Diamond at the nanoscale: applications of diamond nanoparticles from cellular biomarkers to quantum computing

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Although nanocrystalline diamond powders have been produced in industrial quantities, mainly by detonation synthesis, for many decades their use in applications other than traditional polishing and grinding have been limited, until recently. This paper presents the wide-ranging applications of nanodiamond particles to date and discusses future research directions in this field. Owing to the recent commercial availability of these powders and the present interest in nanotechnology, one can predict a huge increase in research with these materials in the very near future. However, to fully exploit these materials, fundamental as well as applied research is required to understand the transition between bulk and surface properties as the size of particles decreases.

Keywords: diamond; nanoparticles; applications

1. Introduction

More than 40 years ago, researchers in the USSR found that diamond nanoparticles were formed as a product of the detonation of carbon-based explosives (Danilenko 2004). For several reasons, including the security measures in place in the USSR and a lack of industrial interest in nanotechnology at the time, the application of this nanodiamond (ND) remained unreported and under-exploited until very recently. However, there has been a clear upturn in interest in the use of ND particles in a wide range of applications in the past few years. Preliminary reports of the use of ND in fields as diverse as catalysis, quantum computing and biology appear to indicate a field on the brink of massive expansion. Other examples of ND application can be found in the formation of hard coatings and composites, polishing and seeding of substrates for chemical vapour deposition (CVD) diamond growth.

Efforts to create diamond synthetically date back many years and have resulted in gemstone quality diamond being commercially available through high-temperature and high-pressure treatment of carbon-based materials. In addition, high-temperature and low-pressure conditions available through CVD have enabled the growth of diamond coatings using a gas-feed mixture of hydrogen and methane. Growth conditions of such films can be tailored to produce micro- or

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nanocrystalline morphology and dopants such as boron added to induce conductivity. Diamond particles of size similar to detonation ND have been discovered in interstellar dust and primitive meteorites, which are believed to be formed from the condensation of primary carbon particles to form diamond as a metastable phase (Lewis et al. 1987). While all of the above examples of diamond synthesis are interesting in themselves, this paper will focus on the properties and applications of ND particles formed through detonation (variously referred to in the literature as detonation ND, ultradispersed diamond and nanocrystalline diamond powder). Some of the applications outlined in the following sections make use of ND particles produced by other methods, but they have been included in this paper as it is anticipated that detonation ND could be similarly exploited.

2. Synthesis of detonation ND

Figure 1 shows the phase diagram for carbon, showing that diamond is metastable at room temperature and pressure. However, the detonation of carbon-containing explosives at high temperature and pressure with a negative oxygen balance results in the condensation of the free atomic carbon products as diamond or liquid carbon. Theoretical calculations show that conditions for diamond stability during this process are only conserved for a very short time (sub-microsecond) and are closely followed by conditions where graphite is the more stable phase (Dolmatov et al. 2004). This is due to a fast decrease in pressure while the system is still at a high temperature, which favours a
To obtain diamond, it is therefore important to control the rate at which the system cools—faster cooling at relatively high pressure results in a higher diamond yield.

The most commonly used explosives for this process are mixtures of trinitrotoluene (TNT) and hexogen or octogen. Explosion commonly takes place in a sealed stainless steel chamber in the absence of oxygen. Diamond yield increases with the quantity of coolant present in the system; gases such as argon are commonly used, as well as water, water-based foams and ice. Optimal cooling rates after detonation are found to be 3000–4000 K min\(^{-1}\). The products of detonation are a complex mix of ND particles of an average size of 5 nm and other graphitic carbon forms, hence rigorous cleaning stages are then employed to remove the non-diamond material. The extent and method of cleaning depends on the source of the ND powder, but generally includes either gaseous ozone treatment or solution-phase nitric acid oxidation to remove sp\(^2\) carbon and metallic impurities. Generally, commercial detonation ND powders contain up to 98% diamond in the form of 2–10 nm particles with very small amounts of sp\(^2\) impurity.

