Application of Computational Nanotechnology in Construction Materials

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Abstract
In this paper, application of nanotechnology in building materials for various civil engineering works is discussed. Since the use of nanotechnology controls the matter at the atomic level, the properties of matter are seriously affected. Strength, durability and other properties of materials are dramatically affected under a scale of nano meter(10-9m).This paper also reveals how the use of nano technology makes concrete more stronger, durable and more easily placed. Different types of nano materials used are discussed with its wide applications.

I. Introduction

Nanotechnology is the use of very small particles of material either by themselves or by their manipulation to create new large scale materials. Nanotechnology is not a new science and it is not a new technology, it is rather an extension of the sciences and technologies that have already been in development for many years. Nanotechnology is the re-engineering of materials by controlling the matter at the atomic level. The key in nanotechnology is the size of particles because the properties of materials are dramatically affected under a scale of nano meter [10-9 meter]. Further, as particles become nano-sized the proportion of atoms on the surface increases relative to those inside and this leads to novel properties. Concrete is stronger, more durable and more easily placed, steel tougher and glass self-cleaning. Increased strength and durability are also a part of the drive to reduce the environmental footprint of the built environment by the efficient use of resources. This is achieved both prior to the construction process by a reduction in pollution during the production of materials (e.g. cement) and also in service, through efficient use of energy due to advancements in insulation. Two nano-sized particles that stand out in their application to construction materials are **titanium dioxide (TiO_2)** and **carbon nanotubes (CNT's)**. The former is being used for its ability to break down dirt or pollution and then allow it to be washed off by rain water on everything from concrete to glass and the latter is being used to strengthen and monitor concrete. Owing to many unique characteristics of nanotechnology derived products, newly developed nano based products can significantly reduce current civil engineering problems. Basically, construction deals with high-tech materials and processes that have been use in construction. Hence, there is huge scope to apply nano technology in construction materials, which can exhibit, probably one of the most prominent, societal impacts.

II. Nanotechnology

Nanotechnology is the use of very small pieces of material by themselves or their manipulation to create new large scale materials. The size of the particles is the critical factor. At the nanoscale (anything from one hundred or more down to a few nanometres, or 10-9m) material properties are altered from that of larger scales. There is a dramatic change in situation and this is what happens at the scale of nanotechnology. Different things start to happen at this level e.g. gravity becomes unimportant, electrostatic forces take over and quantum effects get in. Another important aspect is that, as particles become nano-sized, the proportion of atoms on the surface increases relative to those inside and this leads to change in the properties. Knowledge at the nanoscale of the structure and characteristics of materials (otherwise known as characterization) will promote the development of new applications and new products to repair or improve the properties of construction materials. For example, the structure of the fundamental **calcium-silicate-hydrate (C-S-H) gel** which is responsible for the mechanical and physical properties of cement pastes, including shrinkage, creep, porosity, permeability and elasticity, can be modified to obtain better durability. It is these "nano-effects", however, that ultimately determine all the properties that we are familiar with at our "macro-scale" and this is where the power of nanotechnology comes in. If we can manipulate elements at the nanoscale we can affect the macro-properties and produce significantly new materials and processes.

Types of nano materials:
i) Titanium dioxide (TiO2)
ii) carbon nanotubes (CNT's)
iii) nano silica(ns)
iv) polycarboxilates
v) nano Zro2,etc

III. Application of nano technology in building materials:

Many disciplines of civil engineering including design and construction processes can be benefited from nanotechnology. For example, new structural materials with unique properties, lighter and stronger composites, fire insulator, sound absorber, low maintenance coating, water repellents, nano-clay filled polymers, self-disinfecting surfaces, UN light protector, air cleaners, nano sized sensors, ultra thin-strong- conductive wafers, solar cells etc to name a few. This paper presents, in brief, the areas of application of nanotechnology in civil engineering and the science & technology behind the improved performance. Further, the existing challenges that the scientists and technologists facing towards exploiting the potentiality of nanotechnology is also brought out.

