

Individual Articles

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IN MEMORIAM

Rustum Roy: aeternum vale

(1924-2010)

Employing a clump of few words to describe the complexity of one single human life seems, at best, a futile attempt to encompass the ideals, limitations, dreams, fears, achievements and, finally, the enormous variety of concepts of what we call an actual human being. If, additionally, one must ascertain the proper terms for summarizing a life fully committed to teaching, discovering, outreaching and pioneering one of today's most active and influential areas of R&D in the entire Globe, the task becomes a gargantuan enterprise.

Over sixty years of prolific academic activity of the late Rustum Roy, based primarily on Pennsylvania State University but reaching the whole World, implies describing the emergence of Materials Science as a fully respected scientific discipline, with its own personality and area of influence, both technically as well as politically speaking, to a great extent thanks to the work, effort and personality of Rustum,

I met personally Rustum during my postdoctoral work at IBM in the mid 1980's, both because he was a regular and popular speaker in many scientific meetings and also because he happened to be the father of a friend and fellow postdoc: Ronnen Roy. Furthermore, since at the time I was working on cementitious materials, was familiar with the work of Rustum and Della Martin Roy, who produced some results which are still considered classics in the field. In addition to the imprint that such a personality forged on a (then) young scientist, I quickly learned, every single time a completely "new" and "revolutionary" idea came to my mind, to check whether Rustum had already discovered or invented that before!

The well over 1000 articles, including technical papers, scientific reports, opinions and notes authored and co-authored by Professor Roy during more than 6 decades of intensive labor, truly parallels the history of Materials Science and Engineering in the second half of the 20th Century, for it is really hard to find a relevant area of this discipline in which Rustum had not shared a thought, either through his writings or his enchanting conferences or conversations.

However, despite his many and important achievements as a scientist, there is another facet of Rustum Roy which draws the attention of even outsiders to the scientific community: his impressive ability to reach almost any audience with a convincing and lasting message, which made him not only an effective and favorite communicator, but a real activist, entirely

committed to the message that science really is, at least he was able to convince many of us of this, one of the most effective instruments we have developed as a culture for a human being to transcend, surpassing his/her own limitations as an individual while participating in a collective long-term effort: to sustain knowledge, thus becoming a “citizen scientist”, a term, incidentally, invented by Prof. Roy. It is to no one surprise, then, that Rustum was a champion of interdisciplinary research, in a time when each scientific discipline was kept “pure” from the contamination of other “foreign” influences and was unthinkable for a theoretical physicist to publish a paper with a civil engineer, or even take care of what was intellectually interesting in the Department at the next aisle of the building!

Rustum Roy received numerous recognitions to his valuable efforts, many of which set new standards, not only in terms of quality and influence (tens of thousands of citations in the ISI web of Science can apprise this!) but also opened the path for fellow scientists of a discipline that, 3 decades ago, was considered just a subset of Solid State Physics combined with a little of Chemical Engineering. Rustum was always proud to introduce himself as a Materials Scientist.

Every individual who today receives education in any of the wide variety of disciplines encompassed by what we generally call Materials Science, owns a debt of gratitude to Prof. Roy, not only because of the innumerable discoveries he made, from sol gel to biomaterials, from cementitious materials to high T_c superconductors, from diamond films to novel crystal growth techniques and a long etc., but mainly, because he represents one of the true founders of this discipline as we know it today, with an incredible reservoir of creativity, imagination and stamina which, even during the latter part of his prolific existence, was extremely contagious to those who had the fortune to happen to be around him.

Perhaps one of the most visible and obvious fruits of Rustum’s visionary mind, was this Journal of Materials Education (JME) first started in 1979 as Journal of Educational Modules for Materials Science and Engineering, envisioned as an effective and open tool for educating new generations of materials scientists and engineers, thus becoming one of the oldest and lasting efforts in materials education in the World. For many years, Roy was directly in charge of editing the Journal, in spite of his multiple commitments and obligations, for he was convinced that education, at the highest possible level, was the way for a discipline to prosper. Keeping this publication, JME, with his inclusive editorial policy is, certainly, to honor Rustum and his legacy. Conjointly, Dr. Roy was the founder of the U.S. Materials Education Council, today the International Council on Materials Education, a world-wide organization that, for many decades now, has gathered the great variety of opinions, projects and objectives of the global community of “Materialists”, pretty much along the lines of Rustum’s philosophical and epistemological legacy.

Rustum: we thank you dearly. Farewell forever.

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International Symposium on Materials Education held March 26-28, 2011 at Yashda Pune organized by IISER, C-MET and DIAT Pune, India

Materials Science and Engineering witnessed explosive growth during last three decades. Initially advanced materials (advanced/fine ceramics, advanced polymers and composites, electronic and photonic materials) surpassed several boundaries of performance. Nanostructured Science and Technology revolutionized the ways in which materials and products are created and range of functionalities can be generated. Nature's own technology emerged billions of years ago when molecules began organizing into complex structures that could support life. Macromolecular Science and Engineering has evolved by Materials Science and Engineering bridging the gap by enhancing the secrets of biology and communications to it by latest technologies. Unprecedented developments in Materials Science and Engineering gave rise to breathtaking developments in information and biotechnology.