3. Structure and chemistry of ND particles

Figure 2\(a\) shows a transmission electron microscopic (TEM) image of commercially available 5 nm ND powder. The powder contains diamond particles of very narrow size distribution averaging 5 nm but, as is clear from the image, the particles readily agglomerate to form aggregates up to several micrometres in dimension. Most detonation ND powders contain particles of less than 10 nm and theoretical studies have postulated that this is because diamond particles are in fact more stable than graphite clusters in this size range (Badziag et al. 1989). X-ray and neutron diffraction measurements as well as high-resolution TEM (Kulakova 2004) have confirmed that the core of these nanoparticles is an sp\(^3\)-bonded diamond lattice.

The exact nature of the outer layer remains unclear, but two general models have emerged: (i) an amorphous shell with significant sp\(^2\) carbon content or (ii) an sp\(^2\) graphene-type sheet, of a fullerene structure, giving rise to a structure described as ‘bucky-diamond’. The latter model is at present largely theoretical (Raty & Galli 2003); however, heating ND particles to above 1000 K in vacuum does result in laminates of fullerene shells being formed around the diamond core and ultimately to the formation of ‘carbon onions’. Experimental evidence including Auger spectroscopy, Raman spectroscopy and XPS confirms that the outer shell does have some sp\(^2\) character (Demnt’ev & Maslakov 2004); however, it is probable that the composition (thickness, sp\(^2\)/sp\(^3\) ratio and atomic arrangement) will depend very strongly on the cooling conditions employed during synthesis (Kulakova 2004). Based on the analysis of large-Q neutron diffraction measurements, Palosz et al. (2006) postulated that ND consists of an ordered diamond lattice core, surrounded by a shell of compressed diamond, which is enveloped in a non-crystalline shell of ‘gas-like’ carbon; probably, with a mixture of sp\(^2\) and sp\(^3\) bonding. This model is illustrated in figure 2\(b\).

The chemical composition of detonation ND is found by XPS to be mainly carbon, with approximately 10–20 at% oxygen and 2–3 at% nitrogen. Owing to the oxidative cleaning processes, most surface carbon atoms are terminated with...
oxygen moieties, such as hydroxyl and carbonyl, as confirmed by FTIR spectroscopy. Understanding the chemistry of these surface functionalities as well as the nature of the outer shell of the ND is a key to unlocking the potential of this material for the outlined applications.

The nature of the bonding sites of nitrogen in ND is still the subject of debate; in some studies, FTIR spectroscopy has shown the presence of NH₂ groups on the surface of the ND, while others demonstrate that nitrogen atoms are only present within the core of the ND. It is probable that nitrogen groups present on the surface have been introduced during the acid cleaning stage, whereas...

Figure 2. (a) Transmission electron microscopic (TEM) image of commercial 5 nm detonation ND powder (from Shenzhen Jingangyuan New Material Co., PR China), drop-coated from ethanol onto a TEM grid, using JEOL 100CX TEM. (b) Schematic of a tentative model for a structure of 5 nm detonation ND (adapted from Palosz et al. (2006)). The figure is not drawn to scale.
substitutional core nitrogen impurities come about during the detonation process, as nitrogen is a component of most explosives used. Simulations have predicted that nitrogen is metastable within the core of ND but that surface sites are preferred (Barnard & Sternberg 2007). Practically, it is becoming increasingly important to determine the actual binding sites of nitrogen in order to exploit ND in two important applications: use as qubits in quantum computing and as fluorescent probes for biological imaging.

