to prepare in a biocompatible manner, they may be better suited to certain biomedical applications. Furthermore, Monte Carlo approaches are not restricted to GNPs or even high-Z materials, since non-metallic nanostructures can also be designed to generate ROS. Overall, evaluation of biological enhancement mechanisms by means of Monte Carlo codes incorporates particle-dependent dose deposition modeling, which is essential for advancing this important area of study.

High-Z nanomaterials for dose enhancement

The therapeutic role of High-Z nanoparticles in radiation therapy has received a significant amount of attention in the past years. Gold nanoparticles (AuNPs) have emerged as a well-studied prototype, with an overall strategy relying on the selective accumulation in tumors due to the leaky vasculature that characterize solid tumors. This mechanism has been shown to yield a dose enhancement of the nanoparticle-embedded volume, while high concentrations in organs and tissues surrounding the tumor could produce excessive radiotoxicity. In parallel, the use of high-Z nanomaterials other than gold has been proposed, in order to achieve transverse and longitudinal biodistribution and clearance profiles that could eliminate the current hindrance of AuNPs [180, 181, 182, 183].

In this context, the dose-enhancing effect that High-Z nanomaterials could produce during Radiation Therapy (RT) is analyzed, and the alternatives

that could stand beyond gold are surveyed. Additionally, the production of Non-Uniform Reactive Species (NURS) is examined, with the aim of assessing their possible supportive roles in the therapy.

Reactive oxygen species generation

The therapeutic effectiveness of radiotherapy can be improved by enhancing the radiation dose in the region of interest. One possible enhancement mechanism relies on bioreductive processes, wherein high-Z nanoparticles are produced inside or around a tumor site. For this method to be applied in radiotherapy or combined with other types of treatment, and to avoid possible toxicity, the design of the different nanoparticles could also include the generation of Reactive Oxygen Species (ROS) such as hydroxyl radicals (·OH), hydrogen peroxide (H_2O_2), and superoxide ($\cdot O_2^-$). ROS production can trigger cellular apoptosis; it can also represent a non-targeted therapeutic effect, as high concentrations of these species can induce damage in adjacent cells. Therefore, by quantifying the different pathways that generate ROS, it is possible to evaluate their contribution to the proposed treatment. Computational models that simulate the radiolysis of water and the subsequent generation of ·OH, H_2O_2, and $\cdot O_2^-$ can yield insight into these mechanisms and indicate conditions for efficient ROS generation. Coupling Monte Carlo codes that simulate radiation transport with chemical kinetic models enables tracing the concentration of species responsible for the ROS production in the DT and their respective pathways [184, 185, 186].

Production mechanisms for ROS such as ·OH, H_2O_2, and $\cdot O_2^-$ upon radiation of water are analyzed. The results indicate the concentration of these species in the distilled water and their main formation pathways. The concentrations of ·OH and $\cdot O_2^-$ in close proximity to a population of AuNPs exposed to γ-ray radiation have also been calculated.

Monte Carlo-based dose modeling

In the past decades, the therapeutic use of high-Z materials has been an attractive approach in radiotherapy due to the possibility of enhancing the dose of ionizing radiation in the region of these materials. However, the improvement in the therapeutic ratio is still a major challenge. One possible way to address it is to localize the insertion of these materials, minimizing the scaling of side effects. Monte Carlo simulations offer a flexible tool for this purpose, enabling the calculation of dose distributions in complex geometries. Assimilating the biological effects of radiation in the regions close to the high-Z materials with the amplification mechanisms potentially associated with

them can facilitate a better understanding of these systems and is important for future clinical applications.

The use of Gold Nanoparticles (GNPs) to enhance the dose delivered to malignant cells was initially proposed in 1995. The biological effectiveness associated with the increased dose to detachucleated tissues and the expected effect of GNPs, in terms of concentrations and localization, are evidently the most important aspects for tumor treatment. Nonetheless, some contradictions remain concerning the biodistribution of GNPs and their therapeutic potential. Thus, high-Z nanomaterials other than gold have been explored, such as colloidal bismuth titanate, cerium oxide, hafnium oxide, lanthanum oxide, tantalum oxide, and tungsten disulfide. Proposals for oxidative-stress-induced enhancement mechanisms have also been investigated [187, 188, 189, 190].

Clinical translation challenges

Identifying translation challenges in diagnostic imaging systems based on solid-state or nanomaterials is crucial for enabling implementation. Breakthroughs in basic biomedical research usually precede new medical devices, and diagnostic imaging agents and stimuli-responsive systems are no exception. Nevertheless, successfully bridging the gap remains complex, time-consuming, and expensive. Techniques based on nanomaterials offer high flexibility with relative simplicity at the proof-of-concept stage, yet several obstacles must be overcome before practical application is feasible. Potential approaches currently are more advanced and closer to clinical implementation, namely quantum dots as optical imaging agents and gold nanoparticles as X-ray contrast agents. In both cases, the mechanisms of dose enhancement or signal amplification are well, if not completely, understood, yet the road to clinical use is long due to regulatory hurdles. Other strategies aim to increase sensitivity and specificity for early-stage disease detection by applying stimuli-responsive agents, often leveraging the high biocompatibility of nanoparticles. However, achieving adequate spatial resolution using these systems for early-stage disease is far more challenging than working with more traditional imaging approaches. When the desired resolution and imaging quality are obtained, the breakthrough is only the first step. The long and winding regulatory path must then be traversed.

Recent advances in nanoscience and nanotechnology have provided new perspectives on the existing treatment modalities. Understandably, these developments have led to the suggestion of using gold nanoparticles as carriers for radiotherapy and photothermal therapy. Several mechanisms for radiation dose enhancement and photothermal responses have been proposed. In

physics-based dose distribution modeling, the actual dose distribution around nanoparticles that are mixed with the tumor region is still unclear. Several biodistribution studies have also been performed, revealing a localization tendency toward organs of the reticuloendothelial system. However, the limitations of the concentration levels related to the dose enhancement factor remain to be clarified. Furthermore, localization at the tumor mass level *in vivo* is still far from reality [191, 192, 193, 194].

Chapter - 10

Magnetic and Spintronic Materials in Medical Devices

Magnetic materials, encompassing ferromagnetic elements and compounds as well as paramagnetic systems, are incorporated into medical devices for imaging-contrast enhancement and magnetic field detection as well as for magnetic hyperthermia treatment. Ferromagnetic materials display spontaneous magnetic ordering, the degree of which is dictated by the temperature and magnetic field. Contrast mechanisms involving magnetic nanoparticles in magnetic resonance imaging are closely connected to surface design that controls the nanoparticle-protein corona interaction and influences biosafety. The capabilities of magnetic magnetic-resistive sensors to detect magnetic fields of tiny amplitude are superimposed herein with the minimization of sensor noise. Disorders of either spin-transport or spin-coherence properties can be exploited in novel sensor configurations. In medical magnetic-hyperthermia treatment, magnetic heating undergoes refinement by optimizing the heating versus biosafety relationship.

Ferromagnetic and paramagnetic systems display distinctive properties that enable their application in magnetic-field detection (magnetic-resistive sensors) and imaging (magnetic-resonance imaging), while magnetic nanoparticles in X-ray radiation therapy augment the treatment's efficacy. The use of ferromagnetic materials is justified by the feature of spontaneous magnetic ordering, which permits device operation even in the presence of very low external magnetic fields. Ferromagnetic ordering is, however, disturbed by thermal and external-field effects, both of which necessarily modulate system response and impose operational limitations. Such phenomena are often undesirable for a given sensor specification; understanding their underlying principles thereby becomes crucial in optimizing sensor performance [195, 196, 197, 198].

Ferromagnetic and paramagnetic systems

Exhibit distinctive structures, magnetic properties, and behaviors with significant implications for device design and emerging application areas. Knowledge of the interactions responsible for ferromagnetic order and the

fundamental physics of individual atomic moments paves the way for spintronic device development. In the classical description, magnetic materials contain many localized moments associated with unpaired electron spins mediated by superexchange or double exchange interactions. In the ferromagnetic phase, the moments become ordered, aligning parallel to each other, and macroscopic magnetization emerges. A bifurcation occurs at the Curie temperature, resulting in a second-order phase transition that is usually smooth and continuous.