Prof. Rustum Roy, doyen of Materials Science and the Founder Director of Material Research Laboratory at Pennsylvania State University, USA had established The International Council of Materials Education to further the cause of Material Education in developed and developing countries. Several conferences and symposia have been organized world over, co-organized or co-sponsored by International Council of Materials Education (ICME). India has strong base of Materials Science and Engineering

and Nanotechnology. There are various challenges in the development of these new materials ranging from design of smart materials to energy saving and environmentally safe materials. The aim of this symposium is to sensitize young minds early to these challenges as well as to faculty and researchers in this frontier area. Between 2006-2010, six such symposia have been organized in USA, Singapore, Australia, Italy and Brazil. This symposium is being organized in India by leading Science and Technology Organizations (IISER, NCL, C-MET and DIAT) in Pune on behalf of ICME.

21 invited lectures were delivered by experts from France, Germany, Italy, Japan, UK & USA and eminent Indian Institutions (IITs, IISc, National Laboratories, Central and State Universities). 34 short lectures were delivered by young scientists from India, Nepal and Srilanka. There were 51 poster presentations by young scientists, research scholars and postgraduate students from India and abroad. 50 young scientists and technologists, postgraduate and undergraduate students participated in ISME 2011 from Industries, research laboratories and academic institutions.

A wide range of invited lectures, short lectures and posters on latest trends in Materials Science and Engineering, Nano Technology/Nano-Biotechnology and Materials Education were delivered/ presented. The lectures on Materials Education topics are

being submitted for publication in the Journal of Materials Education. The presentations were on soft matter, multiferroics, iron based high T_c superconductors, graphene, controlled and targeted drug delivery by nanoparticles, nanomaterials synthesis by soft chemistry, surface and volume properties of nanomaterials and their characterization, characterization of nanocomposites, new green bulk composites, spectroscopy of semiconductors, molecular science at surfaces, nanocomposites coatings, rheology of polymer melts and nanoparticle mixtures, dendrimers and hyper branched polymers, processing, characterization and fabrication of nanomaterials and their devices, conducting polymers and devices, fluorination of polymers and composites, turbulent drag reduction and flocculation by polymers. Similarly there were lectures on materials education and integrated education in materials science for teachers at secondary and tertiary levels.

The symposium was inaugurated by Prof. K. N. Ganesh, Director IISER Pune, who emphasized that young minds should be sensitized with challenges in present day Materials Science. Dr. Sourav Pal, Director, National Chemical Laboratory, Pune was Guest of Honour. He hoped that the

deliberations of ISME will address such issues that are posed in front of the faculty and students as well as to enlighten the researchers in the frontier area. Dr. D.P. Amalnerker, Director, C-MET Pune proposed vote of thanks to sponsors of the ISME-2011 and organizers and participants of ISME-2011.

Six prizes were awarded to young scientists and research scholars for their best poster presentations during valedictory function by Dr. S. Sivaram, Former Director of the National Chemical Laboratory, Pune. Prof. M. Hess gave a presentation about IUPAC and presented a presentation on behalf of Dr. John E.E. Baglin on Education About Science - an Urgent Global Challenge. A musical programme by TALAASH band enthralled participants on the 27th March evening.

Professor Rustum Roy, the founder of the International Council of Materials Education, passed away on 26th August, 2010. ISME-2011 was dedicated to him.

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METALS CORROSION AND BIOLOGICAL RESPIRATION: SIMILARITIES AND DISPARITIES: AN OVERVIEW

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ABSTRACT

Both metallic corrosion and biological respiration involve oxidation – reduction reactions, taking place upon electron transfer between the participating entities. Metals corrode as a consequence of their tendency to return to the oxide state prevailing in the original ores. Corrosion occurs by reduction of dissolved oxygen in neutral pH solutions, or by reduction of H⁺ ions in acidic solutions. The involvement of oxygen and redox reactions is also essential for sustaining life in biological systems. Biological respiration in humans relies on the oxidation of carbohydrates, fats and amino acids as a part of the vital network of metabolic processes that generate the energy necessary to maintain normal body function and temperature. In plant systems the biological ‘respiration’ process of photosynthesis, which involves chlorophyll, is a major source of oxygen on the planet. For example, in human biological systems, unlike corrosion processes in metals, oxygen transport by blood is carried out by haemoglobin as the essential process of human respiration. Haemoglobin is a tetrameric protein located in the red blood cells, containing porphyrin-bound Fe²⁺. Haemoglobin picks up oxygen in the lungs, carries it to the tissues and releases it there, where it is actually used. On its way back, haemoglobin picks up the metabolic CO₂ produced in the tissues and releases it into the lungs. In photosynthesis the chlorophyll molecule is the inverse analog to haemoglobin; both molecules are porphyrins with the difference of central metal atoms being Fe in haemoglobin and Mg in chlorophyll. In this report similarities and disparities between metallic corrosion and biological respiration are presented, taking into account the respective reactants, products and catalysts. This comparative study allows for the interaction between teachers and students, in order to explain the similarities and diversities of the fundamentals of natural processes such as metallic corrosion and biological respiration. This paper covers elements from the mineral, animal and vegetable kingdom, with a comparative approach.

