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Inventing a New Africa through Discovery and Innovations in Computational Material Science

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ABSTRACT

Researchers are increasingly relying on computational technologies to help in simulation of properties of new materials and some areas in materials science has enjoyed some level of success which ranges from composites, to polymer science and to advanced ceramics. This review paper discuss certain developments in the area of computational Materials and how Africa can leverage on this technology to develop their emerging Industries, while dwelling more on application of computational material science in energy sector, since energy has been most pressing challenges in Africa which could be addressed by advanced materials. Also, we summarize part of our research work on galvanic corrosion of mild steel bolt in a magnesium alloy (AZ91D) plate simulation using comsol Multiphysics and 2^k factorial experiments on factors that influence the recovery of gold during the upgrade of Ilesha-Itagunmodi, Nigeria gold ore through Froth flotation using Anova software. Attempt have been made to identify existing computational method, challenges of computational materials science deployment in Africa, and how material development can be accelerated through the power of computational material science. With this work, we were able to establish that the strength of computational materials science is in making a connection between the experiment and theories of complex phenomena.

Keywords: Computational material science, Technology, Energy, Africa

INTRODUCTION

The history of civilization can be explained as a step of breakthroughs in material science from Stone Age, we have progressed through Bronze, Iron and Silicon Age. Advances in materials have balance of economic power: Iron and steel, silicon based electronics. Materials have enabled the modern civilization, providing a pathway to innovation in energy industries, health, information technology and agriculture.

For so many years Africa has been battling with effort to develop its own infrastructure through an improved technology, and is also not a gain saying that that Africa is endowed with so many natural resources, part of which if well harnessed can catapult many developing parts of Africa to developed country, as countries of the world are been classified as developed countries based on the valuables numbers of technological problems they are able to solve. Part of these Natural resources is minerals representing important components of many products used daily in Africa (e.g. Energy storage device, Cell phone, and computers electronic parts semiconductor). Computational material science is one of the fastest growing disciplines in materials science [1]. Number of scientist involved in materials modelling has rapidly increased and Africa cannot be left behind [1]. Researchers are increasingly relying on computational technologies to help in simulation of properties of new materials.

In much of materials science, it is the interaction of groups of defects that define the materials response, for example plastic deformation requires the movement of many dislocations. Atomistic, while useful for individual defects,

cannot cover the length and time scales needed for such simulations. A promising approach to study deformation phenomena's called dislocation dynamics, in which the dislocations are treated as the fundamental entities of the simulations [1]. Dislocation forces are calculated and the equations of motions are solved overtime, much as in molecular dynamics. Devincre and Kubin have done an impressive work in this area, which includes the development of fully three-dimensional simulation [2]. However some partial breakthroughs have been recorded, for example developing an understanding of dislocations in strained epilayers [3]. The example shown by grain growth modelling, done with a variety of methods, has nailed down the rate equation of coarsening [4]. Moreover on computational materials simulations has been able to re-describe the study of the effects of texture because they enabled us to make useful predictions across the every range of experiments [5].

Areas in material science that has enjoyed some level of success ranges from composites, to polymer science and to advanced ceramics. In most cases, the modelling provides a guide to a better knowledge of the materials science engineering. With proper coupling of modelling with experiment, progress can be truly made. Here I highlighted certain developments in area of computational materials and how its development can impacts emerging technologies in Africa most especially Energy sector. This work is not is not intended as a review. Instead we summarized our experience and view point on the subject, and use examples from our own work as illustrations.

Engineering materials designed at nanoscale level

Understanding and controlling self-assembly designer materials made of pre-programmed building blocks that spontaneously organize into structures with unique and complex properties exhibited only by biological systems have long been a dream of researcher [6]. Structures whose constituents can assemble, disassemble, and reassemble automatically or on command enable materials capable of self-repair, multi-tasking, and even shape-shifting properties known throughout the biological world [7].