Magnetic systems enter a paramagnetic phase in the high-temperature limit when thermal fluctuations destroy the ferromagnetic order and the interaction-induced coupling of the atomic spins becomes negligible. Atomic moments still persist in the absence of ordering but fluctuate on a timescale that is short relative to experimental measurements. These systems remain isotropic in the paramagnetic phase, but anisotropy becomes important in the ferromagnetic phase. Integrating this physics into magnetoresistive sensors that operate on the Giant Magnetoresistance (GMR) and Tunneling Magnetoresistance (TMR) principles requires consideration of the interplay between thermal noise and the magnetic moment response to an external stimulus. The fabrication of magnetic nanoparticles opens new avenues for Magnetic Resonance Imaging (MRI), magnetic hyberthermia, and magnetic drug delivery [199, 200, 201, 202].

Magnetic nanoparticles for MRI

Magnetic nanoparticles are increasingly exploited as contrast enhancers in Magnetic Resonance Imaging (MRI). Two main mechanisms of contrast enhancement can be identified: T1 enhancement and T2 shortening or darkening. The latter is associated with the utilization of paramagnetic or superparamagnetic particles, for which the relaxation times are decreased by the magnetic susceptibility of surrounding tissue. The T1 contrast enhancement arises from the increased proton density available for longitudinal magnetization recovery when particles are introduced into tissues with high regional rates of diffusion, such as blood vessels. Both mechanisms can, however, be simultaneously generated, depending on the size, magnetic properties, and distribution of the nanoparticles in the biological environment. As a consequence, it is important to carefully control the biodistribution of nanoparticles, particularly their size and surface chemistry.

For clinical use, the nanoparticles must be biocompatible, exhibit negligible toxicity, display desired relaxation properties at the operational magnetic field, and yield sufficient contrast in the examined area for, above

all, T2 shortening. Although T1 enhancement can always be obtained through the introduction of high-density materials into liquids, the biocompatibility conditions present severe restrictions when the contrast agent is administered in blood. The design of suitable nanosystems for MR contrast enhancement thus requires an integrated understanding of the physical mechanisms and their relative importance in the different biophysics environments at stake [203, 204, 205, 206].

Spin transport modeling

Spin transport in magnetic systems governs spin dynamics, coherence, and transfer efficiencies. Spin relaxation emerges from spin-orbit interactions and magnetostatic fields, while spin injection relies on spin-dependent scattering at ferromagnet-metal contacts. Sensor performance hinges on the degree of polarization in magnetic readout structures and the tunneling magnetoresistance effect. Spin-orbit torque mechanisms enable ferromagnet switching through associated currents, while heat exchange with the ferromagnetic element underpins hyperthermia applications. Accurate modeling of these processes improves sensor design and diagnostic device functionality.

In spintronic sensors, proximity contact with a ferromagnetic element and spin-polarized current enhance detection sensitivity through additional noise sources. Thermal properties of the magnetic layer affect signal fidelity, with increased metallic conductivity, scaling laws, and magnetoresistance determining optimal sensor size. Wiring designs that minimize inductance or resistance improve signal quality; larger sensors boost signal strength at the expense of speed. Residual resistance adds to total noise, while flux-gate-type enormous magnetoresistance sensors face bandwidth limitations.

Medical applications of hyperthermia leverage magnetic nanoparticles or films in targeted therapy. Heat generation arises from magnetic hysteresis losses or Brownian/magnetic particle rotation, with cooling of the magnetic element informing safety limits. Hyperthermic response prospects for metallic nanostructures, cement pastes, and oxide-diluted ferromagnets expand the range of potential materials. Modeling individual particle behavior predicts residual loss considering size and spacing, while magnetization describes the collective response of closely packed assemblies with a distribution of magnetic properties [207, 208, 209, 210].

Magnetoresistive sensors

Magnetoresistive sensors are sensitive detectors based on Ferromagnetic

(FM) and ferromagnetic/insulator/ferromagnetic (FM/I/FM) heterostructures, their operation relying on giant magnetoresistance (GMR) or tunnel magnetoresistance (TMR). GMR arises due to the spin-dependence of scattering in FM materials, while TMR exploits tunneling through an insulating barrier, the process driven by the difference in density of up-spin and down-spin states that are coupled through the barrier. Both effects can constitute near-ideal sensors, with noise performance in the shot-noise limit, when the FM stripe dimensions are of the order of 100 nm. However, performance is limited by the low current modulation ratio produced by single tunneling contacts. Alternative configurations involving more than one FM element can push the magnetoresistive response close to the square of the GMR/TMR ratio, resulting in substantial sensor gains, but compromising noise levels. Magnetoresistive sensors find applications in medical fields where very low magnetic fields need to be detected, such as magnetoencephalography [211, 212, 213, 214].

The key operating principle of FM and FM/I/FM devices is that the resistance of the system depends on the relative orientation of the magnetization of the two ferromagnetic elements. Whether in a GMR or a TMR configuration, the sensor resistance is minimal (i.e. the device is in the parallel state) when the magnetization vectors of the two ferromagnetic layers are parallel to one another, and maximal (i.e. the device is in the antiparallel state) when they are antiparallel. The magnetoresistive response is expressed as a percentage of the resistance change: $\Delta R/R = (RAP - RP)/RP \times 100\%$. In addition to the change in resistance with the relative orientation of the ferromagnets, two further characteristics are important in determining sensor performance: the magnitude of the variation (ΔR) and the noise level.

Hyperthermia applications

Hyperthermia treatments harness magnetic nanoparticles, selectively infused within tumors, to enhance radiation therapy effectiveness through local temperature elevation. Despite prospects for improved treatment planning and response modeling, empirical data are scarce. Heating capability depends on the specific absorption rate (SAR) of the nanoparticles under the applied field and is influenced by materials and conditions. To facilitate estimation in radiobiological frameworks, calculations determine the SAR for different materials and field geometries, enabling identification of leading candidates and off-target tissue safety constraints [215, 8, 68, 216].

Heating-enhanced radiotherapy exploits nanoparticle accumulation in tumors to locally elevate temperature. Such tissue modification may intensify

radiation damage or mitigate repair. Magnetic nanoparticle-based heating a spatially defined option with minimal invasiveness offers a promising approach. However, limited SAR data hampers treatment planning and response prediction. Below 200 kHz, SAR is primarily material-dependent; during hyperthermia at frequencies < 1000 kHz, SAR also depends on tissue composition and surrounding tissue bio-heat capacity, ultimately guiding clinical translation choices for each treatment. Uncertainty arises primarily from physiological factors; for suitable NP design, SAR primarily reflects material selection. Severe SAR deviations in clinically relevant conditions may result from strong field inhomogeneities.

SAR facilitates radiation dose-enhancement modeling. In radiobiological contexts that explicitly connect SI units to dose in Gy, evaluating NP concentration or mass without empirical knowledge of spatial dose deposition can lead to misinterpretation. To guide SAR incorporation in Monte Carlo models, calculations determine the specific absorbed rate for various materials, including silica and zinc oxide, and under different field configurations, including zero-field- and constant-frequency-and-amplitude-approaches. SAR in radiobiological frameworks is linked to dose enhancement for gold nanoparticles in NP-augmented radiation therapy.

Chapter - 11

Solid-State Sensors and Biosensing Platforms

Transduction principles underpinning solid-state sensor operation are examined, along with their influence on sensitivity and selectivity.

Gate modulation of FET biosensors upon biomolecular binding is modeled to study readout-capacity trade-offs; electromechanical coupling in piezoelectric nanomaterials enables sensitive detection without potentiometric signal transduction; high graphene mobility facilitates FET sensor design, functionalization impacting selectivity. General signal transduction mechanisms encompassing chemical-electrical and chemical-optical pathways are classified, enabling sensitivity and selectivity modeling as functions of film permittivity, surface-state density, and operating pH.

The rapid growth of solid-state sensors is driven by their inherent transduction advantages, compact devices, and suitability for integration in portable and multiparameter instrumentation. Signal transduction in these sensors is performed by electrochemical, optical, or Piezoelectric coupling. Piezoelectric transduction directly produces an electromechanical response without an intermediate potentiometric signal, eliminating the need for an external voltage source and reducing power consumption. Sensitive FET-based bio- and gas sensors take advantage of the large surface-to-volume ratio of nanoscaled materials. A novel concept for quantitative modeling of signal transduction in solid-state sensors combines all mechanisms into a single framework [217, 218, 219, 220].

These principles are then applied to qualitatively and quantitatively assess sensitivity and selectivity in various sensor configurations, focusing on readout capacity in FET-based sensors, the origin of the electromechanical response in nanowires and nanofibers, and the interplay between permittivity, surface-state density, and operating pH in Opto-Electronic devices.

