

## Nanoparticles and nanotechnology research

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We would like to welcome you to this new journal (JNR) that has its origin in the significant and growing interest in nanoscale science, engineering and technology. The focus of the journal is on the specific properties, phenomena, and processes that are realized because of the nano size. Experimental and theoretical tools of investigation at nanoscale, as well as synthesis, processing and utilization of particles and related nanostructures are integral parts of this publication.

The overall objective is to disseminate knowledge of the physical, chemical and biological phenomena and processes in structures that have at least one length scale ranging from molecular to approximately 100 nm (or submicron in some situations), and exhibit novel properties because of size. The threshold size is a function of the targeted property and system. Research contributions on nanoparticles, clusters, nanotubes, nanocrystals, nanolayers, and macromolecules surrounded either by gases, liquids or solids, are brought together in this single publication. Generation, assembly, transport phenomena, reactivity, and stability of such structures are considered. Realization and application of structures and systems with novel functions obtained via precursor nanoparticles is emphasized. The content of the journal is at the confluence of various scientific and technological areas, including particle technology, colloids, aerosols, multiphase systems, solid state physics, chemistry and macromolecular science, applied mathematics, materials engineering, pharmacy, microcontamination, emission control, environment and health effects, biotechnology and biomedicine, sensors and electronics. The journal will publish original full papers, brief scientific letters to the editor, and communications on novel technologies and applications. The rapid evolution of

discoveries in this field will require matching via a short publication cycle, particularly of the letters to the editor and brief technical communications.

Nanoparticles are seen either as agents of change of various phenomena and processes, or as building blocks of materials and devices with tailored characteristics. Use of nanoparticles aims to take advantage of properties that are caused by the confinement effects, larger surface area, interactions at length scales where wave phenomena have comparable features to the structural features, and the possibility of generating new atomic and macromolecular structures. Important applications of nanoparticles are in dispersions and coatings, functional nanostructures, consolidated materials, biological systems and environment. Research programs on nanoparticles and nanotechnology around the world suggest different strengths have developed in various countries, a fact that would suggest the need of international collaboration (Siegel et al., 1999; Roco, 1998). This editorial highlights issues in nanoparticle research that are the object of the JNR. The journal was initiated in collaboration with the Nanoparticle Group of the Particle Technology Forum in the US, the Nanoparticle Network in Europe (NANO) and the Society of Cluster Science and Technology in Japan.

### **Nanoparticles – essential component of nanotechnology**

Nanotechnology is concerned with development and utilization of structures and devices with organizational features at the intermediate scale between individual

molecules and about 100 nm where novel properties occur as compared to bulk materials. It implies the capability to build up tailored nanostructures and devices for given functions by control at the atomic and molecular levels. Nanotechnology is recognized as an emerging enabling technology for the 21st century, in addition to the already established areas of information technology and biotechnology. This is because of the scientific convergence of physics, chemistry, biology, materials and engineering at nanoscale, and of the importance of the control of matter at nanoscale on almost all technologies. Nanoparticle manufacturing is an essential component of nanotechnology because the specific properties are realized at the nanoparticle, nanocrystal or nanolayer level, and assembling of precursor particles and related structures is the most generic route to generate nanostructured materials.

Nanoparticles have been empirically synthesized for thousands of years, for example, the generation of carbon black. A fourth century Roman masterpiece, known as the Lycurgus Cup, exhibits the unusual property of dichroism, appearing to be green in the reflected light and red in transmitted light, because of nanometer particles suspended in the glass (Lambert, 1997). It is noticeable that very few nanoparticle synthesis processes have developed their scientific base decades ago, long before other nanotechnology areas have emerged. One finds in this category the pyrolysis process for carbon black and the flame reaction for pigments, particle polymerization techniques, self-assembling of micelles in colloidal suspensions, and chemistry self-assembling. Several kinds of nanoparticles are routinely produced for commercial use via aerosol and colloid reactors in the US, Japan and Europe. The wide range of powder prices is a function of market size, from \$0.5/kg for carbon black and Alumina (each with over 5 Mt/year worldwide market) to about \$1,000/kg for superconductors (about 2 t/year) and Silicon Carbide whiskers (about 1 t/year). Important areas of relevance for nanoparticles and nanotechnology are advanced materials, electronics, biotechnology, pharmaceuticals and sensors. Emerging technologies that have been introduced in the last few years already impact tens of billions of dollars production in the 1998 high tech US industries alone. These include hard disks in computers, photographic systems, dispersions with novel optoelectronic properties, information recording layers, bio-detectors, advanced drug delivery systems, chemical-mechanical polishing, a new generation of lasers, chemical catalysts,

nanoparticle reinforced materials, ink jet systems, colorants, and nanosystems on a chip, to name some of the most important.