4. Processing of ND powders to monodisperse solutions

As noted previously, ND powders show a very strong tendency to agglomerate; therefore, many of the applications described in this paper make use of core aggregates of the particles of approximately 100–200 nm, rather than isolated 5 nm particles. The unusually tight aggregation in detonation ND and methods to produce solutions of monodisperse 5 nm particles was first described by Osawa and co-workers (Krüger et al. 2005). According to the analysis using dynamic light scattering ND consisted of aggregates of three discrete sizes: 100–200 nm, 2–3 μm and 20–30 μm, but no particles of size 3–10 nm corresponding to isolated ND particles could be identified. Powerful sonication was able to produce a monodisperse solution with an average particle size of 120 nm, but these core aggregates are remarkably stable and cannot be broken down any further using this method. Stirred-media milling with ceramic beads (0.1 mm in diameter) was therefore successfully used to break down the core agglomerates into the primary ND particles. The ND slurries were turned into a turbid, dark-coloured and increasingly viscous suspension and, remarkably, once the milled slurries were diluted and subjected to ultrasound, the solution turned completely clear as the core aggregates disintegrated to form colloids of primary 5 nm particles. This methodology allows a much greater range of ND applications to be realized as individual 5 nm particles can now be addressed, as well as the aggregates.

5. Optical properties of ND

One of the attractive properties of ND is its ability to fluoresce when excited with light of ultraviolet wavelength (< 400 nm; Aleksenskii et al. 2001). It will also emit when excited by multiphoton excitation at longer wavelengths (Glinka et al. 1999). The emission of 5 nm detonation diamond is dominated by a broad band in the visible region, from 390 to 650 nm (Kompan et al. 1997). The mechanism of photoluminescence has been variously assigned to the emission from impurity sites (e.g. dopants) within the core, defects in the diamond lattice or sp² clusters on the ND surface. To illustrate some of these processes, the energy transitions are shown in figure 3. Some lower energy (red) emissions were found to vary between ND samples and also to decrease after heating, indicating an association with the amount of sp² carbon on the surface of the ND. However, when thicker layers of graphite were formed on the surface, photoluminescence intensity was found to decrease dramatically, demonstrating that graphite itself was not responsible for this emission and it was conjectured that sp² clusters embedded in a sp³ matrix may be responsible (Glinka et al. 1999).
Another ND fluorescence process of note is that resulting from excitation of the negatively charged nitrogen–vacancy (N–V) centre, which absorbs strongly at 560 nm and emits efficiently at 700 nm (red; figure 3). This type of fluorescence has been reported in synthetic type 1b (nitrogen-containing) diamond particles of 35 and 100 nm that have been irradiation damaged to create defects (Yu et al. 2005). Irradiation with an electron beam creates a vacancy in the lattice and the sample is then annealed to bring the vacancy close to the nitrogen atom; this (N–V) centre acts as an ion embedded in a solid matrix. As this fluorescence arises from defects deep within the ND core, it is unaffected by the surface chemistry of the ND. These irradiated ND particles have been used as cellular biomarkers, as will be discussed further in §7.

6. Surface modification of ND

The surface of most commercially available ND is highly oxidized containing different functional groups, including hydroxyl, carboxyl, lactone and ketone. The nature of these groups, and also the presence of remaining sp² carbon, strongly influences the stability of the individual ND particles in solution, leading to agglomeration into larger aggregates. It is therefore desirable to modify the surface groups of ND for several reasons: for better solubility in different solvents; to reduce or prevent agglomeration, hence ND is present as isolated 5 nm particles; and to introduce surface functionalities to allow its use in various applications. A significant amount of the literature on this material to date has been concerned with the mechanical (ultrasound and ball milling) and chemical means of reducing agglomerate size and adding functionalities to the resulting particles.