Field-Effect Transistor (FET) biosensors

exploit the gating action of specific biomolecular binding to an FET-sensing surface. The affinity between probe molecules immobilised on the

gate and the target biomolecules in the solution alters the carrier concentration (or in some cases also the type) in the sensing layer, causing a change in the source-drain current for a constant gate bias. The detection principle thus correlates the change in gate voltage with the concentration of target biomolecules. Depending on the configuration and the type of sensing material, FET biosensors provide several advantages, such as high sensitivity (sub-picomolar detection limit), ease of fabrication, low-cost detection, and a simple read-out circuit. FET sensors have also attracted much interest in infection detection, DNA hybridisation, cancer biomarker testing, auto-immune disorder detection, and toxic biochemical detection.

Further sensitivity enhancement can be achieved by using nanostructured materials with high surface-to-volume ratios. The combination of semiconducting nanostructures with large mobility and high-speed detection capabilities makes these sensors very promising for real-time detection of biomolecules. In addition, the analyte-induced change of electrical transport properties within the nanowire-based FET enables simple doping and sensing measurement. Modelling of potential FET biosensors indicates that resistive gating should be investigated in detail for optimising the sensor performance [221, 222, 223, 224].

Piezoelectric nanomaterials

Nanomaterials with electromechanical coupling display piezoelectricity and are suitable for sensing and actuation applications. Fabrication techniques, support conditions, composition, and electric field influence electromechanical coefficients. Piezoceramic-based energy harvesters are integrated for estimating delivered power; nanogenerators modelled with surface charge dynamics predict harvested power during physiological motion. Optical chemical-to-electrical transduction is achieved with an ion-gel-gated field-effect-transistor (FET) structure and improved response by combining FET and piezoelectric nanomaterials; biosensor performance increases upon gold-nanoparticle (NP) inclusion to silicon nanowires or deposition of functionalized graphene oxide. Oligonucleotide-modified graphene oxide suspension detects goldNP/oligonucleotide conjugate bonding, with FET performance enhanced by gold-NP functionalization.

Allow signal transduction and electromechanical actuation. Relationship between dielectric-permittivity and mechanical-stress change enables evaluation of electromechanical coupling without dedicated characterisation. Sensor systems also employ external-parameter modulation: ions-flooding a planar FET modulates ion-concentration across the gate. Integration with

piezoelectric nanomaterials increases chemical-electrical response, by either harvesting transduction-energy from surrounding events or by triggering localized nanomaterial-dynamics to amplify a proximal stimulus. Simulations of polarization and charge-distribution dynamics within a piezoelectric nanogenerator quantify generated-potential during motion. A gold-nanoparticle array embedded within a silicon-nanowire FET enhances sensor signal by increasing charge transfer within the oxide region; responsive to an oligonucleotide-gold-NP conjugate, the specific FET response is comparably increased by functionalizing an aqueous-formulation of graphene oxide with the over-saturating oligonucleotides [225, 226, 227, 228].

Graphene-based sensors

Combining the highest electron mobility with a two-dimensional structure, graphene leads a promising development in chemical sensors. By making a heterostructure with nanomaterials possessing different energy-band structures, it can have the alteration of electron transmission. Such type of change can be used to detect the existence of specific analytes, providing a range of applications. Sensor precision will be determined by structure and parameters of the integrated chemistry.

Chemical sensors can respond to chemical species by altering electrical, optical or mechanical properties. The primary mechanism of chemical bosensory systems is the interaction of bioreceptors with specific analytes. Such transduction can be considered a kind of chemical modulation of semiconductor field-effect transistors (FETs). In contrast with standard FET-based chemical sensors integrated with conventional bulk substrates, the extremely high mobility of graphene or other two-dimensional materials allows them to respond to chemical ad-operation with a much lower mass as compared to three-dimensional devices. The effective holes or electrons concentration in graphene can be modulated by the addition of chemical species, thus leading to a variation of the source-drain drain-source current in graphene FETs. This variation can serve as a quantitative measurement of that analyte at the interface.

However, such modulation in chemical FET sensors is usually severely obscured due to the weak binding nature between chemicals and the chemical receptor. As a consequence, high reactant concentrations and FET sensor arrays coupled with advanced pattern-recognition methods are needed to improve the detection accuracy. A chemical response mechanism based on tunnelling modulation in a p-n junction has been proposed and theoretically investigated. In this structure, the formation and recombination of p-n junction

carriers as well as the probability of tunnelling of charge carriers through the band-gap can be reversed by the interaction with different species. Such an interaction mechanism has been verified in a wide range of chemical FET devices made from organic, molecular, polymeric and metallic materials [229, 230, 231, 232].

Signal transduction mechanisms

Signal amplification in biosensors is indispensable for the reliable detection of analytes at extremely low concentrations. In a typical biosensor, the binding of a biomolecule modifies the local chemical (for potentiometric and FET sensors), optical (for optical sensors), or mass-induced (for piezoelectric sensors) environments. A signal amplification mechanism enhances the response of the primary transduction process, providing higher signal sensitivity and lowering the detection limit. In signal transduction-based chemical sensors, the detected quantity (e.g., conductivity, resistance, fluorescence/TIRF change, or mass change) depends on the concentration of redox couple; therefore the response is quantitatively modeled based on the temperature-dependent Nernst equation.

Signal transduction in electrochemical and FET sensors is generally governed by the Nernst equation, describing the change in the electrochemical potential difference caused by the transfer of charged species from the bulk of the solution to the active interface. Such processes can be considered as the accumulation of species at the surface, yielding second-order kinetic coefficients and detection limits in the low micromolar range. In optical biosensors, signal amplification occurs in two ways. First, resonance energy transfer between two individual quantum dots can be achieved in the proximity of 2-10 nm. Second, ion-exchanged Ag/Au nanowires can achieve TIRF for exponentially enhanced resonance light near the silver-sensing layer interface. For piezoelectric biosensors, the detection limit is directly related to the volume of target analyte and, hence, a relationship is established for target molecules. Actual detection limits are dependent on many physical factors, such as the nature of the transduction method, the effective surface area, the signal transduction process, the signal amplification mechanism in surface binding, and the detection technique [233, 234, 235, 236, 237].

Sensitivity and selectivity modeling

Diagnostics systems based on solid-state materials usually sense trace biomolecular amounts. Therefore, diagnosis precision increases when transduction events are maximally efficient. Sensitivity and selectivity are the

main performance metrics evaluated to address this goal. The sensing capability is characterized by the Limit of Detection (LOD), defined as the concentration value providing a significant signal reaction against the noise level. The lower the LOD, the higher the sensitivity. Selectivity is the ability to only react with the targeting compound, without cross-sensitivities that cause undesired signal production.

Optimal parameters can only be defined if quantitatively estimated through predictive models, since each sensor is designed and tested in a unique biomolecular environment. Modeling chemical-electrical-optical processes can be obtained from first principles or simplified time-scale analyses. Material properties type, morphology, thickness, choice of dopants and dielectric layer are the main parameters of interest at the moment. Diverse experimental conditions, such as temperature or moisture, are also relevant, but can only be tested after sensor fabrication. Once statistical information becomes available, incorporating these variables in the predictive models will enhance their robustness.

Signal transduction requirements can also be quantitatively assessed. Electrical, optical, and electrochemical readout performances make use of distinct physical principles and material features, thus leading to sensibilities and limits of detection in different ranges. The main route to nonselective sensors is the unintentional involvement of chemical species beside the targeting one in the transduction process. High-sensitivity chemical reactions occurring at the solid-electrolyte interface, whose kinetics is much faster than the diffusion process reacted at the solid-gas interface, are regarded as cross-sensitivities, increasing the response current or laser excitation without being the target analyte. Signal transduction through Piezoelectric field effect signals is quantitatively described earlier in this section [238, 239, 240, 241].

Chapter - 12

Energy Harvesting and Power Systems for Medical Devices

Advances in medical devices and their integration in bioenergetics and homeostasis assertion have propelled developments in materials and technologies for the generation, storage, and use of energy on a nanometric scale. The increasing antenna surface area provides sufficient nanostructured photovoltaic or thermoelectric conversion and nanogenerators for energy-harvesting functions during natural motions. Safe operation during natural usage cycles imposes constraints on junction temperatures, dielectric field strengths, leakage currents of inductive systems, and biocompatibility of energy-storage and supercapacitor units. Efficient wireless power transfer through inductive coupling is demonstrated.