Keywords: *Corrosion; Respiration; Water; Blood; Sap; Iron*

1. INTRODUCTION

From the initiation of the civilized world, human beings have utilized natural materials: wood, stone, leather, vegetable fibres and metals, in order to build their dwellings, tools, cloths, weapons, etc. In the modern era they invented and developed synthetic materials - such as plastics derived from petroleum, metals from metallic minerals and ceramics from earth minerals - in order to build and manufacture their structures, buildings, vehicles and machinery. All these natural and synthetic materials undergo deterioration processes^{1,2}. These are caused by natural aging, due to exposure to the environment and, particularly, when subjected to the action of aggressive chemical, biological and mechanical agents and processes. Recently, the European Federation of Corrosion and NACE International, USA, both professional associations of corrosion scientists, engineers and practitioners, adopted a broad definition of the term "corrosion". It encompasses the deterioration of all engineering materials, such as metallic, plastic, ceramic, and composites, and also includes biomaterial implants and soft materials in the human body such as skin, muscle, cartilage and bones. Osteoporosis, an illness of the osseous tissue, is considered a biocorrosion process³. Comparative studies offer useful tools for understanding the fundamentals and mechanisms of these natural processes and reveal their similar as well as different characteristics. They are used for teaching the basics of chemistry, biology and materials from several points of view. Hence, these studies already steer the students' interest in natural phenomena, particularly the ones that are not fully understood yet.

2. OXIDATION-REDUCTION PROCESSES

Oxidation-reduction (redox) processes involve solids, liquids and gases. They involve transfer of electrons and, therefore, are delineated as electrochemical reactions. Such processes actually proceed by two simultaneous half-

reactions: oxidation and reduction⁴. Corrosion and respiration are typical redox processes, both occurring with the participation of oxygen from the air. In the case of Fe oxidation, electrons are lost and its oxidation number increases:

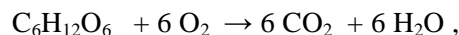


In the case of Fe²⁺ reduction, the ion gains electrons and the oxidation level decreases:

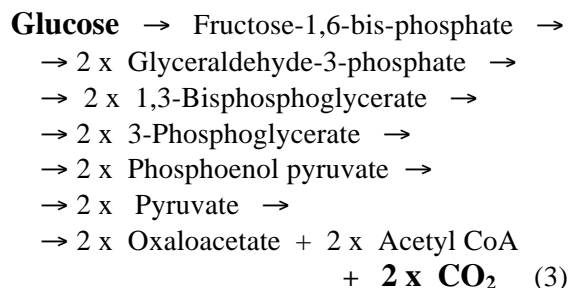


Many redox reactions take place in nature and also are applied in industrial processes as well. Examples of the latter are the fermentation of sugars, *e.g.* glucose, to produce alcoholic beverages, and the combustion of fossil fuels to generate electricity which, in turn, is converted into thermal and mechanical energy.

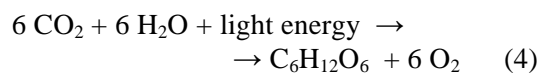
In physiological oxidation, glucose is oxidized to CO₂, while oxygen is reduced to water and, CO₂. And, while the overall reaction can be summarized as



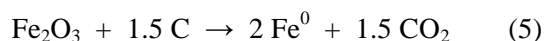
the actual process is much more complex, taking place as a sequence of events. The more representative ones⁵ are indicated in Equation (3):



Plants photosynthesis is the reverse of that reaction, where CO₂ and H₂O are converted into sugars and molecular O₂, a process promoted by the green pigment chlorophyll^{6,7}:

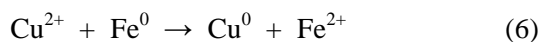


The steel industry produces steel by reducing iron ore with coal:



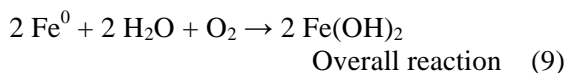
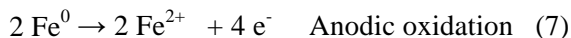
An interesting oxidation-reduction process

takes place during copper production from a solution of CuSO_4 , upon addition of chunks of scrap iron:

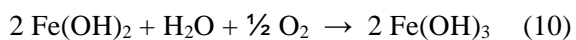


3. CORROSION AND BIOLOGICAL RESPIRATION

Corrosion is derived from the Latin word "roer" (to gnaw). Metals corrode due to their natural tendency to return to the more stable, oxide/salt state prevailing in their ores. In the presence of water, vapour or liquid, metal corrosion takes place by reaction with dissolved molecular oxygen (DO), while the latter is reduced to hydroxyl ion. The overall corrosion process is the combination of two half-cell reactions, this taking place at the metal-environment interface:



Upon further oxidation, $\text{Fe}(\text{OH})_2$ is converted into $\text{Fe}(\text{OH})_3$ (rust):



Corrosion science is concerned with the study of the causes and mechanisms of corrosion processes. Corrosion engineering applies scientific knowledge towards abatement of corrosion by practical and economic means⁸.