Osswald et al. (2006) employed a simple method of heating ND powder in air at 400–430°C to remove sp² carbon impurities. This narrow temperature range was chosen as it allows maximum oxidation of sp² carbon with minimal
loss of diamond. This results in a highly oxidized, but predominantly $sp^3$, product that can be hydrogenated to remove the surface oxygen and introduce hydrogen termination. Reaction of ND with a gaseous fluorine and hydrogen mixture at 150–470°C results in a high degree of covalent surface fluorination, as described by Liu et al. (2004). Fluorinated ND can be used as a precursor for further functionalization using alkyl-lithium reagents, diamines and amino acids (see figure 4 and scheme 1). In addition to improving solubility in polar organic solvents, like ethanol, the chemical modification allows other applications to be explored. Krüger et al. (2006) took another route towards the modification of ND for biological applications, by homogenizing surface termination by reduction of all of the surface oxygen groups to hydroxyl, using borane in THF. Silane-linker molecules were then used to form an amine-terminated surface, which could be further functionalized by direct synthesis of peptides onto the surface (figure 4, scheme 2). This type of functionalization is potentially useful for introducing ND into cells to interact with specific cellular components for targeted drug delivery. ND particles have also been terminated with polymer brushes (Li et al. 2006), which improved solubility and tailored hydrophilic/hydrophobic properties of the nanoparticle. A radical initiator was covalently attached to oxidized ND particles, via an ester linkage, to initiate growth via atom transfer radical polymerization of methacrylate monomers (see figure 4 and scheme 3).

The above examples make use of covalent bonding strategies to modify the ND particles; however, there are also several examples of electrostatic approaches to functionalization, especially for proteins and biological moieties. The protein lysozyme was physisorbed onto the oxidized (carboxylated) ND surface (Chung et al. 2006) and its adsorption was monitored by FTIR spectroscopy. Strong uptake was noted until saturation and strong binding was observed even after washing, due to interaction of the positively charged amine groups of the protein with the negative carboxyl groups of the ND. Other proteins with amine groups can be directly adsorbed onto ND in a similar fashion, as described for poly-L-lysine, cytochrome $c$, myoglobin and bovine serum albumin (Huang & Chang 2004). The same principle can be used to form a self-assembled monolayer of ND onto an amine-modified surface, which can then be further functionalized for potential applications as a biosensor or biochip (Guan et al. 2006).

7. Biological applications of ND

There are many potential biological and medical applications of ND, including its use in biocompatible composites and implants, targeted drug delivery, components of biosensors and stable solid supports for the synthesis of peptides. Some of the surface modification discussed above was carried out with a view to examine these applications. To date, there have been reports of the use of ND in three main biological applications: immobilization of proteins for purification, separation or further analysis; use as a delivery vehicle to introduce biological moieties into cells; and use as a fluorescent marker for cell imaging.

Bondar et al. (2004) demonstrated the use of detonation ND to separate recombinant proteins from *Escherichia coli* using physical adsorption of the protein onto the ND particles (figure 5). The cells were disrupted using ultrasound and the cell debris was removed through centrifugation. Suspended
ND was then added to the solution containing the recombinant protein, stirred and then sedimented using centrifugation. The sediment was then removed from the solution and washed to remove any unadsorbed protein. Finally, the

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ND–protein complex was treated with a buffer containing dithiothreitol, which caused desorption of the protein from the ND. High degrees of purity for the recovered proteins were noted, with yields from 35 to 60%, and the whole separation procedure took 30 min in contrast to the traditional purification by chromatographic means, which took several days.

The same principles have been used to capture proteins for the analysis by mass spectrometry (Kong et al. 2005a, b). The affinity of ND for protein adsorption allows very dilute solution of proteins to be analysed, as they adsorb to ND and so become preconcentrated. The ND–protein complex can then be separated from the solution by centrifugation and directly analysed by matrix-assisted laser desorption/ionization (MALDI) time of flight (TOF) mass spectrometry, where an enhancement in sensitivity of more than two orders of magnitude is reported. The adsorbed protein molecules do not need to be separated from the ND prior to mass spectrometry analysis. The technique was demonstrated in a clinical proteomics application, with the analysis of human blood serum for biomarkers indicating disease. Using the ND, results were obtained that which were up to 10-fold more sensitive and richer in spectral features than existing techniques. The same authors used very similar procedures to perform MALDI-TOF mass spectrometric analysis of DNA oligonucleotides (Kong et al. 2005a, b). In this case, they first modified the ND with poly-L-lysine by electrostatic attachment, which then forms stable complexes with DNA oligonucleotides. Again, no pre-separation of poly-L-lysine or DNA was necessary prior to mass spectrometry analysis.
Perhaps the most exciting developments in biological ND research are those involving the uptake of ND by living cells. Kossovsky et al. (1995) used ND coated with a disaccharide to immobilize an antigen, which was then directly injected into rabbits to elicit an immune response. This method of antigen delivery was found to result in a strong and specific immune response to mussel adhesive protein, in contrast to alternative, traditional delivery methods that produce only a weak response. The antigen carrier plays an important role in controlling the conformation of the antigen and exposing or shielding important functionalities; it is believed that ND immobilization results in less distortion of the protein conformation allowing better binding by antibodies and hence a stronger immune response.