A. Nano technology and concrete:

Concrete is, a macro-material strongly influenced by its nano-properties and understanding it at this new level is yielding new avenues for improvement of strength, durability and monitoring. Much of the analysis of concrete is being done at the nano-level in order to understand its structure using the various techniques developed for study at that scale such as Atomic Force Microscopy (AFM), Scanning Electron Microscopy (SEM) and Focused Ion Beam (FIB). Silica (SiO_2) is present in conventional concrete as part of the normal mix. However, one of the advancements made by the study of concrete at the nano scale is that particle packing in concrete can be improved by using nano-silica which leads to a densifying of the micro and nanostructure resulting in improved mechanical properties. Nano-silica addition to cement based materials can also control the degradation of the fundamental C-S-H (calcium-silicate- hydrate) reaction of concrete caused by calcium leaching in water as well as block water penetration and therefore lead to improvements in durability. Related to improved particle packing, high energy milling of ordinary Portland cement (OPC) clinker and standard sand, produces a greater particle size diminution with respect to conventional OPC and, as a result, the compressive strength of the refined material is also 4 to 6 times higher (at different ages). Another type of nano particle added to concrete to improve its properties is titanium dioxide (TiO_2).TiO_2 is a white pigment and can be used as an excellent reflective coating. It is incorporated, as nano particles and it is added to paints, cements and windows for its sterilizing properties since TiO_2 breaks down organic pollutants, volatile organic compounds and bacterial membranes through powerful catalytic reactions. It can therefore reduce airborne pollutants when applied to outdoor surfaces. Additionally, it is hydrophilic and therefore

gives self cleaning properties to surfaces to which it is applied. The process by which this occurs is that rain water is attracted to the surface and forms sheets which collect the pollutants and dirt particles previously broken down and washes them off. The resulting concrete, already used in projects around the world, has a white colour that retains its whiteness very effectively unlike the stained buildings of the material's pioneering past.

A further type of nanoparticle, which has remarkable properties, is the carbon nano tube (CNT) and current research is being carried out to investigate the benefits of adding CNT's to concrete. Carbon nanotubes are a form of carbon that was first discovered in Russia but came into use in the late ninety's in Japan. They are cylindrical in shape, as shown in figure below, and their name comes from their nanometre diameter. They can be several millimetres in length and can have one "layer" or wall (single walled nanotube) or more than one wall (multi walled nanotube). They have 5 times the Young's modulus and 8 times (theoretically 100 times) the strength of steel while being 1/6th the density. The addition of small amounts (1% wt) of CNT's can improve the mechanical properties of samples consisting of the main Portland cement phase and water. Oxidized multi-walled nanotubes (MWNT's) show the best improvements both in compressive strength (+ 25 N/mm2) and flexural strength (+ 8 N/mm) compared to the reference samples without the reinforcement. It is theorized the high defect concentration on the surface of the oxidized MWNTs could lead to a better linkage between the nanostructures and the binder thus improving the mechanical properties of the composite rather like the deformations on reinforcing bars.

In fact, even some of the rules in structural concrete design are actually empirically derived from observed behaviour Nanotechnology, involving the study of the fundamental components of concrete can lead the way to a real understanding of concrete construction and service life based on a designed material with predetermined properties. This is strongly related to the study of service life through multiscale modelling (covering multiple dimensional scales such as from nm to m). As an example of the kind of additions that have been made to concrete, research has shown that an anaerobic (one that does not require oxygen) microorganism incorporated into concrete mixing water results in a 25% increase in 28-day strength. The **Shewanella microorganism** was used at a concentration of 105 cells/ml and nanoscale observations revealed that there was a deposition of sand-cement matrix on its surface. This led to the growth of filler material within the pores of the cement- sand matrix and resulted in increased strength.