The tendency for corrosion to take place stems from the fundamental law of nature, as expressed by the free-energy change accompanying the electrochemical reactions involved:

$$\Delta G = -nFE \quad (11)$$

where ΔG is the free-energy change associated with the processes considered, n is the number of electrons involved in the reaction, F is the Faraday constant and E is the cell electrical potential. A negative value of ΔG indicates that

the spontaneous corrosion will occur, while a positive value of ΔG indicates that, for corrosion to happen, an investment of energy is required⁹.

The corrosion potential of a metallic material in an electrolyte solution is experimentally determined in an electrochemical cell. The latter contains an anode, a cathode and an auxiliary electrode. The potential is measured relative to a reference electrode, under open circuit conditions. Polarization plots are recorded with a potentiostat, an instrument that maintains an electrode at a constant potential. A polarization cell consists of three electrodes: the metal working electrode, a Pt auxiliary electrode and the reference electrode, such as a saturated calomel electrode. (SCE) This arrangement simulates a corrosion process happening in a natural or industrial environment¹⁰. Electrochemical corrosion tests are conducted according to the practices recommended in ASTM standards G3 and G5¹¹.

Human respiration is an integral part of the body metabolism that carries out the conversion of the food components, such as carbohydrates, fats and proteins, into matter and energy. These are required for achieving tissues renovation, body growth and body vital functions, as well as for maintaining and regulating body temperature¹².

Respiration is a life sustaining physicochemical process based on the oxidation of carbohydrates, fats and amino acids. This process requires reduction of molecular O_2 , as indicated in Equation (3), and the latter is supplied by the haemoglobin carrier in blood. Metabolic CO_2 is excreted from the tissues to the lungs and then expired into the air¹³. Corrosion and respiration are chemical and biological processes, respectively, both based on the fundamental laws of chemistry and biology.

4. WATER, SAP AND BLOOD

Corrosion and respiration take place in two

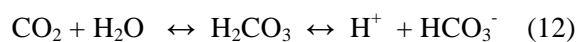
natural, liquid environments, water and sap, with the active participation of DO, and blood with the participation of absorbed O₂. The required oxygen comes from the air.

Many natural processes take place in water. On the one hand, great varieties of organisms live and thrive in water and, therefore, without water, human, animal and vegetable life cannot exist. On the other hand, without water aqueous corrosion will not occur. Water ionizes slightly, yielding hydrogen and hydroxyl ions, in a state of equilibrium:



As a matter of fact, H₂O and H⁺ are associated and form the hydronium ion H₃O⁺. Water is a polar solvent, dissolving acids, minerals, salts, sugars and proteins, thus forming ionic or molecular solutions. The salt content of seawater and river water and pertinent electrical conductivity are different. In river water, salt concentration and electrical conductivity are low.

Water contains dissolved gases, in particular O₂ and CO₂ that are involved in corrosion and respiration. CO₂, a greenhouse-gas product, acidifies water, according to the following equilibrium:



The DO content of water varies with temperature; it is high in cold water and decreases as water temperature increases, in accordance with Henry's Law for dissolution of gases in liquids. The gas solubility depends on gas pressure, as well as on solvent nature and temperature¹³.

The principal component of the human body is water (about 70% of the body weight). It contains about 1.0% of various salts, mainly NaCl. Blood is the most important and dynamic body fluid, since it carries and delivers nutrients and O₂ to the whole body. It is composed of plasma, an aqueous phase containing dissolved proteins, carbohydrates, fats and salts, and of cellular elements such as red and white blood cells. Within the red cells there is haemoglobin, an iron-containing protein, which transports O₂

from the lungs to the body tissues. On its way back, haemoglobin picks up metabolic CO₂ produced in the tissues and releases it into the lungs, which perform as an efficient air pump¹⁴. Some basic properties of water and blood, related to corrosion and biological respiration, are listed in Table 1.

Table 1. Physical and chemical properties of water and blood.

Property	Water	Blood
Density, g/ml	1.00 (25 ⁰ C)	1.06 (37 ⁰ C)
Viscosity, cP	0.894	3-4 times water viscosity
Specific heat, cal/g	1	
pH	6.5-8.1	7.35-7.45
DO, mg/l	8.5(25°)	4.2 Plasma 28.0 Blood
pO ₂ , mmHg		80-100
pCO ₂ , mmHg		35-45

5. WATER AND BLOOD CIRCULATION

The circulation of water in industrial equipment, the movement of blood within the human body and sap in plants are distinctly different. In most cases industrial water flows in an open system, while blood and sap always does so in a closed one.

A complex network of pipelines, pumps and valves is used to conduct water from its source to the consumers. This equipment is fabricated from steels, concrete and/or plastics, with or without internal and/or external coatings and linings. Within this network corrosion may take place. Its occurrence is a nuisance. However, upon applying preventive corrosion control technology, its extent can be minimized or even completely eliminated.

Blood flows in a fully closed circuit. It is pumped by the heart through arteries to the capillaries and through veins back to the heart

again. Blood carries oxygenated blood for O₂ supply. In the lungs O₂ and CO₂ are interchanged: O₂ is absorbed and CO₂ is expelled¹⁵.