As discussed earlier, the presence of the nitrogen–vacancy (N–V)− centre within diamond nanoparticles results in very strong fluorescence at 700 nm after excitation at 560 nm (Yu et al. 2005). This is very advantageous for imaging in biological cells, as certain cell components, such as flavins and porphyrins, produce very high background fluorescence in the region 300–400 nm, so probes that fluoresce at higher wavelengths are desirable. Impressively, ND showed very intense fluorescence, sufficient for single-particle tracking within a cell, with no photobleaching observed over 300 s (in contrast with approx. 10 s for a dye molecule). The fluorescent intensity is similar to quantum dots, such as CdSe/ZnS, but without the associated toxicity. As the emission results from defect sites within the core of the ND, the surface of the particle can be modified without altering the fluorescence signal. Uptake of 100 nm NDs by human kidney cells was confirmed using confocal fluorescence microscopy, where the ND was found to form aggregates within the cytoplasm of the cell, but not in the nucleus. A particle size of 35 nm ND was introduced to living HeLa cells and a single particle was tracked as it diffused throughout the cytoplasm (Fu et al. 2006).

An extension of this research could be to modify the fluorescent particles to become drug or gene carriers, where the interaction of the ND with the target site within the cell could be monitored using fluorescence microscopy.

An important consideration for medical and biological application of ND is its potential cytotoxicity; it is of little use to have a cellular probe that kills the cells after uptake. Diamond is considered an excellent candidate for these applications because in its bulk form it is chemically inert; however, it is unclear whether the same is true of ND, as the surface chemistry of the nano-sized particles will dominate that of the bulk. Yu et al. (2005) investigated the cytotoxicity of fluorescent NDs on human kidney cells using an assay based on the reduction activity of methyl thiazolyl tetrazolium. They found that cell viability only diminished slightly upon the addition of relatively large quantities of ND. A recent paper titled ‘Are diamond nanoparticles cytotoxic?’ (Schrand et al. 2007) examined neuroblastoma cell viability in the presence of 5 nm ND by monitoring mitochondrial function and luminescent ATP production. Oxidative stress on the cells was measured by detecting generated reactive oxygen species (ROS). It was found that the presence of ND does not affect the integrity of the mitochondrial membrane and there was no significant ROS production attributed to the presence of ND. In addition, it was possible to grow cells onto a surface modified with ND. The authors concluded that ND shows good biocompatibility, but noted that ND tends to localize within the cell cytoplasm, forming aggregates of approximately 500 nm that may be hard to clear from the
cell. The long-term effects of ND on a cell or an animal remain to be investigated. Bakowicz-Mitura et al. (2007) took a different approach to this problem, by studying the effects of ND upon human gene expression of stress-responsive genes. When cells become stressed by the presence of ROS or other toxic agents, certain genes are expressed in response and can be detected using PCR methods. ND was found to result in an increase in the expression of genes responding to oxidative stress (i.e. in the presence of ROS) and a decrease in genes responding to toxic and genotoxic substances. It is unclear what to conclude from these results, but it is certainly true that, while apparently biocompatible, ND is certainly not bio-inactive. While this is a research area that is relatively unexplored to date, it is crucially important that the bioactivity of ND is clarified. Owing to its large surface to bulk ratio, ND cannot be considered to behave in the same manner as the larger diamond crystallites, for example, found in CVD diamond films.