Self Compacting Concrete (SCC) is one that does not need vibration in order to level off and achieve consolidation. This represents a significant advance in the reduction of the energy needed to build concrete structures and is therefore a sustainability issue. In addition SCC can offer benefits of up to 50% in labour costs, due to it being poured up to 80% faster and having reduced wear and tear on formwork. The material behaves like a thick fluid and is made possible by the use of **polycarboxylates** (a material similar to plastic developed using nanotechnology). SCC mixes, which contain a high content of fine particles, need a very effective dispersing system in order to be fluid and workable overtime at low water/cement ratio (high W/C ratios would lead to risk of segregation) and only polycarboxylates can meet these requirements. In addition, while long term strengths of conventionally super plasticized concrete are very high, the very early strengths, especially in winter, are not high enough for a quick and safe removal of formwork and steam curing is therefore used to accelerate the hydration of cement. This can be eliminated in the precast industry through the use of the latest generations of polycarboxylates resulting in further time and energy savings.

Finally, fibre wrapping of concrete is quite common today for increasing the strength of pre- existing concrete structural elements. Advancement in the procedure involves the use of a **fibre sheet (matrix)** containing nano-silica particles and hardeners. These nanoparticles penetrate and close small cracks on the concrete surface and, in strengthening applications, the matrices form a strong bond between the surface of the concrete and the fibre reinforcement. In the strengthening process pre-cut carbon tows (fibres) and sheets impregnated with the matrix are placed on the prepared concrete surface and bonded using grooved rollers. The ability of the samples to sustain load after cracking is greatly improved by the carbon tows and both the matrix and the interface are durable under wetting and drying and scaling (scraping) conditions. Additionally, there is no decrease in the maximum load capacity after repeated cycles of wetting and drying or scaling.

B. Nanotechnology and Steel

Steel has been widely available since the second industrial revolution in the late part of the 19th and early part of the 20th Century and has played a major part in the construction industry since that time. Fatigue is a significant issue that can lead to the structural failure of steel subject to cyclic loading, such as in bridges or towers. This can happen at stresses significantly lower than the yield stress of the material and lead to a significant shortening of useful life of the structure. The current design philosophy entails one or more of three limiting measures: a design based on a dramatic reduction in the allowable stress, a shortened allowable service life or the need for a regular inspection regime. **Stress risers** are responsible for initiating cracks from which fatigue failure results and research has shown that the addition of **copper nanoparticles** reduces the surface unevenness of steel which then limits the number of stress risers and hence fatigue cracking. Advancements in this technology would lead to increased safety, less need for monitoring and more efficient materials use in construction prone to fatigue issues.

Welds and the Heat Affected Zone (HAZ) adjacent to welds can be brittle and fail without warning when subjected to sudden dynamic loading, and weld toughness is a significant issue especially in zones of high seismic activity. Weld and HAZ failures led to the re-evaluation of welded structural joints in the aftermath of the 1994 Northridge earthquake in the Los Angeles area and current design philosophies include selective weakening of structures to produce controlled deformation away from brittle welded joints or the deliberate over-sizing of structures to keep all stresses low. Research currently under way, however, has shown that the addition of nanoparticles of magnesium and calcium makes the HAZ grains finer (about 1/5the size of conventional material) in plate steel and this leads to an increase in weld toughness. This is sustainability as well as a safety issue, as an increase in toughness at welded joints would result in a smaller resource requirement because less material is required in order to keep stresses within allowable limits.

Two relatively new products that are available today are **Sandvik Nanoflex** and **MMFX2** steel .Both are corrosion resistant, but have different mechanical properties and are the result of different applications of nano technology. Traditionally, the trade off between steel strength and ductility is a significant issue for steel; the forces in modern construction require high strength, whereas safety (especially in seismic areas) and stress redistribution require high ductility. This has led to the use of low strength ductile material in larger sizes than would otherwise be possible with high strength brittle material and consequently it is an issue of sustainability and efficient use of resources. **Sandvik Nanoflex** has both the desirable qualities of a high Young's Modulus and high strength and it is also resistant to corrosion due to the presence of very hard nanometre-sized particles in the steel matrix. It effectively matches high strength with exceptional formability and currently it is being used in the production of parts as diverse as medical instruments and bicycle components, however, its applications are growing. The use of stainless steel reinforcement in concrete structures has normally been limited to high risk environments as its use is cost prohibitive. However, MMFX2 steel, while having the mechanical properties of conventional steel, has a modified nano-structure that makes it corrosion resistant and it is an alternative to conventional stainless steel, but at a lower cost.