6. MATERIALS DETERIORATION

Deterioration or degradation of materials implies the loss of their useful properties. Among the latter, loss of mechanical strength deserves particular consideration. This is the case for industrial engineering materials, as well as for organic and organic-inorganic hybrid materials that constitute the body organs and tissues. Hard metallic and soft biological materials undergo specific deterioration processes, with mechanisms related to their physical and chemical nature, microstructure and surface texture, and with detrimental effects on their functional characteristics.

Corrosion, scaling and fouling appear equally in sea, river, potable and industrial waters. These phenomena depend on the chemical, biological and thermal characteristics of water. Also, thick, tightly adherent scales form on metal surfaces by sedimentation and crystallization of dissolved and suspended minerals, such as carbonates, silicates and hydroxides. Special chemical inhibitors are added to water to prevent corrosion and scaling. Macro and microorganisms, such as bacteria, algae, fungi and molluscs, form layered fouling films on materials' surfaces and they enhance corrosion. Chemical biocides and mechanical cleaning methods are applied to remove fouling and scaling.

Body organs, blood vessels and tissues involved in respiration suffer from deterioration due to natural aging. Concomitantly, physiological regeneration "repairs" some of them. Of particular concern are the arteries and veins, which lose their flexibility. Blood clots and plaques form inside blood vessels and impair or even completely interrupt normal blood flow. The appearance of these malfunctions are prevented and/or avoided by administration of appropriate medication. Special surgical

procedures - such as angioplasty - are applied to maintain open the blood vessels and to assure the supply of nutrients and oxygen to vital body organs, particularly the brain. Insertion of the more advanced metallic or polymeric stents into the blood vessels, following angioplasty, averts their collapse and prevents the life-threatening restenosis process.

7. COMPARATIVE OVERVIEW

A comparative summary of corrosion and biological respiration, emphasizing their similar and distinct aspects, is presented in Table 2. We note that, while the basic oxidation and reduction reactions involved similar participants, the properties of the fluids involved and their circulation systems are completely different. Nevertheless, both processes obey the fundamental laws of nature, including those of fluid mechanics.

Related to these phenomena one notice that, in blood cells, the oxidation-reduction processes and the concentrations of materials involved, are well balanced, satisfying the requirements of a healthy metabolism. However, when – for whatever reason – this balance is impaired, the organism runs into critical metabolic disorders. Among them is the Iron Deficiency Anemia. It affects some two billion people worldwide, with negative consequences mainly on child development, child and maternal mortality and work productivity¹⁶.

8. EDUCATIONAL ASPECTS

This paper addresses apparently unrelated phenomena. On the one hand, we consider biological respiration and its related phenomenon of biological photosynthesis. On the other hand, we address the chemical corrosion of metals, a process that usually does not involve biological-type activity. The back-to-back consideration of these phenomena has an outstanding educational value that stems from following two well established pedagogical avenues: "from complex-to basics-to complex" and "from learning-to-doing".

Table 2. Metals corrosion and biological respiration: similarities and disparities

System	Metallic materials	Human body	Plant
Process	Corrosion	Respiration	Respiration
Type	Chemical	Biological	Biological
Mechanism	Electrochemical	Biochemical	Biochemical
Chemistry	Metals	Organics	Vegetables
Liquid, gases	Water, O ₂	Blood, O ₂ , CO ₂	Sap, O ₂ , CO ₂
Circulation	Pumps, pipelines	Heart, blood vessels	Vascular bundles
pH range	5 – 8	6.5-7.5	Acidic, neutral ¹
Products	Metallic oxides/salts	H ₂ O, CO ₂ , energy	H ₂ O, CO ₂ , energy
Protection	Inhibitors, coating	Drugs, stents	Greenhouse

Note 1: Varies according to parts: roots, leaves, fruit.

Thus, the first lap along this route allows one the mastering of fundamental chemical, physical and thermodynamic principles that govern the structure and structural stability of the highly complex biological entities considered. In so doing, one can reach a thorough understanding of the specific and unique mode of action of these entities.

In the second lap along this route one relies on the understanding thus reached. And, using appropriate computational tools, one can now design, assemble and operate novel systems that will perform pre-determined functions. Such functions are otherwise not achievable.

This second lap is now known as Molecular Engineering¹⁷. This field of endeavor already lead to the development of basic components

for Biomolecular Information Processing Systems (BIPS), particularly enzyme-based switches¹⁸ and enzyme-based logic gates¹⁹. These systems were subsequently extended to neural network-type configurations²⁰. Moreover, the biomolecular switches and biomolecular logic gates are being implemented in the development of multi-functional biosensors for medical and environment-monitoring applications²¹.

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INTEGRATION OF MATERIALS SCIENCE IN THE EDUCATION OF HIGH SCHOOL TEACHERS IN AN ADVANCED COURSE PROGRAM

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Dedicated to Prof. Jung-Il Jin, Seoul, Republic of Korea, former President of IUPAC, on the occasion of his 70th birthday.

