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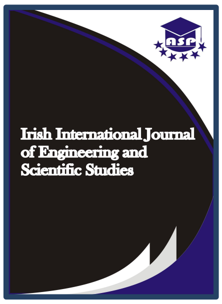

IMPROVING MATERIALS ENGINEERING RESEARCH IN NIGERIA THROUGH COMPUTATIONAL MODELLING AND SIMULATION.

Paul S. Nnamchi[1,2] and Camillus S. Obayi[3]
[1]*Department of Materials Science and Engineering, University of Sheffield, Mapping St, Sheffield, S1 3JD, United Kingdom.*
[2]*Department of Metallurgical and Material Engineering, University of Nigeria, Nsukka. Nigeria.*
[3]*Directorate of training and research, Council for regulation of Engineering in Nigeria (COREN), Abuja.*

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Abstract: *Generally, experimental research in materials science and engineering is tasking and expensive and often the required equipment are lacking in developing countries and Nigeria is not an exception. It is a common knowledge that the laboratories in Nigerian Universities lack the basic amenities that make them stringent enough to be called a science laboratory, hence, the need for a faster and cost-effective ways of research. Computational materials science and engineering is defined as the computer-based employment of modelling and simulation to understand and predict materials behaviour. The present work addresses and proffers solutions to the factors that have hindered the adoption and deployment of this convenient and faster means of research in Nigeria higher educational system. In effect, this work recommends that we take advantage of the development and deployment of very fast computers to speed up and enhance our ability to increase our knowledge base as well as productivity.*

1. Introduction

Computational materials Science and Engineering have been defined in the most general terms as the computer based employment of modelling and simulation to understand and predict materials behaviour. Although, the methods are similar, in practice, we generally make a distinction in application between computational materials science, in which the goals are to better understand and predict materials behaviour and computational materials engineering, which is focused on the practical application of materials, typically with an emphasis on products [1]. Considering the above, and the ease in accessing material modelling and simulation soft wares, certain advantages which includes new opportunities for using computational modelling to carry out profound intensive materials design studies that could greatly advance the development and refinement of materials and materials processing abound.

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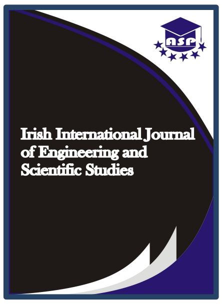

Additionally, the recent development of inexpensive, yet very fast computers and the availability of software for many applications have given a comparative advantage to workers in this field of research. The development and increasing complexity of industries have recently necessitated the separation between doing and knowing. The antecedence today, is that empirical computational modelling and simulation of materials have moved from being entirely in the hands of specialists to being accessible to those who are modelling not as their principal activity, but as an adjunct to their primary interests.

Despite that computational materials research has since reached advance status in many developed and developing countries [2-8], the current educational process for developing computational materials research is lacking in Nigeria. Hence, the focus of the present work is devoted to addressing the factors that have hindered the adoption and deployment of this convenient and faster means of research in Nigeria higher educational system.

There are multiple ways to advance the understanding of the lag in computational materials modelling and future of technological research in general in Nigeria. One, which I do not adopt here, is to try to predict or identify the socio/economic and political factors which may be affecting most technological developments of the future in Nigeria. The other is to identify some respects in which our kind or pattern of education by its nature, brings about lag in technological development and offer solutions. It is along the later that I speculate in what follows, restricting myself largely to the Nigerian scene.

2. The basic problems:

(1) Most materials scientists receive little training in quantum mechanics beyond a solid state physics course (see Table1).

(2) Most materials scientists receive little training in physics beyond a basic solid state physics course.

(3) There is almost no training in chemistry beyond freshmen chemistry; the lack is most important in quantum chemistry (Hartree-Fock) and organic chemistry.

(4) The understanding of polymeric and ceramic systems is often very limited (sometimes even for materials scientists).

(5) There is often little formal training in programming beyond a Fortran course for all categories of science and engineering students,

(6) The training of materials scientists and engineers in numerical analysis is often minimal or lacking.

(7) Most quantum mechanics courses do not cover the computational aspect relevant to electronic structure calculations.

(8) Perhaps most importantly, most graduate students, mostly PhDs learn little or nothing about basic simulation techniques, and those who do, have little grasp of other methods. Implicitly, most computational materials scientist and physicists have had to fill the above voids in their knowledge on their own; there is often little in their formal training that prepares them for a broad career.

