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Short Communication

The Realm of Materials Science: A Playground for Physicists, Chemists, and Engineers

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Beyond MATTER consisting of atoms bonded together through their chemical affinities with a wealth of natural (Geological as quartz α-SiO_2 and the rarely occurring high pressure form Stishovite) and man-made compounds like boron nitride BN, the concept of MATERIAL comes as enlarged scope of science, where Material = Matter + properties. This is especially relevant when it comes to applications.

In this acceptation, Materials Science is a discipline of Matter "make-up", spanning physics, and chemistry, as well as the technologies building upon them where the syntheses consider the shape, which can be bulk (3D; D for dimensionality), 2D/surface, or even 1D/chains, and the size ranging from the atomic nanoscale (1 nm= 10^{-9} m) up to macroscale. The relevant characterizations call for X-ray and neutron diffractions, high pressures -gas, liquid, solid media- , spectroscopies -NMR, IR-VIS, XANES, EXAFS; and shape analyses with electron microscopy EM (transmission TEM and scanning SEM). Besides basic research in academic and public laboratories that can be considered as the cradle of ideas and inventions, further developments are achieved in start-up companies and industries, the final (noble) aim remains the compliance with the everlasting demand of Industry and Society (ex. medicine and healthcare, *vide infra*). For the purpose, physicists, chemists and materials scientists must work together for the benefit of all. At this point, it is interesting to relate a true story for events that happened when I was young researcher in France. In the research institute where I used to work as well as in another one, solid-state chemists synthesized copper-oxide-based La_2CuO_4 and $YBa_2Cu_3O_7$ shown later to undergo a superconducting transition below T_C (critical temperature) of ~33 K, which was the highest critical temperature observed at that time. In fact, the measurements down to such low temperatures were carried out by two physicists from the IBM -Zurich research institute: K. A. Müller and J.G. Bednorz who were awarded the Nobel Prize in 1987 for their discovery of superconductivity in an oxide. That was a breakthrough, knowing that such a property was exclusive to metals and alloys which obeyed the BCS theory (Bardeen, Cooper, and Schrieffer also awarded the Nobel prize in Physics in 1972), providing the long-sought explanation for superconductivity in terms of the interaction of electrons and phonons (quanta of vibrations). This prize could have been won by French physicists and chemists were they to work mutually. The underlying problem was that at the academic research institutes, the chemists could carry out measurements down to liquid nitrogen (-195.79°C), while the physicists in another neighboring laboratory had the possibility of going down to liquid helium (-269°C, knowing that absolute zero temperature is -273°C). But unfortunately, due to missing scientific exchange they missed the Nobel Prize! Lastly it needs to be mentioned that the sample of $YBa_2Cu_3O_7$ measured by the Swiss scientists was a mixture of three phases, in which only the minority one exhibited the superconductivity. Such mixed-phase sample is horrified by chemists (and also physicists) who prefer to work on single phase samples. Serendipity in Science is frequent and sometimes fortunate for humanity such as the discovery of penicillin y Alexander Fleming in 1928.