ABSTRACT

A concept for an advanced course in polymer materials science for students of Chemical Education is described in which creativity and curiosity for scientific problems are challenged. This ambitious concept that can be conducted with small groups and well-equipped laboratories can uncover otherwise hidden potentials of the students.

Keywords: *interactive lab course, Advanced Materials Science Education, interactive instruction manual, creativity, motivation, encouragement*

INTRODUCTION

In courses for students of Chemistry who want to become teachers it is frequently observed that the content of the classes is separated from the lab course and that the correlation of the lectures and the lab course is often poor. The students do not have much influence on the specific content of the course; they perform prescribed experiments generations of students have done before in the same way. In materials

science, the students do not only deal with the general properties of materials and their determination, for example mechanical behaviour, thermal properties etc., an important issue is the correlation of structure, morphology and properties of the material. Understanding complex interactions and non-linear chains of cause and effect is an essential learning target where inflexible teaching concepts are not really satisfying. We can teach many facts in a course but essentially is what remains with the

students as real knowledge. In the particular case of students who want to become teachers, there is a strong demand for showing them not so much a collection of separate techniques and properties but a broader perspective of how things cooperate^{1, 2}. Having experienced this in a specific field with a particular substance and with certain techniques they should be able to transfer this picture to other systems and other techniques without major problems.

This is a report of a project-focused approach with a range of flexibility left for the students' creativity that has been carried out at the Gerhard-Mercator University, Duisburg, Germany, in advanced courses for students of Materials Science Education.

During this specific course, the students were allowed some degree of interactive freedom to decide which experiments they think should be conducted and in which sequence. In Materials Science, in particular in the field of organic polymeric materials, one can start from the very basics, means from monomers that can be polymerized to different kinds of polymeric materials such as homo- and copolymeric bulk polymers, polymer blends or composites. The students can become creators of the materials they are working with, a very important experience with respect to the measurements they perform later with exactly these substances. They continue their experiments not with some kind of anonymous sample from the lab assistant but with their own material. This concept in some sense puts into practice Peter Mahaffy's tetrahedral view on chemical education.³

In international courses, means in courses where there are students from different countries, modern teaching instruments like electronically available manuscripts provide a chance incorporating and combining matter-of-fact information with language information in a very useful way which is not only comfortable for students from foreign countries. These options should also be considered in up-to-date teaching.⁴⁻⁶

RESULTS AND DISCUSSION

During recent years several courses in (polymer) Materials Science were conducted with the scope to show the students not only how materials behave but also why they behave as they do and in which way this can be controlled. So, the questions are, for example, why is this material strong (and what does it mean "strong") and another one "weak", why does this sample (of the same material) pass a test but another sample fails, how can we control the properties of a material and to which extend.

The basic idea is to give the students an idea of a material, literally a "feeling" for a material. Therefore, after some weeks of introductory class room teaching where the very basics of Polymer Chemistry are presented, the lab course starts with the synthesis of a particular polymer. This can be done applying different techniques or varying experimental conditions, see Figure. 1. A certain general direction is of course predetermined, say, let us study polystyrene or how to cover a metal surface with a polymer. The students are then asked to develop a strategy how to conduct the investigation. Provided there are not too many students in a course and that there is a good hardware background, the students can develop many different ways to discover their unknown territory actively.

The students work in groups of two to four. The feeling of putting into shape their own practical course wakes up hidden potentials of creativity and encourages using their brain and following their own ideas, eventually forming a real research team. The tutor observes, guides with "slackened reins", helps and assists and only interferes when really necessary. Guidance has to be strict only in the beginning and it was observed that very soon a team forms from the accidentally assembled group, and an increasing degree of self-confidence is formed where even weak students find their strength and grow with their task and success. Because the individuals can play their part (one student is good at synthesis, the other good at physical

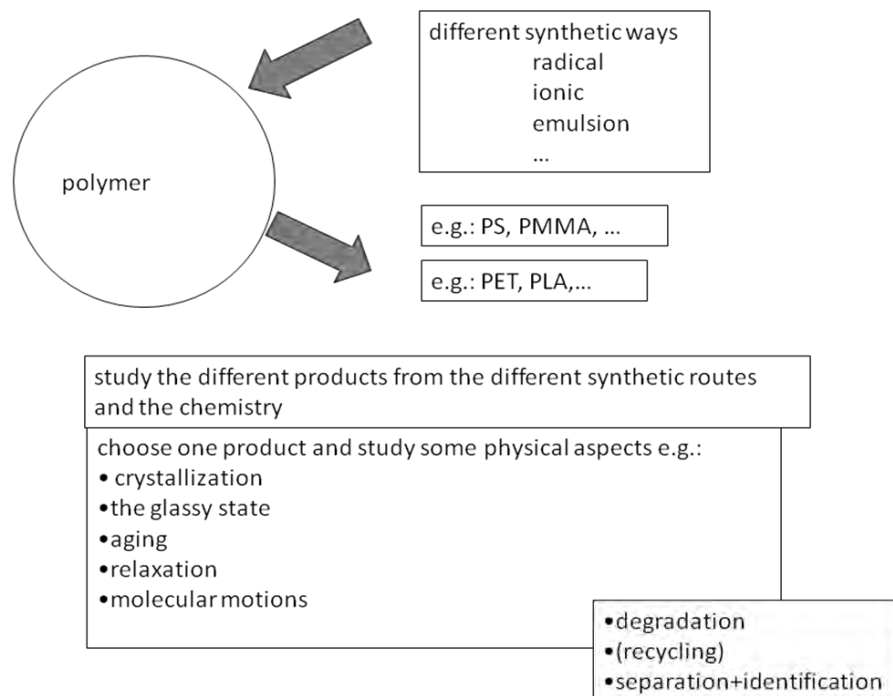


Figure 1. General scheme how a Materials Science project can be started from the synthesis of a polymer