8. Applications of ND in catalysis

The reported applications for ND in catalysis mainly concern its use as a solid catalyst support; however, a direct role for ND itself in the catalysis of the oxidation of CO to CO₂ has been suggested (Bogatyreva et al. 2004). Untreated ND powder was found to oxidize CO to CO₂ starting at 230°C and reaching a maximum 80% yield by 380°C. ‘Electrochemical treatment’ (experimental conditions not given) of the ND in hydrochloric acid was found to enhance the catalytic properties, resulting in the conversion of CO to CO₂ from 80°C and proceeding to almost 100% yield by approximately 400°C. It was proposed that there was a relationship between the catalytic activity and the ratio of different oxygen species on the ND surface, although no mechanism has been given.

A more straightforward case of the use of ND as a solid support for the metallocene catalysis of ethylene polymerization was reported by Yuan et al. (2002). Interestingly, the activity of the catalyst immobilized onto ND was significantly greater than that immobilized onto Al₂O₃ particles and polymerization proceeded at a much more regular rate, indicating greater catalyst stability. The ND was able to incorporate greater quantities of the catalyst onto its surface than the alumina, possibly due to the presence of oxygen functionalities. The interaction of the catalyst with the ND surface was also found to be an important factor in the work of Tsoncheva et al. (2006a,b), who investigated iron oxide ND and nickel-modified ND in the catalysis of methanol decomposition. In general, ND-based catalytic materials exhibited better activity, with a direct correlation between the rate of methanol decomposition and the amount of ND incorporated in the catalyst. Compared with activated carbon or mesoporous silica supports, catalytic activity was more stable for the ND support; the authors suggested that this is due to the formation of larger and more easily reducible iron species on the ND. It is postulated that the reduction state of Fe species is determined by their interaction with ND surface groups or by the reductive effect of some defect sites. In this case, the ND is not acting simply as a support for the catalyst, but the interaction between the catalyst and the ND results in the formation of complex and more effective catalytic centres.

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The catalytic studies outlined in §8 emphasize that diamond is far more chemically active in the form of nanoparticles than it is as a bulk crystal. This is further demonstrated by the reports of the use of ND in electrochemical applications or as an electrode component. The idea that an undoped diamond material might find electrochemical application is initially surprising, as diamond is a textbook example of an insulator, with a band gap of 5.47 eV. However, Novoselova et al. (2004) fabricated electrodes from detonation ND by sintering the powder at 1600°C and 8 GaP applied pressure to form compacts of DC resistivity $10^3$ Ω cm. In the absence of a redox couple, the electrode was found to exhibit redox peaks at approximately 0.7 V, which were attributed to reactions of carbon phases present in the electrode. In the presence of the well-known redox probe ferricyanide, $\text{Fe(CN)}_6^{3-/4-}$, peaks for the reduction and oxidation of this couple were observed, but with very small currents and significant irreversibility. Much more complex behaviour was noted with the $\text{Ce}^{3+/4+}$ couple, where not only were the peaks for the redox couple observed, but also other peaks that could only be attributed to the ND itself. Zang et al. (2007) also fabricated an electrode using detonation ND powder. They formed a cavity electrode by sealing a platinum wire in glass and treating with aqua regia to form a microcavity; the cavity was then filled with ND powder. The powder was found to be electroactive in ferricyanide solution and the authors postulated that the conductivity of the diamond was due to sp$^2$ groups on the surface of the particles. ND powder has also been incorporated into an electrochemical glucose biosensor by forming a self-assembled monolayer of ND onto a gold electrode modified with amine groups (Zhao et al. 2006). Glucose oxidase was then bound to the ND. After the ND was electrochemically oxidized by applying a potential of 0.7 V to the electrode, the electrochemical oxygen reduction reaction was found to be significantly enhanced. The reduction of ferricyanide was also enhanced at the ND-containing biosensor, in comparison with a similar biosensor without ND incorporation. The authors suggested that the enhancement of electrochemical activity of the ND on oxidation may be due to the destruction of the basal plane of the ND and the appearance of the more reactive edge plane.