(9) There have been little or no computational laboratory with dedicated softwares and programmes beyond the basic DOS, Microsoft office and outdated mathematics programs in most part of the country. In effect, there are few or no competent computational materials scientists or theoretical physicists to educate others.

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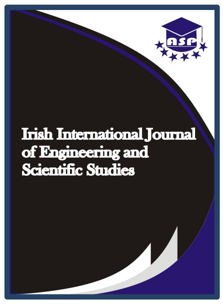

(10) Although, it is a very common knowledge that there is scientific conferences to attend, there are relatively few opportunities to attend external workshops on particular advanced aspects of computational materials science; such workshops can be a highly efficient way to advance the skills of researchers beyond their university days. I believe that it is time to reform the educational process to fill those gaps, since computational research is accessible, fast, efficient, and cost effective and the data compete favourably with experimental research [9-15].

3. **Possible solutions**:

3.2. Short-term

In the near term, a number of new courses could be added to existing curricula to greatly increase the depth and breadth of students' knowledge. For materials science students: (1) at least 1-2 courses in quantum mechanics and at a graduate-level chemistry course that emphasize chemical bonding, organic chemistry, re- action pathways and catalysis; (2) a numerical analysis course; (3) a computer science course (CS) that includes computer architecture, data structures, and especially programming methodology (the problem is that most CS courses treat these in separate courses, which is too heavy a load for most non-CS students); coverage of parallel algorithms is a possibility as well; (4) a course on computational quantum mechanics that covers Hartree-Fock, Quantum Monte Carlo (briefly) and, especially, the generalised-gradient approximation (GGA) and Local density approximation (LDA) (5) a course on macroscopic modelling that covers finite differencing, finite elements, lattice methods and kinetic rate equations, such as Thermocalc and Dictra; (6) a course on atomistic simulation methods that covers bonding, molecular dynamics, energy minimization, Monte Carlo, applications to materials, and coupling to macroscopic models.

3.3. Long term

In the long term, Nigerian universities should consider developing a program or a section of Materials science department focusing on computational materials science and engineering. Such a program could be flexible enough to handle both computer scientists, chemist and physicists who wish to specialize in materials science computing, as well as scientists and engineers who wish to specialize in computational methods. In addition to offering and sponsoring attendants to series of seminars.

(II) Engineering students must take some of the following courses (although I would change the requirement to one of the following, allowing more space for electives): (1) numerical methods for partial differential equations; (2) numerical linear algebra; (3) numerical approximation and ordinary differential equations; (4) geometric and symbolic computation; (5) finite element analysis; (6) grid generation and multigrid techniques; (7) parallel numerical algorithms; (8) materials studio; Monte Carlo and simulation methods; (9) numerical methods in fluid dynamics.

(III) Students choosing the computational materials option must take five of the following (there are similar sets for other engineering disciplines): (1) thermodynamics/statistical mechanics; (2) quantum mechanics (undergraduate); (3) quantum mechanics (graduate); (4) computational quantum mechanics; (5) solid state physics; (6) atomistic simulation methods; (7) surface

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physics. In addition to the above PhD program, a reduced program could be available as a minor within a materials department.

4. Conclusion

It is widely and ritually repeated these days that a technological world is a world of change, i.e., new technology creates new possibilities. To this extent, the statement is implicit of how computational research or virtual laboratory might be used to bring about a whole world of change and shape the future of empirical studies in Nigeria. It is a common knowledge that the laboratories in Nigerian Universities lack the basic amenities that makes them stringent enough to be called a science laboratory. Although a stock of such equipment lacked is beyond the scope of this paper, but evidently anyone would agree that we are still a research consumer country. Therefore, taking advantage of the development of inexpensive, yet very fast, computers and the availability of software cannot be a mistake, rather could speed up and enhance our ability to increase our knowledge base as well as productivity.

In effect, it is recommended that the universities should acquire the state of the art soft wares used for high tech researches that are usually very expensive for the researchers to get individually as well as encouraging effective collaborative research arrangements with other research institutions.

We also recommend attendance and streamlined sponsorship of local and international computational /modelling workshops, such as the one done in Oxford University in the United Kingdom quarterly or that instituted by Accelrys user group [16] should be encouraged. Such workshops and conferences can be the most efficient way to advance the skills of researchers beyond their university days.