Assemblies of nano-particles, droplets, bubbles, fibers and tubes with an interstitial medium are defined here as 'ultradispersions'. This term will mark the difference as compared to ordinary dispersions because of the specific properties and phenomena developed at nanoscale (dispersed phase dimension or interstitial gap).

### Why nanoparticles?

Nanoparticle, crystal and nanolayer manufacturing processes aim to take advantage of four kinds of effects:

- a) *New physical, chemical or biological properties are caused by size scaling.* Smaller particle size determines larger interfacial area, an increased number of molecules on the particle interfaces, quantum electromagnetic interactions, increased surface tension, and size confinement effects (from electronic and optic to confined crystallization and flow structures). The wavelike properties of the electrons inside matter are affected by shape and volume variations on the nanometer scale. Quantum effects become significant for organizational structures under 50 nm, and they manifest even at room temperature if their size is under 10 nm.
- b) *New phenomena are due to size reduction to the point where interaction length scales of physical, chemical and biological phenomena (for instance, the magnetic, laser, photonic, and heat radiation wavelengths) become comparable to the size of the particle, crystal, or respective microstructure grain.* Examples are unusual optoelectronic and magnetic properties of nanostructured materials, changes of color of suspensions with particle size, and placing artificial components inside cells.
- c) *Generation of new atomic, molecular and macromolecular structures of materials by using various routes: chemistry (three-dimensional macromolecular structures, chemical self-assembling), nanofabrication (creating nanostructures on surfaces, manipulation of three-dimensional structures), or biotechnology (evolutionary approach, bio-templating, and three-dimensional molecular folding).*
- d) *Significant increase of the degree of complexity and speed of processes in particulate systems.* Time scales change because of smaller distances and the

increased spectrum of forces with intrinsically short time scales (electrostatic, magnetic, electrophoresis, radiation pressure, others).

Nanoscale phenomena and processes are yet to be understood and the resulting structures to be controlled and manipulated. Critical length and time scales, surface and interface phenomena are essential aspects to be defined. Novel mechanical, optical, electric, magnetic, thermal, chemical and biological properties occur as compared to bulk behavior because of the small structure size and short time scale, but only a small part of these properties have been fully identified and quantified.

### Investigative tools

The nanostructures are difficult to characterize because they are much smaller than visible light wavelengths and significantly larger than individual molecules. Likewise, simulation at the nanoscale is equally difficult, as the structures are mostly too small for continuum treatments and too large for simulations involving individual atoms and molecules. Investigative tools have played a critical role in the advancement of the entire nano field. Besides modeling, simulation and experimental methods, information technology and control theory are increasingly important as we decipher the intimate nature of nanostructures and advance with complex processing techniques. The main research and design tools may be grouped as:

a) *Modeling and simulation of the connection between structure, properties, functions and processing* using atom-based quantum mechanics, molecular dynamics and macromolecular approaches. Use of hierarchical multi-scale modeling and simulation is necessary in order to complement and generalize the increasing body of experimental data and make the connection between fundamentals and applications. Simulations aims to incorporate phenomena at scales from quantum (0.1 nm), molecular (1 nm) and nanoscale macromolecular (10 nm) dimensions, to mesoscale molecular assemblies (100 nm), microscale (1000 nm), and macroscale. A critical aspect is bridging the spatial and temporal scales. Study of multibody interactions combined with simplified molecular dynamics techniques is a possible avenue for an approach to the mesoscale. One may use fractals, statistical mechanics, genetic

and other methods depending on the application. The *ab-initio* methods to calculate electronic transport properties and the semi-empirical electronic structure theories provide insight to the understanding of molecular properties. Interaction force-based molecular dynamics methods provide a way to connect molecular properties to those of the nanoparticle systems (material and thermodynamics properties, flow characteristics).

- b) *Testing and measurement*. There are a wide range of instruments and techniques, from scanning tunneling mapping of surfaces to atomic force chemistry, nuclear chemistry and near-field visualization. Scanning probes and optical and laser-based diagnostic techniques are the most widely applied experimental tools.
- c) *Information technology*, including pattern recognition, molecular organization mechanisms, and nanorobotics. Information on surfaces play a key role in selforganization and selfassembling.
- d) *Reaction pathways and process control*. Such techniques can be used in order to obtain a predetermined structure or function, and integrate the operation of nanosystems with complex architectures.