Recent work carried out in our laboratory has found that 5 nm undoped ND is indeed electroactive, but cannot be considered as conducting (Holt et al. submitted). In its dry powder form, its resistivity is very high and it gives the IR response of a resistor when pelletted to form an electrode. However, when a thin layer of ND is drop-coated onto a graphite electrode, a significant enhancement in the redox response of ferricyanide, $\text{Ru(NH}_3)_6^{3+}$ and oxygen reduction is observed, compared with the unmodified electrode. In addition, other redox peaks are sometimes present which appear to be attributed to redox reactions of the ND itself, as shown in figure 6a. Immobilization of a thin layer of the ND onto an electrode using a mineral oil binder allows the investigation of the electron transfer between the ND layer and the underlying electrode. It appears that ND can indeed undergo oxidation and reduction at specific and well-defined potentials (figure 6b). The oxidation of the powder by heating in air resulted in an increase in its redox activity, but the reduction of the ND by hydrogenation inhibited the electrochemical behaviour. This has lead us to postulate that the observed electron transfer
processes of ND can be attributed to electron injection into unoccupied surface states, available as a consequence of unsaturated bonding in the surface layer of the ND. As noted in all of the examples discussed previously, the exact nature of the surface is still unclear, but it contains a proportion of sp$^2$-bonded carbon (but not necessarily graphite) and when highly oxidized it comprises a great number of C=O bonds. The surface layers of ND are therefore able to act as a sink and source of electrons and hence have a promoting effect on redox reactions.

The exact mechanisms for these processes remain to be elucidated; however, the ND may also play a similar role when used as a catalyst support. The redox activity of ND and, in particular, its promoting effect on the oxygen reduction...
reaction with potential generation of ROS may also have significant repercussions for its use in biological environments. These electrochemical investigations again suggest that ND cannot be treated as an inert and bio-inactive material and further work is needed to fully understand this material.

10. Towards quantum computing: a role for ND?

It has been speculated that ND particles could form the basis of a quantum computer (Barnard & Sternberg 2005), due to the desirable properties of the \((N–V)^-\) defect centre: it is a photostable, single-photon source, allowing the use of this centre as a solid-state room temperature qubit (quantum bit). For the potential of this material to be realized, various practical issues need to be considered, including how to pattern individual \((N–V)^-\) centres at distinct locations within the diamond and then register them to electrical gates. In addition, the centres emit over a range of frequencies, hence they would require optical tuning for use as qubits. Many researchers are currently addressing the structure and properties of the \((N–V)^-\) centre, with optimism that it will find its use in quantum computing and other applications such as quantum key distribution (Greentree et al. 2006; Wrachtrup & Jelezko 2006).

11. Conclusions

The above examples illustrate the potential for use of detonation ND in a wide range of applications in disciplines spanning chemistry, materials chemistry, life sciences, medicine and physics. At present, most of the referenced studies represent short communications and preliminary investigations, which have been published within the last three or four years. Clearly, this is a field on the brink of expansion, and it should be expected that publication rates will increase rapidly over the coming years.

At this point, it is instructive to consider how the property of a material changes as its size is decreased from a bulk quantity to nano-dimensions. The 5 nm detonation ND used in most studies has nearly 20% of its atoms located on the surface. At these dimensions, it is not difficult to imagine that the chemical properties of ND will be dominated by the chemistry of the surface. This leads to behaviour, such as catalytic and redox activity, which one does not find with diamond in its bulk form. Although the exact physical, chemical and electronic structure of the surface is still not known, it is probable that there is a large degree of delocalization due to the presence of unsaturated carbon sp² and C=O bonds arranged over the whole surface. The unsaturated nature of the bonding may be the origin of the unexpected chemistry, which is observed for a material that was previously thought to be inert.

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Applications of diamond nanoparticles


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