Back to Materials Science, an example of properties of relevance at both levels of academic and industrial developments is offered by ultrahard materials. Sustained research efforts started in the first half of the 20th century for the industrial applications of the hardest known material, Diamond characterized by the highest hardness (Vickers' H_V ~100 GPa) and large bulk modulus B_0~ 450 GPa (GPa is the pressure unit Pascal (Pa) and 1 Giga =10^9. Its applications raised problems limiting its use such as in tooling machinery on one hand, and the high cost of using natural Diamond sources, on the other hand. In fact, at high temperatures, in addition to graphitization, diamond oxidizes with air oxygen and interacts chemically with ferrous alloys, which essentially limits its use in cutting tools. The other issue of high cost was solved by the first diamond synthesis performed in 1953 by the Swedish company ASEA then by General Electric Company (Schenectady, USA) back in the fifties of last century, by the first synthesis of man-made Diamond at high temperature and pressures: P ~10 GPa and T~ 1300-1400°C. Such conditions are met in the overlapping tectonic plates and near volcanoes, allowing Nature to make natural Diamond over long periods of time (low kinetics). However, it was shown later that large-scale synthesis of bulk nano-diamonds could be achieved near 9 GPa and milder temperatures T~ 1250-1300°C. Furthermore, surface coating nano-diamonds can be achieved by CVD (chemical vapor deposition) even at ambient pressure. Consequently, size matters, and this feature demonstrates that the research in Materials Science involves engineers, besides chemists and physicists. Despite the solution brought by synthetic diamond for coating tooling machines, its instability at elevated temperature was a problem awaiting solution. The answer was brought by man-made boron nitride BN, which takes over all the polymorphs of carbon. Regarding layered structures (2D), both graphite and layered BN (also called white graphite), are soft materials that can be used as lubricants. Oppositely, diamond and cubic boron nitride c-BN are super-hard with a smaller zero pressure bulk modulus for the latter: B_0 ~ 380 GPa and large hardness. With such properties c-BN was considered in the second half of last century for cutting tools replacing synthetic diamond while remaining stable at high temperature. Note that regarding morphology, nano-BN can be synthesized thanks to metal particle catalysis. The close relationship of physical properties of carbon and BN promoted research within the B-C-N ternary system characterized by light elements with small radii leading to small interatomic distances and reduced volumes; -all these parameters being 'recipes' for high toughness and hardness. The research activity in this domain, which is ongoing, started in the second half of last century involving physicists (high pressure), chemists (crystal chemistry) as well as engineers to come up with propositions of new compounds with exceptional properties. Interestingly, large number of such experimental studies were backed with strong propositions from quantum mechanical calculations based on density functional theory DFT (Hohenberg, Kohn and Sham, 1964-1965), extensively used by the author in close collaboration with experimentalists (the reader is kindly referred to the author's ORCID web site containing links to publications mainly at Google scholar and Research Gate). Regarding hard materials taken as an illustrative example the quantum mechanical calculations through DFT based methods in the last four decades, have proven DFT with its improved exchange-correlation functionals, its reliability in accounting for energy related physical quantities as mechanical, dynamic, thermal and spectroscopic ones to be predictive of new materials likely to replace diamond in applications. Besides new forms of carbon close to diamond, original binary B-N and ternary B-C-N candidates for super-hard phases were proposed and identified.

In the realm of the Quantum, a context must be introduced here in what is called Modern Physics. It is the branch of physics that deals with the post-Newtonian concepts, involving the schism between the two worlds of physics: On the one hand Classical Physics whose father is Isaac Newton (17^{th}-18^{th} century) involving a continuity of the physical phenomena, and on the other hand, the physics at the subatomic scale or Quantum Physics initiated by Max Planck in the early years of the 20^{th} century and brought to light for explaining phenomena as the black body radiation that couldn't be understood by classical physics. In this field Quantum Materials were developed such as strongly electron-correlated cerium hexaboride CeB_6, which has challenging properties that are little understood presently (see recent papers in Scientific Reports), and some type of superconducting materials with electronic order or particular magnetic order. Add to that, the Special (and General) Relativity introduced by Albert Einstein in the beginning of 20^{th} century, changing our vision of space and time by relativizing them while keeping one physical constant, the speed of light c = 300.000 km/s. (in vacuum). Quantum Physics and Relativity are recognized as the major breakthroughs of the twentieth century, but one shouldn't ignore the invention of the transistor in the 1950's. The Quantum world is not only in laboratories and in computers for fundamental research, but also in technologies. This is the case of healthcare where it heralds a new era of integrative medicines, by using complex rules of quantum mechanics, and hence making medicine faster, less painful, and more personalized. Quantum technology is likely to modify the way we think about healthcare and medicine. Let's work, Materials Scientists, physicist and chemists (experimental and theorists) as well engineers for a better world.

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