Thermoelectric-generation materials are estimated in terms of figure of merit, biocompatibility, and producing zones, thus paving the way for targeted future experimental investigations. Nanogenerators enable the synthesis and harvesting of energy during physiological motion. Safety assessment during implantation, exposure to sunlight, and natural functions is required for photovoltaic nanostructures deployed in high-energy-density supporting cushions. Energy storage and supply systems must function without breakdown during operation. Energy transfers must be effective during natural ranges of motion. Transferring energy from device to implant is preferable over sources asides batteries.

Photovoltaic nanostructures: The extent of human interaction with light in daylight and medical installations is enormous. Manmade archaeological/architectural strategies utilize sunlight as energy source. Thus, also implantable and noninvasive devices controlling during normal individual maintenance-repair cycles may incorporate photovoltaic action generating energy sources for control and actuation in electronic, optical, and other materials/applications. Piezoelectric nanocomposite power-generating systems: Delivery of energy-generating nanostructures on a power system basis for implantation in nanohomedics is considered [242, 243, 244, 245].

Thermoelectric materials

are able to convert temperature differences into electric voltage. They allow electrical power generation through thermal gradients and can also produce thermal gradients that may be used for heating or cooling in a solid-state fashion. Both applications are desirable in medical devices: thermal-electric generators can be used to exploit temperature differences between human body and environment, and thermal-electric coolers can be used to build solid-state coolant for solid-state cooling applications for chips and in portable dehumidifying solution. Thermoelectric material performance is characterized in terms of a dimensionless figure of merit (ZT). Materials with a higher ZT are desired to build smaller and more efficient power generators and coolers. Furthermore, biocompatibility and safety must be taken into consideration for the development of thermoelectric devices that will be placed inside the human body, and that are meant to be in direct contact with biological fluids.

Advanced nanostructuring of thermoelectric materials is a promising approach to enlarge the ZT figure of merit. It has been largely demonstrated that the figure of merit can be enhanced by introducing nanoscale features in both alloy- and oxide-based materials or by dimensioning the material down to the nanoscale (zero-dimensional nanoparticles, one-dimensional nanowires/nanotubes, and two-dimensional thin films). However, most of the published works in the field focus only on a part of the problem in the design of efficient thermoelectric materials; a proper thermoelectric material for energy harvesting and cooling applications must also achieve biocompatibility and safety when used in the medical sector. Biocompatibility of thermoelectric materials has not yet been assessed in detail, and safe usage in a medical context cannot be assumed yet.

Piezoelectric nanogenerators

Nanogenerators based on piezoelectric nanomaterials harness electromechanical properties for energy harvesting. Nanostructures with large surface-to-volume ratios facilitate electromechanical coupling, enabling operation in low-frequency, low-magnitude mechanical stimulation regimes. These systems may also utilize network architectures capable of responding to higher-magnitude physiological motions.

Energy-generating technologies rely on electrochemical or thermoelectric mechanisms. Electrochemical cells are commonly employed in implantable devices, yet the limited operation duration necessitates external replacement,

implantation, or recharging. Thermoelectric modules utilize temperature gradients, typically between blood and surrounding tissue, to generate power. Nanogenerators based on mechanically stimulated piezoelectric nanomaterials offer an additional energy-harvesting mechanism. Power generation is often achieved via networks of nanowires subjected to mechanical deformation induced either by external means or physiological motions from heartbeat, respiration, arteries, veins, or other skeletal and soft tissues. Coupling nanomaterials with piezoelectric properties allows low-frequency nanoscale stretching or vibrating motions to be transduced into electric energy.

Using piezoelectric nanomaterials as nanogenerators requires careful consideration of the operating conditions. In many previous demonstrations, networks of ZnO or $BaTiO_3$ nanowires were deformed using mechanical testing equipment, thereby characterizing the devices under conditions that were not representative of physiological stimuli. Sensorimotor action potentials associated with body and limb motions operate in the Hertz regime, necessitating the ability to harvest energy from low-frequency mechanical movements. Persistent nanostructures, assembled into device configurations that can horizontally or vertically expand and contract under externally applied forces or physiological stimuli from muscles, skin, or organs, may therefore be more suitable for coupling with piezoelectricity to harness energy for low-frequency operation.

Photovoltaic nanostructures

Photovoltaic efficiency is limited by parasitic absorption processes in the substrate or other adjacent layers. To mitigate these effects, a Transparent Conducting Oxide (TCO) layer is usually deposited on the absorbing layer, with the main function of boosting light transmission into the semiconductor. Nevertheless, increasing the thickness of this layer may eventually lead to unwanted losses, which naturally reconstitutes the trade-off between TCO thickness and solar cell performance. Optical-engineering calculations may help overcome this limitation by determining the best TCO thickness with respect to the cell structure and size.

In the case of solar cells designed for implantation into the human body, biocompatibility should also be taken into account along with efficiency. The materials commonly employed for TCO layers must be replaced by undoped oxides, which, in addition to being optically transparent in the working wavelength range and providing good transmission to the underlying cell, must also have thermal, electrical, and chemical stabilities. Nevertheless, both metal and ceramic oxides could be operating as TCOs for these devices by

achieving appropriate doping levels without losing any of these stability features.

Life-threatening diseases like cancer that presently have no effective curative approaches appear amenable to photothermal ablation with almost 100% tissue penetration depth by using appropriately sized noble-metal nanoparticles. These particles convert near-infrared radiation (NIR) into heat, rapidly raise the temperature of surrounding biological media, and induce cell death. However, when considering the spatial resolution of this modality, the use of these metals during the treatment should be avoided; for that reason, all the metals reactive in the NIR region are of interest, and such multi-NIR devices should be prepared using a mixture of these metals with proper wavelenghts so that they would induce an enhanced-temperature around the CTML region where the cancer cells are devasted [246, 247, 248, 249, 246, 247, 248, 249, 246, 247, 248, 249].

Wireless power transfer modeling

A generic wireless transfer system is modeled through electromagnetic field equations with a simple-source approximation. A circular dipole configuration is considered, and the radiated power field is computed. The electric field around the body of a representative patient is then calculated, helping to identify tissue leakages, patient safety limits, and transfer efficiency for a possible application on a wireless power supply for medical implants.

Current implantable conditioning devices consume a few μW of power in their active parts without wireless activation. Near-field wireless power transfer can enable their autonomous operation through electromagnetic coupling between a patient-worn surface coil and a properly designed device antenna. Nevertheless, modelling power supply efficiency requires a full characterization of energy leakages in the near-field transfer system, especially in patient tissues. A generic configuration for the wireless transfer system is defined. Power is transferred by a circular dipole positioned on the surface of the powering unit, which radiates an alternating electric field. The analytical characterization of safety limits for the powering configuration can be extended to other wireless power supply systems, improving their design while ensuring patients' safety [250, 251, 252, 253].

Biocompatible energy storage systems

Wearable and implantable biomedical devices generally require stable energy delivery, which can be achieved through energy storage systems integrated with the devices. A biocompatible energy supply can also enable

wireless powering of medical devices in contact with pathological fluids, such as monitoring implants and drug-reserve systems. Biocompatible batteries and supercapacitors have been developed for this purpose. Biocompatible batteries have been manufactured from trees and sea sponges, but their efficiency is still low. Supercapacitors are often made with activated carbon, and their development is focused on high surface area and improved ion transport.

The limitations of metals (low energy density, stray current) make lithium-ion batteries less beneficial, but Li-metal, Li-Co, and Li-Mn batteries have still been used to power medical implants. Investigations on ion gels, ionic liquids, polymer gel electrolytes, polymeric organic ionic plastic crystal electrolytes, and gel polymer membranes exhibit the reliability of supercapacitors in implantable devices. To guarantee patient safety during holding time and implantation of medical devices, low-leakage wireless energy transfer through resonant inductive coupling is favorable. A wireless leakage level comparable to any medical safety standard could allow the safe use of a wireless electric power supply during surgery.

Metal oxide electrolyte (MgO2), gel polymer (TEBA), and bio-soaked TiO2 nanowire electrodes with high pore size are tested in supercapacitor systems to store energy in natural rooting vivarium. Gel polymer electrolytes are considered suitable for an implantable multilayer device with capacitance good enough for powering 2 LEDs connected in series with a photometric brightness similar to a simple lab experiment.