measurements, another one good at data evaluation etc.) literally everyone finds her/his field of expertise, brings it in, finds her/his value in the team. This definitely increases the individual learning efficiency. The effect that weak students are only carried forward by better students decreases. The weak students rather improve their skills and understanding in such a team and gain confidence.

Another effect is that students look at a sample specimen that has to be characterized with much different eyes when they have prepared the sample themselves, when they have some degree of freedom to decide what to do with it. As an example could serve polystyrene as polymeric material: polystyrene is synthesized with different techniques. Different methods to characterize the product are chosen and compared. After the first results, say determination of the different molar mass averages, automatically the question arises what happens when experimental conditions are changed. At the same time handling the experimental data wakes up curiosity, this leads the students deeper into the matter and hence to

a better understanding – literally "grasping" – of the physical meaning of the terms they are dealing with. Having the results from, say, chromatography, the question might arise: does this fit in with osmometry and viscosity,..., what if we change the conditions of the synthesis...

Now, what kind of a material do we have got? Is it brittle or elastic? What exactly does that mean? Calorimetric and dynamic mechanical analysis can help with hard physical data. Soon the students find out that they are dealing with solid state properties, terms like glass transition, etc., one could use microscopy for analysis of the fracture... Many branches of materials science open up once a material is produced, with careful guidance by the tutor a general strategy can be followed with a lot of input from the students.

Smart students can be allowed to follow unexpected effects they might identify such as the enthalpy relaxation that leads to physical aging processes and general relaxation phenomena. In the class and in seminars it is

then possible to go deeper into the matter.

Another example is silicon chemistry that can lead into the fields of rheology of liquid polymeric products, rubber elasticity and even the effects of frequency-dependent deformation behaviour when "bouncing putty" is synthesized. There are many more examples which can be taken from what is present in daily life and deals with the general question: why does this material behave in this way, can I change the behaviour, how and to which extend. After all, this can lead to an understanding of how to think and approach a problem where a material has to be tailored, see Figures 2 and 3.

The students experience that they are not

(passively) taught but they are actively learning, that they are the ones who go forward once their curiosity and enthusiasm woke up and they find out that their ideas are taken seriously. The effect is that the students are much more going for good and consistent results than "just for the grade points". They learn more because they just want to know, and exactly this is what they later as teachers at high schools and colleges have to forward to their pupils. To show them that the materials we are dealing with in daily life did not just fall out of the sky but were developed, can be created by careful and mindful observation followed by applying proper science and combining different disciplines of science and engineering. Basis of all is reveille curiosity and create self-confidence in the students