Self-assembly also permits material structures far more complex than traditional metals, ceramics, and polymers, with many levels of hierarchical organization and compartmentalization typical of biological structures such as cells and organelles. Such structural complexity is demanded by the sophisticated properties and behaviour we desire of next-generation materials capable of meeting future energy demands, most especially active materials that must perform functionally in ways that will not be possible today for traditional, nonbiological matter [6]. Over the past decade, investments and advances in nanoscience have made possible the characterization, creation, imaging, and manipulation of highly complex building blocks ranging from single molecules to supramolecular objects nanometers to microns in size [6]. The design space for self-assembled materials is now so vast that computational tools are required for the rapid screening and prototyping of building blocks that will predictably self-assemble into desired structures. In recent years, promising new theoretical and computational approaches to the study of self-assembly have been discovered to guide experiments, but these are in their initiation stage [7]. Moreover, continued investments in high-performance computing (HPC) have produced computing platforms that are now fast enough to permit predictive simulations of self-assembly for complex building blocks, and new experimental analysis promise the needed resolution of nanoscale structure to monitor assembly processes in their original position, parameterize models and validate simulations [7]. These combined advances in synthesis, characterization and modeling capabilities set the stage for a starting point in our ability to discover the underlying principles controlling self-assembly and to develop robust, predictive simulation-based tools to achieve materials by design [8].

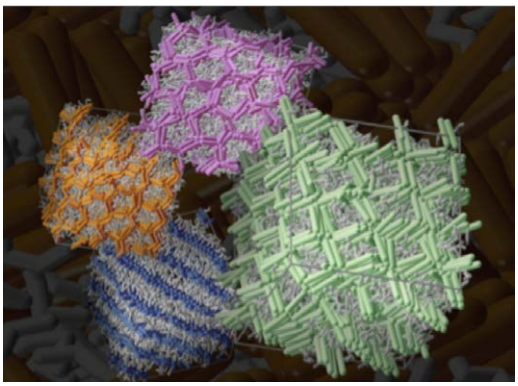

Figure 1: Predictions of computer simulations [15]

Self-assembly and reconfigurability of nanomaterials

Figure 1, shows the predictions of computer simulations of polymer-tethered rod-like nanoparticles [15]. Depending on rod length, different structures result [6]. Each structure exhibits different geometries and consequently different properties [6]. By using "active" nanorods capable of lengthening and shortening, simulations show how the assemblies can be made to be reconfigurable, toggling among different structures on command.

Materials deployment challenges

Incorporating new classes of materials into applications usually take long, usually between 10 to 20 years from initial research to first use; it took 20 years to move the idea of lithium ion battery from a laboratory concept to wide market adoption. Today scientist and Engineers should explore the capabilities in computational material science [9]. To solve the grand challenges of 21st century, reducing the time required to bring discovery to market will be a key driving force for economic growth. The long time frame for materials to move from discovery to market is due in part to the continued reliance of materials research and development on scientific institution and trial and error experimentation. Most design and testing of materials is performed through time consuming and repetitive experiment, characterization loops [9].

Advanced materials share a common characteristic: They are complex. Achieving the required performance gains depends on exploiting the many degrees of freedom of materials development including multiple chemical components, nanoscale architectures and tailored electronic structures [7]. This introduces enormous complexity in the discovery process, complexity that must be understood and managed. Early steels have three to four essential chemical components as its constituent and a relatively simple microstructure. Today's advanced high-strength, high-temperature steels average six to eight chemical components and require complex, multiphase nanostructures. The parameter space for exploration has increased enormously, making continued development by trial and error impractical. There are billions of options: chemical combinations, local morphologies, atomic-scale structure. Sifting through the options using predictive modeling is the only intelligent and efficient path forward. The superconductors of the 1980s were typically two-component systems with a simple crystal structure. Again, high performance comes with a significant increase in complexity and with a corresponding need to narrow discovery possibilities to a manageable number of the most promising options [6].

Accelerating material development by computational tools

Integrated computational and experimental tools should be developed. The software and integration tools should span the entire material continuum, which should be open source. Infrastructure created by this initiative will enable scientists and Engineers to create any number of advanced materials, which will solve engineering problems and addresses issues of pressing national importance [9].