Chapter - 13

Biocompatibility and Toxicological Modeling of Nanomaterials

Biocompatibility is a crucial consideration for implantable nanomaterials and any medical devices in contact with living tissues. Although *in vivo* testing remains essential, modeling offers a scalable approach to predicting the toxicological impact of nanomaterials through in-depth studies using a small set of candidates. Furthermore, patient cytotoxicity screening tests can facilitate rapid patience-specific material screening, protecting vulnerable populations and minimizing adverse effects.

Biocompatibility determines the degree to which materials induce adverse biological responses. Biocompatible surfaces elicit a negligible immune response, exhibit low cytotoxicity, and support protein adsorption for efficient clearance. Protein adsorption onto the material surface can have a decisive influence on these interactions, promoting or inhibiting inflammatory cellular responses. Several review articles describe the general mechanisms of protein corona formation and the subsequent effects on *in vivo* stability and cytotoxicity of nanomaterials. Following implantation, protein molecules are the first biological components to establish contact with nanomaterials. The competitive adsorption of native serum proteins and their respective concentrations determine the composition of the adsorbed layer. The protein coating modifies the surface chemistry of the nanoparticles, impacting protein-cell interactions and subsequently determining cytotoxicity. Depending on their properties, certain proteins from the corona can promote an immune response, while others can reduce it.

Appropriate modeling of the interaction of proteins with nanomaterials in biological media can support faster patient-specific biocompatibility assessment. Such modules form a component of a broader biocompatibility testing framework, enabling patients to be classified according to their sensitivity to specific nanomaterials. Additionally, regulatory sample screening frameworks can facilitate patient-targeted therapy. Bacteria are often the originating source of infections, and biocompatibility with bacteria

represents an important test for medical devices. While preventing biofilm formation on an implanted device is strongly desired, killing bacteria surrounding the device is generally unfavorable. Therefore, the targeting of nanoparticles to cell membranes and/or the internalization of antibacterial agents must be handled with care, balancing bioactivity and protein prevention. These aspects must also be addressed in future modeling efforts [254, 255, 256, 257, 258].

Surface chemistry and protein corona formation

Surface chemistry critically affects nanomaterial biocompatibility and biofunctionality. Following exposure to biological fluids, a protein corona comprising serum/biological fluid proteins coats nanoparticles. This shell mediates cell interaction and recognition and considerable influences the response to stimuli. The corona is modifiable via tailoring the surface chemistry before use. The tendency of different surface atoms to attract specific proteins allows for enhancing predetermining responses by grafting crown moieties. The transition from a hydrophobic to a hydrophilic surface - e.g. by attaching additional hydroxyl groups- generally favours biocompatibility during *in vitro* and *in vivo* testing. Protein adsorption is favoured in small nanoparticles compared to micrometric ones of the same material. An effective strategy to improve cellular Uptake is approaching targeting by attaching ligands that promote selective noncovalent bindings by pairs of bifunctional ligands.

Nanoparticle biodistribution and plasma clearance rely on their interaction with the reticuloendothelial systems of the liver and spleen and remain a safety concern in nanomedicine. By including gadolinium or iron cores, the dynamics within the organism became easier to trace with *in vivo* magnetic resonance imaging or gamma camera and SPECT techniques. Several parameters influence the biodistribution of nanomaterials. Size is critical; nanoparticles with diameter below 6 nm or larger than 200 nm are more prone to accumulate at specific sites. In the intermediate range, the relative concentrations in different organs depends on the exposed time. More significant accumulation in the liver is observed with longer exposure time while the spleen area has higher concentration when exposure is reduced. The residence time within organs also changes with time; the blood-brain barrier remains almost insensitive to size and shape [259, 164, 260, 80].

Cytotoxicity mechanisms

The elucidation of cytotoxicity mechanisms is crucial for the safe use of

engineered nanomaterials in medical physics applications. Nanoscale systems can trigger harmful biological responses upon cellular internalization, and predictive modeling is increasingly required by regulatory authorities. Several studies have investigated the toxicity of different families of nanomaterials, proposing different mechanisms responsible for deleterious interactions with biological systems.

A recent review article has grouped these effects into three main categories: direct interactions with cell membranes; production of reactive oxidative species (ROS) upon internalization; and toxicity due to dissolved metal ions. In the first case, excessive membrane penetration can lead to cell swelling and lysis; in the second, the generation of excess ROS can produce oxidative stress with consequent intracellular damage to lipids, proteins, and DNA; in the third, the lethal dose and residence time of dissolved ions in the blood circulation must be low enough for the cytotoxicity to be negligible. Mathematical descriptions of these effects could help predict the safety of any engineered system [261, 262, 263, 264].

***In vivo* biodistribution modeling**

Modeling organ accumulation and clearance of nanomaterials is crucial for toxicological assessments. Data for verified formulations of nanoparticles can be used not only to evaluate expected body residence but also to determine pharmacokinetic parameters. The proposed approach combines *in vitro* distribution and clearance data acquired along the time course with a distribution model based on the well-stirred compartmental model of pharmacokinetics. The model predicts the concentration of nanoparticles in a specific organ as a function of time based on the parameters governing their distribution and clearance. The model can also be used to estimate clearance rates for the liver and spleen based on direct *in vivo* injected biodistribution data of the nanoparticles during a 24-hour period. Such biodistribution modeling of nanoparticles could be applied to any system with already defined parameters considering the bulk solution properties and could represent a valuable component of the toxicology modeling toolbox.

Modeling organ accumulation and clearance of nanoparticles is important for toxicological assessments. *In vivo* biodistribution data of verified formulations provide insight not only into expected body residence but also into pharmacokinetic parameters. Combining *in vitro* distribution and clearance data acquired at successive time points with the well-stirred compartmental distribution model allows characterization of the concentration of nanoparticles in a specific organ as a function of time. The model predicts

organ concentration based on parameters governing distribution and clearance, enabling estimation of clearance rates for the liver and spleen based on direct biodistribution data during a 24-hour period. This approach thus supports biodistribution modeling for any system with defined parameters, contributing to toxicological understanding [265, 266, 267, 268].

Clearance pathways

Silver, gold, and zeolite nanoparticles have been reported to enhance malignancy radiotherapy by increasing the absorbed dose due to their high atomic numbers and high ratios of mass energy absorption coefficients. Cellular and animal studies have shown a certain biological response (e.g., enhanced mortality rate, change of growing speed) during treatment with various types and amounts of nanoparticles. However, there are still some problems to solve, such as the biocompatibility and biodistribution of nanoparticles in the human body for clinical use.

For silver nanoparticles, the route of injection (intratumoral or intravenous) and the number of injections affect the particle distribution in different organs. Gold nanoparticles are well known for their radiosensitive effects; however, their higher toxicity has also been reported. The concentration and surface properties of gold nanoparticles have been determined to affect the biodistribution. Glioma therapy should focus on the overall therapeutic benefit and seek a balance of both the therapeutic efficacy and the side effects. nontoxic high-Z nanomaterials with potential radiotherapy-enhanced effect and small (-30 nm) size suitable for *in vivo* nanomedicine [269, 270, 271, 272].

Regulatory safety frameworks

Nanomaterial safety assessment and approval are typically regulated by agencies, such as the US Environmental Protection Agency, US Food and Drug Administration, and European Medicines Agency. A list of chemical and physical properties suspected to be hazardous to human health has been compiled, along with corresponding initial tests. For metallic and inorganic nanoparticles, the list includes reactivity; distribution within the body; generation of Reactive Oxygen Species (ROS); the need for a corona of specific proteins, e.g., apolipoproteins; dissolution and stability in body fluids; and penetration of biological barriers (cell membrane, blood-brain barrier). When assessing the safety of organic nanoparticles, additional criteria must be added, such as polymer degradation, long-term accumulation, and immune-system responses.

Nanomaterials must be tested and considered at three levels: individual components, the final product, and large-scale use. At the first level, if either the material or the subsequent products are produced on a zero-scale basis, they must satisfy existing chemical regulation obligations. At the second level, if nanomaterials are present in the product as a colorant, additive, preservative, or other function, or when deliberately included for functional effects or improvement of physical or chemical properties, the product is subjected to existing obligation approvals. At the third level, products containing nanomaterials in reactive mixtures must be registered, tested, and assessed as a whole [273, 274, 275, 276, 277].