### Manufacturing processes

A major issue in nanoscale research is how scientific paradigm changes will translate into novel technological processes. Nanoparticle systems, including nanoclusters, -tubes, nanostructured particles, and other three-dimensional nanostructures in the size range between 1 and about 100 nm are seen as tailored precursors for nanostructures materials and devices. Particle processing (sintering, extrusion, plasma activation, selfassembling, etc.) is the most general method of preparation of nanostructured materials and devices. Nanoparticle manufacturing processes may be separated into the following groups:

a) *Nanoparticle synthesis*. At the beginning of any investigation, one is confronted with the selection of the synthesis method, the experimental and simulation techniques to be used, and the choice of materials (metals, ceramics, polymers, organics or carbon-based, composites). The main challenge is relating the final product properties and production rates to the material properties of the precursors and process conditions. The product may be either homogeneous or composite nanostructured

particles, with one or multi chemical species, consolidated or aerogels, including coated and doped particles. The synthesis methods includes precipitation from solutions (colloids), gas condensation (aerosols), chemical, plasma, combustion, spray pyrolysis, laser ablation, supercritical fluid expansion, polymerization, mechanical attrition, molecular selfassembling, hydrodynamic cavitation, and other processes. Particle synthesis at high production rates has been a major research objective in the last few years. Particle nucleation and growth mechanisms are important scientific challenges.

- b) *Processing and conversion of nanoparticles into nanostructured materials (such as advanced ceramics), nanocomponents (such as thin layers), and nanodevices (such as sensors and transistors).* Examples of processing methods include sintering, generation of nanostructures on surfaces, evolutionary biotechnology, and molecular self-organization techniques. Research challenges include continuous particle synthesis and processing into functional nanostructures and devices.
- c) *Utilization of nanoparticles in order to produce or enhance a process or a phenomenon of mechanical, chemical, electrical, magnetic and biological nature.* Examples of the more frequently used manufacturing processes are particle contamination control, chemical vapor deposition, use of particles as agents of surface modification, filtration, mass spectroscopy, bioseparation, combustion pollution control, drug delivery and health diagnostics, and use of nanoparticles as catalysts and pigments in chemical plants. The multiphase transport aspects (particle-fluid and interparticle forces, rheological properties of powders, sorting, mixing, filtration, sintering, assembling, and interaction with external fields, to name a few) and transient aspects (reactions, nanostructure stability issues) have received less attention than the analysis of other physical, chemical and biological aspects.
- d) *Process control and instrumentation aspects.* Important problems include off- and on-line measuring techniques for fine particles and their structures. In parallel with the better established characterization methods for particle size, shape and composition, new instruments are needed to measure particle interaction forces, their roughness, electric, magnetic and thermal properties.

### Aims of this journal

JNR aims to promote the dissemination of original scientific concepts, interdisciplinary research, manufacturing techniques and novel applications in several areas.

- Unique size dependent properties, phenomena, and processes of nano-particle, droplet, bubble, tube, fiber and layer systems.
- Fundamental physical (mechanical, thermal, optical, electronic, etc.), chemical and biological characterization of nanoparticles and their interfaces, and development of *in-situ* and *ex-situ* instrumentation based on new principles for probing properties and phenomena not well understood at the nanometer scale.
- Synthesis and processing of nanoparticles and related nanoprecursor structures, including clusters, aerosol and colloid particles, nanotubes, nanolayers, biological structures and self-assembled systems. Approaches may include gas-, liquid-, solid-, and vacuum-based processes, size reduction, chemical- and bio-selfassembly.
- Modeling and simulation: atom-based quantum mechanics; molecular dynamics; single-particle, multi-body and continuum based models; fractals; other methods suitable for modeling particle synthesis, assembling and interaction processes.
- Utilization of nanoparticle systems for enhancing a phenomenon or process, such as chemical reactions, nano-electronics, nano-ionics, magnetic processes, optical processes, heat transfer, bioseparation, bio- and chemical reactivity.
- Utilization of nanoparticles for generating one- to three- dimensional hierarchical structures by assembling, including functional nanostructures in dispersions, structural materials and electronic devices. JNR will focus on the molecular and multi-particle interaction mechanisms and less on the bulk behavior of nanostructured materials.
- Utilization of nanoparticles for the formulation and the administration of drugs, including drug and gene delivery systems, transport of molecules in biotechnology, and the use of nanoparticles in the field of the diagnosis.
- Presentation of innovative education approaches in the areas of nanoparticles, nanostructures and

nanosystems will be encouraged. Use of a ‘fabric’ of disciplines – physics, chemistry, biology, mathematics, and engineering – is expected in this field. Courses on surface science, molecular dynamics, quantum effects, and manufacturing at molecular scale need to be promoted and disseminated.

We further comment on three areas of interest to this publication.