Materials science modelling areas that have enjoyed incorporation of computational material science

- Galvanic Corrosion of Mild Steel Bolt In A Magnesium Alloy (AZ91D) Plate Simulation Using Comsol Multiphysics [10].
- 2^k Factorial Experiments on Factors that Influence the Recovery of Gold during the Upgrade of Ilesha-Itagunmodi, Nigeria Gold Ore through Froth Flotation using Anova software [11].
- Computational Molecular Nanotechnology carbon nanotubes are considered as potential building block in future nanoscale materials, machines and computers.
- Large scale simulation of crack propagation, Molecular dynamic simulation can be used to illustrates crack propagation in a ductile metal.
- Deformation of nanocrystalline Aluminium. Molecular Dynamic for Aluminium have carried out under constant tensile load, Mechanical twinning plays an important role in plastic deformation of nanocrystalline Aluminium [12].
- Growth of fractal structures in fullerene layers using monte carlo simulation.
- Molecular Dynamic simulation of the ejection of carbon nanotubes in MAPLE [13].

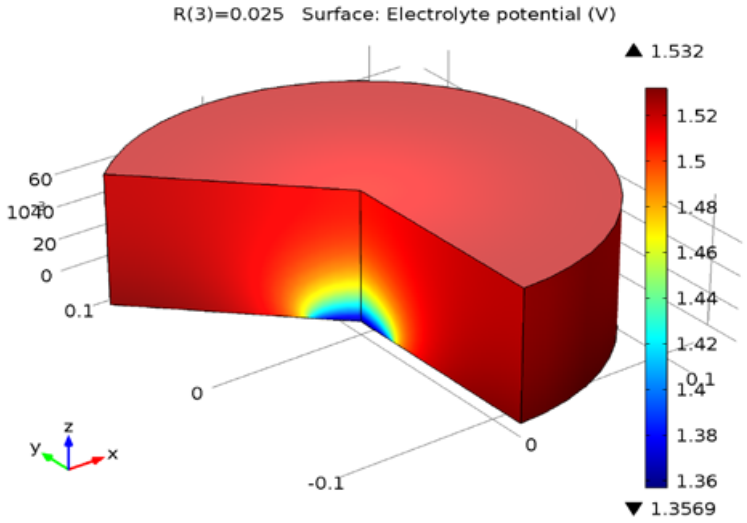

Figure 2: Showing 3D representation of electrolyte potential for a 25 mm disc radius. Galvanic corrosion of a mild steel bolt in a magnesium alloy (AZ91D) plate simulation using comsol multiphysics [10]