Chapter - 14

Artificial Intelligence in Materials Modeling

Recent advances in Machine Learning (ML) and Artificial Intelligence (AI) offer exciting opportunities for materials research and development. ML enables the discovery of new materials and design of devices with optimized properties through the automatic identification of structure-property relationships in existing datasets, which are then used for prediction or guidance at reduced computational cost. Innovative strategy development can also benefit from an AI-driven approach using multi-level models, where the ML component complements physical descriptions to speed up computationally intensive tasks.

Despite the ever-increasing accumulation of experimentally measured and computationally generated materials data, identifying optimal materials remains challenging. A related problem is the lack of suitable models for predicting the properties of materials for which only relatively few examples are available. However, directed efforts can help alleviate this situation. In particular, databases of materials properties for a wide range of quantities (the Materials Project, Open Quantum Materials Database) and descriptors relevant for computing these properties are publicly available and can be conveniently queried and downloaded. In addition, a comprehensive ML formalism is being developed within AIST for the prediction of a wide range of physical properties.

The section reviews recent developments and prospects in the application of AI methods for materials modeling and optimization in solid-state and nanostructured systems, highlighting ongoing directions of activity. Data-driven models are expected to play a major role in advancing materials discovery for applications in radiation and medical physics [278, 279, 280, 281, 282].

Machine learning for material discovery

Machine learning methods, in combination with density functional theory, ab initio molecular dynamics, and classical molecular dynamics, can enable the rapid and efficient discovery of new materials. To drive data generation for discovery, material property data across several classes are

compiled. The curated data set includes chemical reaction formation energies, phonon dynamics, elastic properties, band gaps, and defect energetics. The strategic development of data-driven discovery hinges on the careful selection of high-performing features through recursive feature elimination. These contributions bear the significant potential to empower future discovery projects in the materials domain and bring artificial intelligence-enabled development of novel materials closer to reality.

The synergy of machine learning with density function theory, combined with ab initio molecular dynamics and classical molecular dynamics methods, constitutes a route for the accelerated discovery of new materials. Material properties of diverse nature (formation energy of chemical reactions, phonon properties, elastic moduli, band gap, defect mechanisms) are collected and analysed in order to provide foundational data for guided data generation. Smart feature construction and the subsequent determination of optimal sets of high-performing descriptors for property prediction using recursive feature elimination support the complete predictive modelling workflow, thereby enabling automated data generation to assist high-throughput materials discovery [283, 284, 285, 286, 287].

Neural networks in property prediction

Concepts and eigenstates of spin filaments in magnetic systems and materials

The analysis of magnetic systems and materials is performed in the framework of a quantum magnetic structure feature - a magnetic filament, which is considered as the main object of the spin processes. The concepts of a quantum magnetic filament, its eigenstates, a spin filament and a spin chain, as well as the energy of a filament in an external magnetic field perpendicular to the axis of the filament are formulated. The spin interactions in the filament can be described with a spin Hamiltonian of a different order depending on the width of the filament and the distance R between the filament axes (for a system of parallel filaments).

Thermally activated self-ordering of magnetic filaments, as well as the presence of filaments in the bulk of magnetic crystals at room temperature, account for the connection between internal and external fields through an effective mean-field model. Based on these notions, the conceptual model of spin diffusion by a wave mechanism is developed. It can explain processes associated with the fast magnetic response of a set of nanoparticles and among others, the signal transduction quantum dot behavior after flashing. Spin

filaments are applied to the interpretation of transport and photo-induced effects in nanostructured ferromagnetic thin films, which contain ferromagnetic inclusions and exhibit ferromagnetic resonance at room temperature.

The identification of spin-waves in the electron modes of directly neighboring spin-filaments is proposed. Spin-filament eigenstates generate a system response to external influences in the vicinity of different-fabrication-layer ferromagnetic films. These quantum and classical manifestations enhance information coding with spin processes and technologies.

Data-driven radiation modeling

Empirical data can be used to complement physics-based particle transport models by providing quantities, such as interaction cross-sections and linear attenuation coefficients, that require a large number of experimental results for validation; or they can help reduce the number of layers in a system by taking into account the associated probability of radiation-induced interactions.

For example, the modeling of linear attenuation coefficients for photon energies below the K-edge energies of relevant elements can be controlled by a generalized data-driven empirical model of the form \[\lambda=\sum_{i=1}^M \frac{K_i}{E^{a_i}},\] where \(K_i\) and \(a_i\) refer to the empirical parameters of a specific database for a chosen category of materials, while M is usually set to 6 in the case of compounds. The computed model can be validated with the known experimental data and subsequently integrated with well-established Monte Carlo or deterministic particle transport codes [288, 289, 290, 291].

Optimization algorithms

Selection of various materials with given properties and development of the associated device technology can be facilitated through a procedure based on optimization algorithms. Optimization is needed in numerous applications including material selection, device design, fabrication processes, and operating procedures. The idea of optimization consists of selecting the best material or the best combination of processing parameters out of numerous possible choices, so as to achieve the desired end product with minimum costs. The term "best" is defined in terms of a figure of merit which is to be minimized or maximized, and the optimization procedure identifies the materials, structures or processes that best satisfy this definition. In principle, no optimization can deliver results which are better than those given by the

original models. The predictions are only high-quality when applied to the same region of the input space from which they were constructed. Nevertheless, for many applications the predictions can be sufficiently accurate even in an extended interpolation regime. Optimization methods can therefore be combined with accurate physical models in order to suggest the best choice of materials or processing conditions. This union is particularly powerful in the synthesis of new materials, since physics-based models are available that predict many of the essential properties of materials from their composition and microstructure.

Machine learning investigates the development of algorithms and techniques that allow computers to learn, improve, adapt and generalize through experience. The basic strategy is to define an appropriate mathematical description of a particular class of problems, such that known data sets can be used to construct effective predictive algorithms. In the context of materials modelling, it is possible to formulate a series of machine learning approaches that are of relevance to materials discovery [292, 293, 294, 295].

Integration with medical device design

Emerging medical physics devices must be safe and effective, compatible with regulatory standards, and capable of addressing real clinical needs. Thematically aligned research enables novel-solution development, yet AI models may not independently identify validation requirements. Physics-informed models for material discovery and sensor design must therefore explicitly consider FDA and OECD guidelines for nanomaterial safety assessment, functionality validation, and clinical evaluation.

Fundamental biocompatibility questions include: How does native protein adsorption influence nanomaterial behavior? What cellular processes mediate toxicity? What determine nanoparticle biodistribution and clearance during *in vivo* exposure? Answering these questions hinges on two distinct model classes: predictive exposure/toxicity models and models for assessing nanomaterials' clinical readiness. Protein-corona modeling elucidates the origins of biocompatibility and selectivity, while toxicity-mechanistic models explore the pathways affected by nanomaterial exposure and quantify the produced effect strength. Describing dispersive-kinetic and clearance models applied to real experimental data highlights these topics' cross-cutting nature [296, 297].

Chapter - 15

Fabrication Technologies for Solid-State Medical Devices

Medical physics devices and, particularly, their solid-state parts rely on several aspects for achieving the required performance. Novel and/or complex device architectures often come with increased fabrication difficulty and production cost. These aspects are usually traded off against innovative functionalities or increased performances. Areas covered in device fabrication technology discussions include thin-film repro-duction processes, nanolithographic methods, three-dimensional microfabrication, cleanroom producing technology, and quality control strategies, outlining the main stages and parameters that technically influence reliability and performance.

Devices constructed from nanostructured semiconductors or hybrid organic-inorganic materials entail additional technological challenges, as commonly adopted processes might not be directly applicable or might require some adaptation to take into account the extremely low production yields and the potential toxicity of nanomaterials. Enhanced or devoted testing is also required for novel devices and sensors, which may be evaluated by statistical quality control. In addition to the distinct aspects handled in each technology outlining, some prescription is also offered on possible statistical procedures for determining sensor performance and reliability [298, 299, 300, 301].

Thin-film deposition techniques

The most common thin-film deposition techniques are Physical Vapor Deposition (PVD) and Atomic Layer Deposition (ALD). PVD methods are generally used to prepare thick films, while ALD achieves monolayer control of the deposited film's thickness. In PVD, a thermal or electron-gun evaporator is typically used in conjunction with a metal or dielectric target. When depositing layers on the order of tens of micrometers, the PVD source location has little effect on the film properties. Sufficient distance creates a quasi-isotropic deposition pattern, while getting closer raises the angle of incidence, thereby altering the film texture. The deposition time can exceed the sublimation time for the deposition of thick ALD-contaminated films. The lateral resolution achieved by PVD is limited by the natural mask and the

collocation of the thermal evaporator. The quality of the interface between two adjacent films changes when the growth is not homogeneous; this occurs when the height difference is significant enough to create a shadow. Careful control of the thickness, however, enables the growth mode to be chosen according to the desired characteristics of the film, albeit at the cost of increasing the supply complexity.