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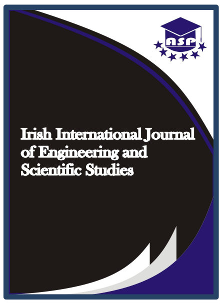

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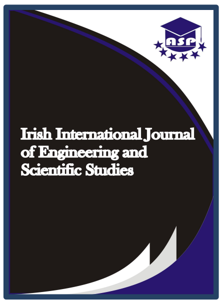

Table 1: A typical B.Eng. degree programme in Metallurgical and Materials Engineering

THIRD YEAR			
FIRST SEMESTER			
a) Required ancillary courses	CED 341	Introduction to Entrepreneurship I	2
	STA 205	Statistics for Physical Sciences & Engr. I	2
	ME 314	Mechanical Engineering Design I	3
	MEC 313	Workshop Practices	2
b) Core/Compulsory Courses	MME 301	Metallurgical Thermodynamics and Kinetics	2
	MME 311	Physical Metallurgy Laboratory	-
	MME 331	Physical Metallurgy I	2
	MME 333	Basic Electron Theory of Materials	2
	MME 341	Mechanical Metallurgy I	2
	MME 381	Ceramic Engineering	2
	MME323	Corrosion Engineering	3
SECOND SEMESTER			
a) Required ancillary courses	CED 342	Business Development and Management	2
	ENGR 301	Engineering Analysis	4
	MEC 351	Mechanics of Fluids I	2
	ME 343	Measurement and Instrumentation	2
b) Core/Compulsory Courses	MME 302	X-ray Diffraction and Electro-optical Techniques	2
	MME 322	Mineral Processing	2

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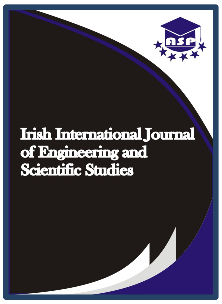

	MME 332	Structure, Properties and Heat Treatment of Alloys	2
	MME 342	Metallurgical Furnaces & Principles of Foundry Engineering	3
FOURTH YEAR			
FIRST SEMESTER			
a) Required ancillary courses	ENGR 401	Computational Methods	3
	ME 471	Heat and Mass Transfer	3
b) Core/Compulsory Courses	MME 411	Corrosion and Chemical Metallurgy Laboratory	-
	MME 413	Mechanical Metallurgy Laboratory	-
	MME 421	Extractive Metallurgy	2
	MME 431	Physical Metallurgy II	2
	MME 443	Production Metallurgy	2
	MME 451	Welding Engineering	2
	MME 461	Polymer Engineering	2
SECOND SEMESTER			
b) Core/Compulsory Courses	ENGR 402	Student Industrial Work Experience Scheme (SIWES)	-
	MME491	Technical Report Writing	3
	ME 481	Technology Development Policy	2
FIFTH YEAR			
FIRST SEMESTER			
a) Required ancillary courses	ME 581	Engineering Law and Management	4
b) Core/Compulsory Courses	MME 521	Tools Steels: Metallurgy, Manufacture and Applications	2
	MME 543	Iron and Steel Making	2
	MME 531	Transport Phenomena in Materials Engineering	2
	MME 541	Theory and Design of Engineering Alloys	2

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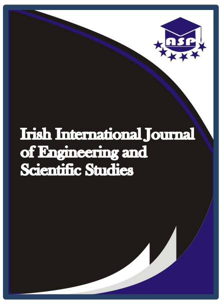

	MME 551	Introduction to Composites	3
	MME 581	Nano-science and Nanotechnology	2
	MME 561	Engineering Materials Selection and Economics	2
SECOND SEMESTER			
a) Core/Compulsory Courses	MME 524	Metallurgical Plant Design	3
	MME 532	Theory of Dislocations	2
	MME 542	Mechanical Metallurgy II	2
	MME 592	B.Eng. Project	-
b) Elective courses	MME 538	Advanced Phase Transformations and Heat Treatment	2
	MME 546	Powder Metallurgy	2
	MME 552	Coal and Coke Technology	2
	MME 556	Refractory Materials and Industrial Furnaces	2
	MME 574	Paper Production Technology	2
	MME 582	Solid State Materials & Electronics	2
	MME 584	Special Materials	2