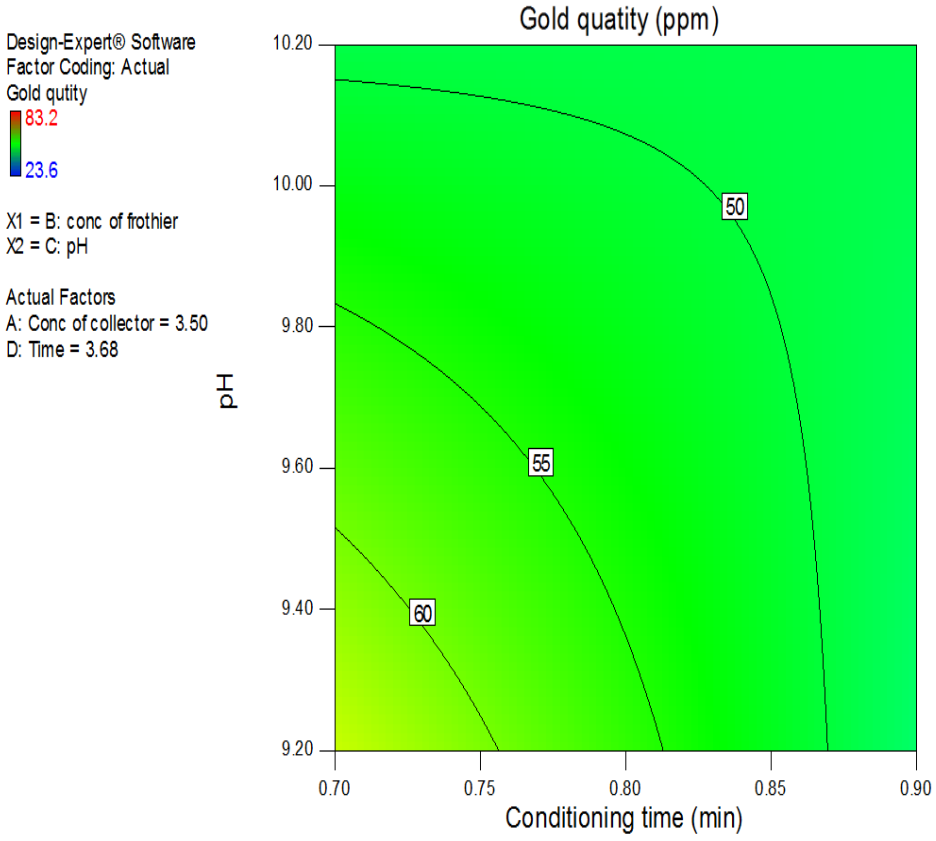

Figure 3: 3D surface graphs showing influence of factors on Gold yield and contour line showing the mutual interaction of the parameters. Nigeria Gold Ore through Froth Flotation using Anova software [11]

Figure 4: The ejection and transport of polymer molecules and carbon nanotubes in matrix-assisted pulsed laser evaporation (MAPLE) [13]

Figure 2, shows a revolved surface plot of the electrolyte potential for a steel disc radius of 25 mm using comsol Multiphysics [10], Figure 3 is a 3D surface graphs showing influence of factors on Gold yield and contour line showing the mutual interaction of the parameters. Nigeria Gold Ore through Froth Flotation using Anova software [11]. Figure 4 shows MAPLE modelling of the ejection and transport of polymer molecules and carbon nanotubes in matrix-assisted pulsed laser evaporation [13].

Infrastructural Innovations through computational materials

Infrastructure created by this initiative will facilitate the discovery and development of myriad of advanced materials that will benefit African economy or National economy. Most pressing challenge in Africa is energy which could be addressed by advance materials development [9]. A typical example is seen through a research that can help us to find new technologies such as better catalysts for the production of bio-fuel, high-efficiency solar photovoltaic, portable energy storage devices, and artificial photosynthesis to drive energy directly from sunlight [14].

University of Limpopo South Africa, computational modeling scientist Phuti Ngoepe and his associates use supercomputers to develop models of minerals that bear precious group metals. Their models help optimize reagents that extract minerals from such ores, and could lead to the discovery of uncharted reefs [14]. According to Ngoepe [14] "Since related simulations are computationally-intensive, remote access to Lengau via the South African National Research Network (SANReN)'s high-speed network allows us to progress at a competitive pace from our Limpopo lab more than 1,700 km away from Lengau". As the world transitions away from fossil fuels, batteries are expected to gain prominence with transportation and electrical applications. Battery research requires mastery of computational physics, chemistry and materials science and there's a global competition to develop batteries that charge faster and last longer, while being smaller, safer and affordable to the masses [14]. Research scholar Sylvia Ledwaba is helping Ngoepe develop simulations of synthesized complex structures to help predict the performance of lithium battery electrodes. They are exploring a variety of materials that promise to be more powerful and smarter. Manganese, for example, is abundant in South Africa and widely used in battery cathodes [14].

CONCLUSION

Integrated relativity between material theorist, experimentalist, computer scientists and engineer could facilitate the development of computational material technology in Africa.

Computational material science and experimental tools has provided basic research opportunities for researchers in the most important aspects of contributing to infrastructural development. The use of modelling and simulation must be coupled with new experimental and characterization tools to achieve this [6]. Computational science has also offers an innumerable opportunity that increase industrial competitiveness by reducing design times, thereby accelerating the development and incorporation of new materials and processes, and minimizing testing requirements.

CONFLICT OF INTERESTS

The authors declares that there is no conflict of Interests regarding the publication of this paper.

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