C. Nanotechnology and Wood

Carbon nanotubes are a new discovery, whereas wood is an ancient material which has been used since the dawn of civilization. However, perhaps not surprisingly given nature's evolutionary process, wood is also composed of nanotubes or **"nanofibrils"; namely**, **lignocellulosic (woody tissue)** elements which are twice as strong as nanofibrils would lead to a new paradigm in sustainable construction as both the production and use would be part of a renewable cycle. Some developers have speculated that building functionality onto lignocellulosic surfaces at the nano scale could open new opportunities for such things as self-sterilizing surfaces, internal self-repair, and electronic lignocellulosic devices. Due to its natural origins, wood is leading the way in cross-disciplinary research and modelling techniques. Firstly, BASF have developed a highly water repellent coating based on the actions of the lotus leaf as a result of the incorporation of silica and alumina nano particles and hydrophobic polymers. And, secondly, mechanical studies of bones have been adapted to model wood, for instance in the drying process.

D. Nano technology in waterproofing building materials

Waterproofing of building materials has been a problem since last 1000 years. The problem has not been addressed completely due to lack of understanding at nano level of the building material. The new development in science & technology has allowed using the latest nano technology to produce eco-friendly **Organo-Silicon products** to waterproof practically all the different kinds of building materials. The nano technology has ensured that service life of this approach will lead to life cycles beyond 20 to 30 years at very economical cost. Building materials are known to have water seepage, water leakages due to inherent porosity and micro cracks. Waterproofing is a treatment, which is expected to make the material impervious to water. Lots of technology and product development has taken place in various waterproofing products for the last 50 years, particularly using polymeric backbone and variety of other materials. Another serious issue waterproofing addresses is to prevent loss of structural strength of concrete building materials, particularly due to ASR (alkali silica reaction), acid rain, sulphate attacked. It also prevents chloride penetration which can result in corrosion of the reinforced steel bars.

a). Water related problems: Most of the building materials are very porous and have **surface hydroxyl groups**. These hydroxyl groups attract water because of the hydrophilic nature and similarity with the structure of water. Therefore, most of the building material easily wet and absorb water in the pores. The size of the water molecule is 0.18 nm (i.e. 0.00018 microns).The size of the pores in most of the building materials, range from 5 to 200 nm. The size of most of the pollutants like acids, chlorides & sulphates would range between 1 to 2 nm. Even with the dense concrete and stones the pore size is much larger than water allowing easy entry with the hydrophilic nature of the building material. The essential requirements waterproofing materials are

- Resistance it can impart to water absorption.
- Preventing of water soluble salts, particularly chloride salts.
- Penetration of waterproofing treatment to a measurable depth.
- Non-staining of treated surface areas.
- Long-term stability in an alkaline environment.
- Low environmental and health risk.
- UV stability (20+ years).

There are two classes of waterproofing products:

a). Film Formers

b). Penetrants

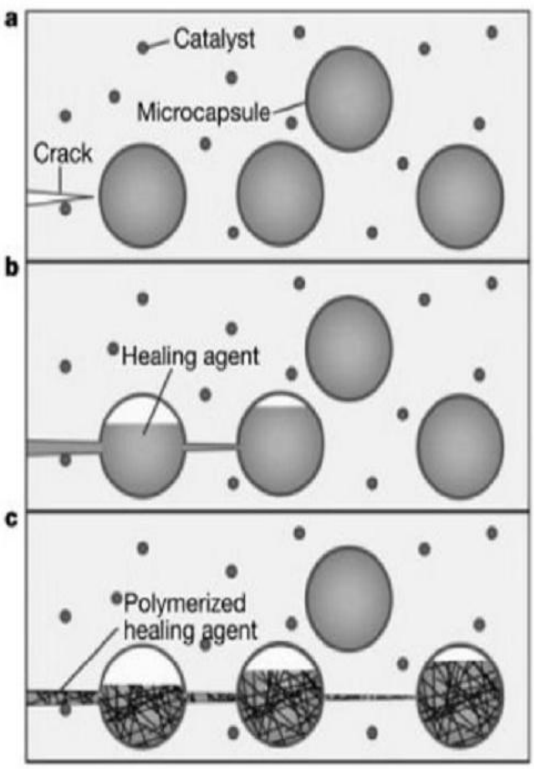
Film Formers: The economics and the ease of application have led to widespread use of film forming water repellents. The products like acrylic paint, silicon polymers are commonly used in the world for waterproofing application. These film formers have particle size greater than 100 nm, which will not allow them to penetrate inside the pores of the building materials but form a film covering and preventing the surface from water absorption. Generally, these polymer films are hydrophobic but they need to be continuous and defect-free and also must be UV resistant. It is found that during application ensuring continuous film on rough surface is not easy which leads to weak points for film former. All the typical polymer films tend to break down under UV leading to cracking of the films in 2-5 years, which leads to failure in terms of losing of hydrophobicity and water repellency.

Penetrants: Most penetrants are solvent based, soluble monomeric material with less than 6nm size. They easily penetrate inside the pores and sub-branches of the pores. There are two types of penetrants i.e. **non reactive and reactive**. Non-reactive penetrants are oils and other low viscosity hydrophobic material, which coats the pore of the substrates, and provide water repellency. However, these types of materials are also biodegradable and loose hydrophobicity within a year. Additionally, these products also provide food for mold or fungus growth. The reactive penetrants chemically react with the substrate and provide molecular level hydrophobicity to the treated surface and 3-5mm deep in the substrate. Therefore, these types of waterproofing products provide protection for a very long period. Additionally, the product is bound chemically on a molecular level to the substrate as a result; weathering (UV radiation) and natural abrasion have virtually no effect and hence very limited effect on the waterproofing characteristics.

Experimentally it has been seen that **Silane** based waterproofing products are desirable for long-term performance. Silanes and Silane/Siloxanes are known as new class of waterproofing products. These products are used in USA and Europe for last 30 years. However only last few years they became available in India. The solvent based silane waterproofing compounds are proven to provide long lasting performance and are used very widely in USA and Europe. The various alkyl silanes that are used for waterproofing are (i) isobutyltrialkoxysilane (ii) n-octyltrialkoxysilane. Silanes are monomeric materials. The products used for waterproofing are known as alkylalkoxysilane. Most building materials contains hydroxyl (OH) group. These OH groups can chemically react with alkoxy groups of Silane forming permanent siloxanes bonds with the substrate. The alkyl group R' provides hydrophobicity (water repellency) to the surface. Therefore, these types of products impart water repellency by modifying surface characteristics from hydrophilic to hydrophobic.

E. Nano technology and self healing concrete:

Experimentation is also underway on self-healing concrete. When self-healing concrete cracks, embedded microcapsules rupture and release a healing agent into the damaged region through capillary action. The released healing agent contacts an embedded catalyst, polymerizing to bond the crack face closed. In fracture tests, self-healed composites recovered as much as 75 percent of their original strength. They could increase the life of structural components by as much as two or three times. When cracks form in this self-healing concrete, they rupture microcapsules, releasing a healing agent which then contacts a catalyst, triggering polymerization that bonds the crack closed fig2.



Fi g2: Mechanism of self healing concrete

IV. Strength comparisons

The compressive strength results of series C0 and N mixtures are shown in table 1 Comparison of the results from the 7, 28 and 90 days samples shows that the compressive strength increases with nano-ZrO2 particles chemical up to 1.0% replacement (N2) and then it decreases, although the results of 2.0% replacement (N4) is still higher than those of the plain cement concrete (C0). It was shown that the use of 2.0% nano-ZrO2 particles decreases the compressive strength to a value which is near to the control concrete. This may be due to the fact that the quantity of nano-ZrO2 particles (pozzolan) present in the mix is higher than the amount required to combine with the liberated lime during the process of hydration thus leading to excess silica leaching out and causing a deficiency in strength as it replaces part of the cementitous material but does not contribute to strength. Also, it may be due to the defects generated in dispersion of nanoparticles that causes weak zones.