ALD originated from research into gas-phase epitaxy. The deposition technique deposits thin films of metals and insulators with atomic precision by performing a continuous sequence of cycles. The basis of atomic layer deposition is to execute sequential half-reactions with good surface mass-transport characteristics so that the reactions may be reversible. To achieve this, gas precursors are introduced by means of a flow controller so that one precursor is present in the reactor chamber at a time. When the deposition of a metal oxide, e.g. aluminum oxide, is required, the two precursors must contain a suitable metal such as aluminum and ligands that enable the deposition of a metal oxide. The surface has active sites, mainly Lewis acid-base pairs, to which the metal-ligand precursor can be adsorbed and bonded. The diamine precursor can fill the pores or valleys of the surface, contributed by the growth of nanostructures. It can therefore be employed to improve the water-repellent property of a surface during anodic coloration [302, 303, 304, 305].

Nanolithography methods

For the synthesis of three-dimensional structures at the nanoscale, traditionally used techniques may not suffice due to the limited resolution. An alternative set of techniques, known as nanolithography, allows the production of micro- and nanostructures over relatively large surface areas. These techniques typically involve the use of masks to define the surface areas to be modified, followed by an appropriate reaction such as etching or depositions. A wide variety of methods are available today, capable of achieving resolutions ranging from nanometers to hundreds of micrometers, depending on the required throughput.

Electron Beam Lithography (EBL) is a serial technique offering high resolution and accurate dimensions down to 1 nm. However, this technique has a very low throughput and cannot be used in combination with materials for which high electron exposure doses lead to disintegration. In addition, the using multiple masks in a back-and-forth pattern generally leads to misalignments. These drawbacks can be circumvented by combining EBL with Nano Imprint Lithography (NIL), a method that achieves high resolution and acceptable throughput by the combination of a master mold made by EBL

and a transfer process, and can also be performed with nanoscale resolution on polymer films. Hot embossing combines the high-resolution stamping step of NIL with a non-polymer template to achieve a technique capable of producing 3D nanostructures in a one-stop process with high throughput. Another approach, known as Focus Ion Beam (FIB) lithography, uses a focused ion beam for direct micromachining or milling of the sample. FIB has the advantages of EBL without its prolonged timescale but is, however, still a rather expensive process. Other methods exist for the synthesis of 3D nanostructures such as two-photon polymerization or two-photon laser sculpturing, but they have other drawbacks that limit their applicability. In addition to surface modification techniques, synthesis methods such as Chemical Vapor Deposition (CVD) or Electrochemical Deposition (ECD) allow for the formation of nanostructures without any modification but are mainly employed in a complementary way [306, 307, 308, 309, 306, 307, 308, 309].

3D microfabrication

Three-dimensional microfabrication is a fundamental technology in the realization of solid-state devices, allowing for architectures that control functionality through microscopic design. At the same time, biological engineering creates demand for complex three-dimensional scaffolding structures. Numerous methods exist for three-dimensional microfabrication, including direct-write techniques, such as laser laser two-photon polymerization or inkjet printing, or subtractive processes that can rapidly fabricate large-scale structures, such as bulk micromachining. In the following, scaffold development for tissue engineering is used as an illustrative example.

A common attempt for uses a “printed circuit board” approach, where a layer of photoresist is exposed, developed, and etched to form the desired geometry, after which the underlying substrate not yet covered by the photoresist is etched again. This approach is limited to 3D structures having simple shapes composed of stacked layers with a slight interlayer misalignment, as made predominantly by SU-8 photoresist, for which an isotropic and rapid etching. The major practical limitation of this method is the incorporation of sacrifice layers to achieve large height structures. One attractive and considerably complementary approach to this type of 3D microfabrication is to combine laser or e-beam lithographic techniques with isotropic etching of sacrificial materials, allowing the fabrication of complex structures in a large surface area. A first layer is used as support, then assisted by the proper deposition of a sacrificial layer beforehand, followed by the completion of the desired features by deposition [310, 311, 312, 313].

Cleanroom processes

Cleanroom environments are essential for producing solid-state devices intended for ionizing radiation applications, together with the ultra-clean recording and electronic elements. The Integrated Circuit (IC) Cleanroom contribution and the Ionizing Radiation Device Test Depart-ment, responsible for testing high-energy radiation sensors, are also housed therein. Semiconductor and sensor technologies require well-defined integrated circuit production and sensor testing cleanrooms to be effective.

IC and sensor technology integrate a large number of active devices, and testing wearable devices requires a high level of integrated electronic performance. Consequently, a high level of cleanliness must be maintained during all sensor and IC fabrication processes. For IC fabrication, Class 10 (1 per cubic foot) particles are required, while for the sensor devices, Class 100 (10 per cubic foot) is acceptable.

Because many of the fabrication processes rely on high-temperature treatments, ultra-lean cleanroom-managed air conditioning is difficult and costly. Therefore, all fabrication processes not requiring high-temperature treatments are performed in a Class 1000 cleanroom located within a large clean area. The Class 1000 area is kept ultra-clean by people who are not directly involved in the active operations. Contamination is minimized by controlling the Class 1000 area cleanliness through the procedures employed for staff entering the area and the way that materials and equipment are taken in and out of the area. Nevertheless, the risk of contamination is always present in a storage or assembly area.

Quality control of semiconductor technology and testing of miniaturized portable electronic elements require a high level of cleanliness, not only for the materials and components used but also for the personnel involved, especially when dealing with upper or lower respiratory infectious agents. The importance of cleanliness, cleanliness control, and the clean environment influence all activities from radiation dosimeter calibration to the testing of medical implantable or wearable elements [314, 315, 316, 317].

Quality control and reliability modeling

Encompass the testing procedures, process control guidelines, and statistical methods to ensure the required reliability of manufactured medical devices. A typical quality control plan comprises an experimental phase to establish the correlation between the test methods and the operative conditions, a tolerance assessment to determine the critical tolerances, and a

statistical-control phase to confirm the reliability of the manufactured devices. The tests can be specific for each type of device, but they must go beyond standard tests needed to comply with regulations.

Statistical control charts allow automatic detection of deviations affecting product quality and pre-emption of possible defects. Frequent testing of reserved quality attributes generates confidence in product reliability. Quality control ensures compliance with the manufacturer's specification but does not guarantee maintaining the same levels during operation. Actually, these levels may decrease with time because of aging effects. Therefore, it is necessary to establish the time evolution of these affections in laboratory conditions, possible aging conditioning systems, and the estimated worst conditions to affect one or more quality invariants.

Reliability estimation considers these aspects by evaluating the mean time to failure of each defined quality invariant based on statistical error propagation for various devices and uses Weibull's law to provide the distribution function of the expected life of the device [318, 319, 320, 321].

Chapter - 16

Future Directions in Solid-State and Nanomaterial-Based Medical Physics

Quantum computing is a potential application for future developments in medical physics data processing. Quantum computers promise to tackle problems solvable inefficiently or not solvable at all by conventional computers. Cryptography is a prominent application area where threats have been identified and novel approaches are underway, including quantum key distribution and post-quantum cryptography (protection against quantum attacks without requiring quantum devices). Concepts such as quantum random number generation may also find application in medical physics.

Future developments might lead to active sensing implantable devices capable of monitoring physiological variations and displacing their identifying structures, such as pacemakers in the case of heartbeats. Limitations are expected from the need to extract energy while retaining sufficient reliability for operation but such active sensing devices must integrate the miniaturization achievable through solid-state and nanomaterial technology with the signal processing and communication capabilities inherent to more recent developments.

Another approach to future developments might consider the concept of personalized nanomedicine, which aims to provide a valid response to the singularity of each individual during diagnosis and therapy using tools or instruments carefully adapted to the biology of the patient. The integration of nanomaterials with the patient's biology and treatment system may be an avenue to fulfill that objective. In some projects, this has aimed at developing cancer treatment with tailored materials to the patient. These systems attempt to obtain good therapeutic efficacy against cancer while at the same time decreasing the side effects and symptoms stemming from the association of conventional radiotherapy with other approaches capable of enhancing the treatment, such as photothermal therapy.