- a) *Multiphase transport*: Most studies in nanoparticle manufacturing have focused on steady-state chemical, material and biological aspects. However, fundamental transport mechanisms for mass, momentum and heat exhibit particularities as compared to bulk systems and will require further investigation in order to understand particle interactions, nanophase formation, heat and mass transfer at interfaces, and many other basic processes. This implies the study of the system rather than individual grains. The analysis should include basic aspects of multiphase transport processes, such as interaction between phases, rheology, particle settling and fluidization, mixing and segregation, separation, and then move to aerosol or colloidal reactors.
- b) *Nanoscale assembling by design*: The promise of nanotechnology is being realized through the confluence of advances in scientific discovery that has enabled the atomic and molecular control of material building blocks, and engineering that has provided the means to assemble and utilize these tailored building blocks for new processes and devices in a wide variety of applications. Current theoretical understanding and trial-and-error experiments have generated rudimentary nanostructures that cannot be generated ‘by design’, rigorously simulated and measured, generalized or scaled-up. Assembling of atoms, molecules and collections of assemblies of molecules into nanostructures with a defined function by design, under controlled conditions, is a critical component of nanoscale science and technology. There is no generic method or theory of assembling in order to overcome interfacial barriers at different hierarchical levels, from atom and molecules to nanoclusters and larger nanostructure assembling. Possible paths may be the use of electrical fields, magnetic fields, pressure, chemical reactivity, rearrangement before selforganization and surface recognition as in biological systems.

- c) *Biological concepts*: Biological molecules and molecular assemblies have a number of attributes that make them either suitable for direct nanotechnology applications or to be used as models for developing nanostructures. Examples of applications are proteins that fold into precisely defined three-dimensional shapes, and nucleic acids and lipids that assemble according to defined rules. Chemical diversity of these molecules and the different ways in which they can be polymerized or assembled provide a broad range of possible structures. Advances in chemical synthesis and biotechnology will enable one to combine these building blocks to produce new materials and structures that have not yet been observed in nature. The selforganization and selfassembly concepts may be applied to inorganic materials to generate other groups of materials and structures. The use of materials of biological origin or biologically inspired structures, and development at the interfaces with materials science, chemistry, physics and engineering, offer an excellent opportunity for scientific and technological developments. Typical applications are in drug and gene delivery systems, synthesis of bio-compatible materials, templating techniques, membranes for biological separations, molecular computation, opto-electronic devices, molecular motors, bioelectronics, ceramic and biological magnets, and in the longer term bioreplication.

## Remarks

A few nanoparticle synthesis processes have developed their scientific base decades ago, well before other nanotechnology areas have emerged. However, most of the scientific base is currently in development. Research in USA, Japan and Europe is advancing towards developing a suitable infrastructure for nanostructure science and engineering. A variety of nanoparticle manufacturing processes are moving from the basic question that was asked one decade ago ‘what if?’ to new questions ‘how to do it’, ‘at what production rate’ and ‘at what cost?’

While current investigations have focused on the generation of nanoparticles and nanostructures, a shift towards nanoparticle processing and imaginative utilization is noticeable. Future work is expected to expand basic understanding of nanoscale phenomena and mechanisms, combine synthesis and assembling

into functional materials and devices into continuous processes, introduction of new principles of operation for devices, enlarge the use of biological concepts, hierarchical simulation techniques at mesoscale, and development of new experimental tools.

JNR is especially addressed to universities, laboratories and R&D facilities in industry that cover chemistry, materials science, physics, engineering, and biology. Industrial units producing dispersions, chemicals, pharmaceuticals, electronics, miniaturized and biomedical devices and sensors, advanced materials, and defense-related products will benefit from this publication.

The journal encourages submission of interdisciplinary research topics, fast publication of 'letters to the editor' for timely dissemination of scientific breakthroughs ('Brief Communications'), and inclusion of technical reports on novel technologies and nanoparticle applications ('Technology and Applications'). While full scientific papers will constitute the main part of JNR space, the other two sections will allow fast communication between various communities in a very dynamic scientific and technological field. All the papers will be subject to a rigorous peer review. A commentary page called 'Perspectives' written by leaders in the field will be included at the beginning of each issue, and experts will be invited to review new areas of research. The journal will include a section entitled 'Reports' with summaries of recent meetings, research and educational programs, book reviews, and relevant nanotechnology websites.

The excitement of nanoscale research in recent years has brought this field to a roller coaster of discoveries and expectations without an end in sight. We plan to cover such research in JNR by bringing together interdisciplinary research contributions on the basic building components of the nanosystems – the nanoparticles and similar organization features at nanoscale.

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