Sample designation	Nano ZrO_2 Particle (%)	Compressive strength(Mpa)		
		7 days	28 days	91 days
C0	0	27.3	36.8	42.3
N1	0.5	31.6	42.7	46.5
N2	1.0	33.1	43.6	48.1
N3	1.5	32.2	42.9	47.7
N4	2.0	28.5	39.7	44.3

Table 1: compressive strength results of series C0 and N mixtures

V. Nano technology and green building

Nanotechnology, the manipulation of matter at the molecular scale, is bringing new materials and new possibilities to industries as diverse as electronics, medicine, energy and aeronautics. Our ability to design new materials from the bottom up is impacting the building industry as well. New materials and products based on nanotechnology can be found in building insulation, coatings, and solar technologies. Work now underway in nanotech labs will soon result in new products for lighting, structures, and energy. In the building industry, nanotechnology has already brought to market self-cleaning windows, smog-eating concrete, and many other advances. But these advances and currently available products are minor compared to those incubating in the world's nanotech labs today. There, work is underway on illuminating walls that change colour with the flip of a switch, nanocomposites as thin as glass yet capable of supporting entire buildings, and photosynthetic surfaces making any building facade a source of free energy.

VI. Concluding remarks and Perspectives for the Future.

The application of nanotechnology in construction presents a myriad of opportunities and challenges. The use of micro nano materials (MNMs) in the construction industry should be considered not only for enhancing material properties and functions but also in the context of energy conservation. This is a particularly important prospect since a high percentage of all energy used) is consumed by commercial buildings and residential houses (including heating, lighting, and air conditioning). Opportunities for energy savings (other than using MNMs to harvest solar or other forms of renewable energy) include improved thermal management by using silica nano particles in insulating ceramics and paint/coating that enable energy conservation and solar-powered self-cleaning nano-TiO2-coated surfaces. Additional opportunities include the use of QDs and CNTs to improve the efficiency of energy transmission, lighting, and or heating devices, as well as incorporation of fullerenes and graphene to enhance energy storage systems such as batteries and capacitors that harvest energy from intermittent, renewable sources (e.g., solar and wind).Furthermore, MNMs that extend the durability of structures (e.g., through enhanced resistance to corrosion, fatigue, wear, and abrasion)also contribute indirectly to saving energy that would otherwise be used to repair or replace deteriorated infrastructure. MNMs can also contribute to a greener construction industry when used as substitutes for materials that can become harmful environmental pollutants, such as lead and mercury. In addition to prevention of potential exposure and resulting hazardous impacts, such replacement facilitates handling and waste management. MNMs as proxy additives include iron oxide nano particles for lead (as pigment) in paint and silica nano particles for polychlorinated biphenyl (PCB) insulators in electrical devices. Contamination due to disposal of mercury containing devices, such as fluorescent bulbs, flow meters, pressure gauges, and thermostats, can be mitigated by using QD-based light-emitting diodes (LEDs) and CNT or ZnO nanowire-based sensors. As new materials are designed and brought into use, it is important to understand their potential mobility and impacts in and across air, water, soil, and biota. Advanced analytical capabilities are among the first priorities to detect and characterize MNMs (released from or incorporated into construction materials) at environmentally relevant concentrations within the complex environmental and biological matrices. Environmentally responsible lifecycle engineering of MNMs in construction also needs to be prioritized. Overall, beyond the current excitement about the possibilities of MNMs to enhance our infrastructure, there are reasonable concerns about unintended consequences. This underscores the need to support research into safe design, production, use, and disposal practices and associated recycling, reuse, and remanufacturing initiatives that enhance the sustainability of both the nanotechnology and construction industries.

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