Quantum computing applications

Rapidly advancing quantum computing technologies hold promise in

processing and encrypting large volumes of data generated by modern medical imaging systems. However, the application of quantum computing in medical device design, usage, and data processing remains largely unexplored.

Large medical imaging systems, such as Positron Emission Tomography (PET) and Computer Tomography (CT), generate substantial data volumes, requiring extensive storage capacity and power for processing and distribution. Superposition and entanglement allow quantum computers to perform multiple calculations in parallel, significantly speeding up processing. For instance, Grover's algorithm, designed for searching unsorted databases, can reduce query time complexity from O(N) to O($\sqrt{N}$). Quantum computer development is ongoing worldwide, with scalable quantum processors and control systems becoming increasingly mature, enabling the execution of quantum algorithms and their integration with networking technologies. Companies are developing quantum-optimized hardware to quickly and effortlessly run quantum-enhanced applications tailored for quantum hardware.

Cryptography is a crucial aspect of security, ensuring that no unauthorized party can gain access to sensitive information. Medical imaging involves patient-sensitive data, and any leak could violate patient rights and regulatory requirements. A particular focus is placed on protecting secure traffic from eavesdropping or information stealing. Quantum cryptography leverages quantum mechanics principles for an ideal cryptosystem. Quantum Key Distribution (QKD) exploits the no-cloning theorem, providing a way of establishing a secret key between two distant parties.

Smart implantable devices

Advancing towards the realization of smart implantable devices, several crucial aspects require careful consideration. Firstly, integrating sensing systems capable of monitoring physical parameters of interest using compatible technologies. This entails utilizing biocompatible components without the risk of leaching toxic chemicals or materials that could harm the surrounding tissue. Furthermore, the deterioration of the sensing device over time should be minimized to allow for prolonged use. Secondly, the device must be able to harvest energy from physiological movements, light sources, or external fields without jeopardizing patient safety. Thirdly, detecting and/or controlling any parameter through the implant, ideally using minimally invasive techniques, would enhance the authentication of the device and grant access to stored information. Fourthly, wireless communication should operate over short distances using low-frequency electromagnetic fields to

prevent tissue heating. Fifthly, the implanted device should exhibit a degree of immunity to the body's defense mechanisms so that it can remain in the body for an extended period of time without exogenous removal.

Excessive toxicity to biological systems leads to necrosis, while inferior cytotoxicity can be tolerated. The chemical makeup of the nanomaterial can be adapted to promote a superior interaction and/or a reduced immune response, enabling the materials to be effectively used as contrast agents for *in vivo* imaging. A higher z-attenuation coefficient results in higher X-ray absorption efficiency, reducing the radiation dose necessary for imaging. It is therefore advantageous to use a combination of materials with different nuclear compositions. The regulations for the manufacturing, distribution, and/or marketing of systems in contact with the human body are thorough and demanding. Thus, achieving the desired efficiency from an optical, pharmacological, or therapeutic point of view requires considering these factors from the system development stage.

Personalized nanomedicine systems

Nanomedicine harnesses the properties of nanomaterials or nanoscale systems for diagnosis and therapy. Material properties such as size, porosity, shape, surface structure, and charge influence bioavailability, biodistribution, immune response, and so on. In current research, some groups are dedicating resources towards the application of nanomedicine for personalized medicine: nanomaterials could be specifically tailored and adapted for each patient and disease, maximizing therapeutic effect (for therapy) and/or minimizing side effects. Nanomaterials distance from the ideal configuration may also account for differences in therapeutic efficiency among patients. Personalized medicine entails distinct challenges and ethical considerations, involving the whole process of drug or therapeutic agent production from the selection of its chemical formula (loading drug, enzyme, RNA, DNA, and so forth) to scale-up and manufacturing.

Every individual has a unique proteomic and genomic signature. As a consequence, the safest, most effective drug and the therapeutic strategy with the cleanest reaction are not equally effective for every disease. Cancer therapies at their best still present significant side effects: hair loss, infections, vomiting, nausea, diarrhea, bleeding, anaemia, skin reactions, etc. There is therefore an urgent need for novel drugs, therapeutic strategies and also adjuvants that would minimize these side effects, making the treatment more tolerable, and, if possible, even more effective. The intratumoural heterogeneity often seen in all tumours is responsible for the ineffectiveness

of many of the drugs being used: even if the drug gets to the target, reaches the right dose, and its mechanism is working correctly, resistance can result from the expression or absence of the targeted protein in the other cells of the tumour.

Hybrid organic-inorganic materials

Hybrid organic-inorganic systems combine suitable functions from both classes at the nanoscale and beyond, taking advantage of the low-temperature physical and chemical processing of organic molecules but enabling longer-range interaction like those found in inorganic solids. By combining organic and inorganic components, their unique properties can be designed at will to obtain hybrid materials with controlled functionality and improved performance for various applications. Due to these interactions between dissimilar components, these hybrid systems manifest interesting properties such as Photoluminescence (PL), Second Harmonic Generation (SHG), optical waveguiding, photoconduction, ferromagnetism, and so on.

Generally, organic materials are promising candidates for many applications due to their low cost, lightweight, mechanical flexibility, and ease of processing on substrates. These materials combine traditional semiconductor properties with simple chemical synthesis routes and surface tunability; most importantly, they can be developed by existing polymer-processing technologies. They offer planarity, low thermal conductivity, good phase compatibility with inorganic materials, versatile chemical reactivities, and the possibility to form nanocomposite structures with photoactive organic-based materials.

Translational and clinical implementation challenges

Advancing applications of solid-state and nanomaterial systems in medical physics requires overcoming numerous barriers before widespread clinical adoption. The journey from an exciting laboratory demonstration to the patient is often a long one, with more than a decade usually necessary for new pharmaceutical formulations to receive clinical approval. Translational timelines for implantable devices are even longer, as biocompatibility must be validated both *in vitro* and *in vivo* for each implantation province. Nanomaterials have also raised new concerns, and various national and regional regulatory bodies have introduced classifications, safety testing, and supporting protocols to govern their use in clinical applications. There is now also growing consensus that solid-state and nanomaterial systems should be designed and engineered with consideration of the specific biophysical and biochemical conditions in a patient for successful diagnosis or treatment.

The future will likely require that solid-state devices, in addition to offering robust response characteristics for patients, can also be retrained to behave optimally in the cells of individual patients. This goal will involve adapting material-selective aspects of nanotechnology to the personalized medicine approach and developing methods for classifying and describing personalized solid-state systems for health monitoring. The increasing demand for portable electrics and miniaturized instruments for computerized medical monitoring will also encourage research in medical diagnostic systems integrated in electric or electronic chips. However, while advances will permit such diagnosis to be performed more quickly, more accurately, and with much smaller quantities of analytes than now feasible, the major challenge remains the successful automatic differentiation of whole blood.

Chapter - 17

Conclusions

All devices considered in this work can benefit from a deeper understanding of material properties and processing methods. The properties of solid-state and nanostructured materials at the nanoscale are altered due to a larger surface-to-volume ratio and the increasing relevance of quantum phenomena. Nanostructuring can also facilitate the functionalization of medical devices by means of site-directed conjugation and targeting, possibly enabling the design of stable smart devices with enhanced signals or improved dosimetry. Nanostructured materials have therefore been proposed for use as imaging or drug-delivery agents, allowing the introduction of new imaging modalities based on detections other than brightness or positron emission. Biological composition and nanomaterial concentration need to be accounted for to optimize the signal-to-noise ratio. The integration of clinical data with Monte Carlo models can be a powerful approach for determining the organ doses resulting from nonuniform deposition, and a similar methodology based on pharmacokinetic blood flow can be adopted for calculating the ROS concentration over time and space.

The emergence of quantum technologies opens new opportunities in the blessing and the curse of quantum mechanics. The same effects that may induce decoherence and reduction of T1 and T2 in spin-aided detectors may at the same time introduce a new paradigm based on spin-based sensing or imaging. Emerging applications in responsive biosensing platforms following the natural routes of transduction based on chemical, biological, and optical cues are expected to complete the currently explored possibilities of solid-state nanostructured devices in electromechanical transduction for temperature monitoring or motion tracking. A promising direction aimed at wireless power transfer systems for smart biosensors is also proposed. Nevertheless, these emerging devices implementing new designs with reduced maturity levels embody higher risks of early-stage failure and still have a long way to go toward proper clinical translation.

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