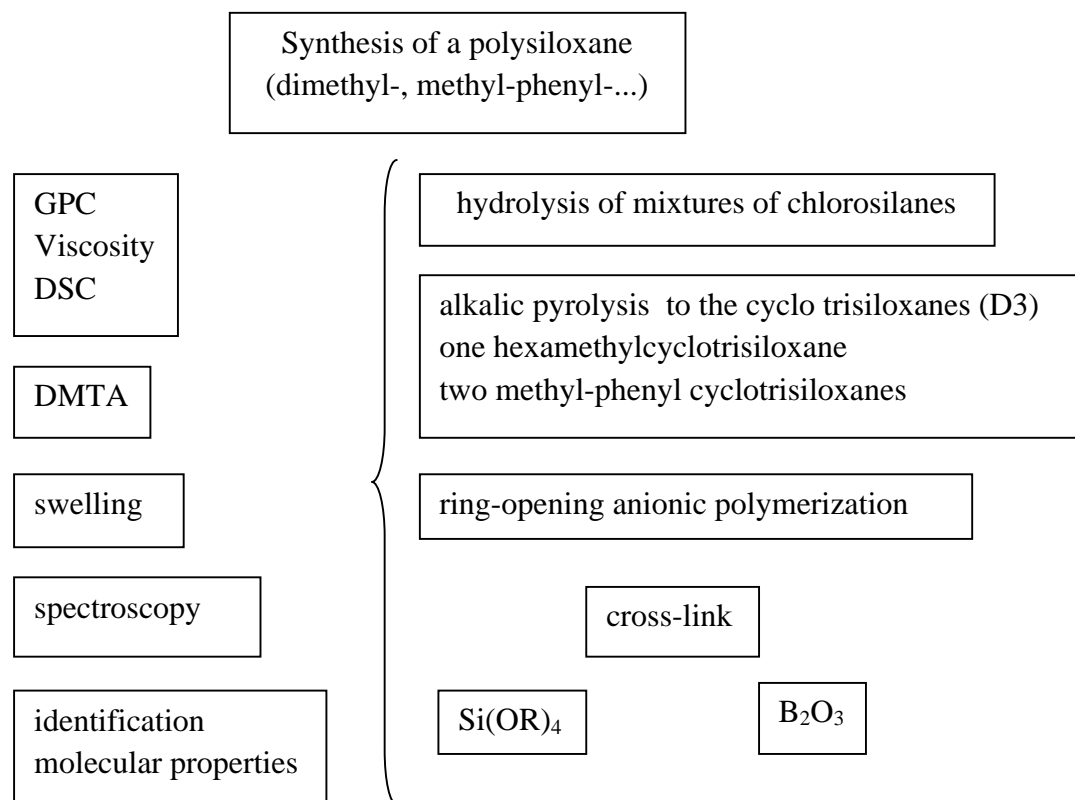


Figure 2. Example of an experimental project starting from the synthesis of a polysiloxane via different synthetical routes and analysing the properties with different methods

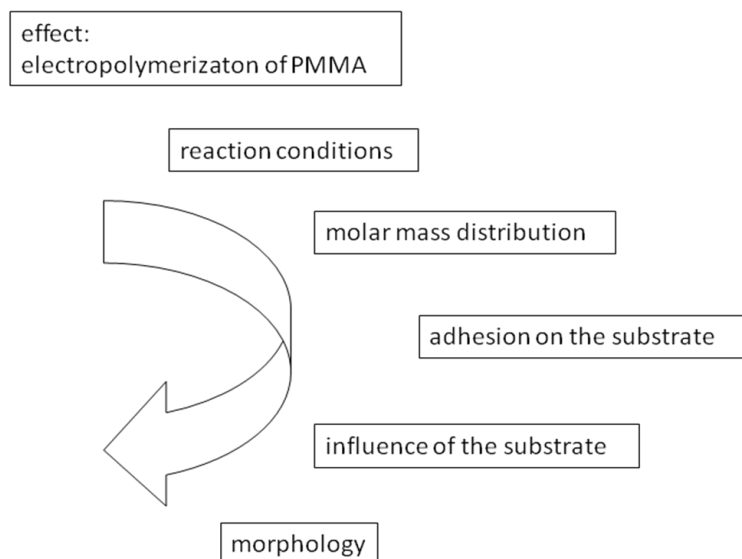


Figure 3. Correlation between experimental parameters and different materials properties: electropolymerization on to a surface as an example

In groups of students of different mother tongue the learning effect can be significantly enhanced by the use of electronic teaching media that allow not only matter-of-fact information about the proper terms of the equipment used and links to general sources of information such as the IUPAC recommendations on terminology and nomenclature^{7, 8} but that also provide terms in different languages on demand in the teaching material like in an on-line dictionary in a "click-and-translate-mode". For example, a liquid-liquid extractor is mentioned in the text. A link leads to a corresponding figure giving the names of the individual parts with further links to translations to different languages. This can be in particular of interest for languages using special characters such as Chinese, Hindi, Arabic or Korean. Same can be done with chemical terms that can be linked to the online version of the IUPAC Gold Book (Compendium of Chemical Terminology)⁹ that contains more than 7,000 entries providing the correct definition.

Further reading for integrating of the tre-

mendously growing fields of nano-technology and biomedical materials science can be found in Skoulidis et al.¹⁰ and Shieh et al.¹¹ New trends and developments in Materials Science have to be incorporated in a curriculum as early as possible to make the teaching up-to-date, another way to generate the students interest in the problems of Materials Science. Giving a solid scientific 'stem' with the historic development of materials science together with 'young shoots', i.e. the most recent developments, on the 'old stem' and realtime active involvement of the students makes the curriculum most attractive. Sometimes boosting areas of Materials Science do not exactly come with advertizing, popular adjectives like 'nano', 'high performance' or 'sustainable' but have an amazingly close 'hand on problems' relation to our daily life, as for example shown by Brostow et al.^{12, 13}

It is a big difference to explain the principles of Materials Science to university students, to college undergraduates or to high-and middle school students.¹⁴ This also has to be considered in the educational curricula.

CONCLUSION

Controlled self-developing lab-courses in Materials Science can provide a more profound learning effect in contrast to a rigid, inflexible curriculum. This has to go along with a correspondingly flexible class respectively seminars that go deeper into special topics of a problem as it becomes necessary. Good results can be obtained with a small number of students allowing them to identify problems or interesting questions worth to investigate by themselves with only a limited guidance by a tutor. Starting with the synthesis of a polymeric material following lines of interest identified by the students themselves guided only by a minimum of "tutorial reins" result in a higher engagement and more enthusiasm, leading to a kind of a self-propelled learning that strengthens the self-confidence of the students. This type of a practical education is often more effective compared with pre-programmed learning.

The advantage of this concept leads to a deeper interest of the students in their subject, a faster process of learning, activation of the student's potential of imagination, curiosity, brain storming and teamwork. They actively start creating ideas and do not so much follow described routines, they feel challenged.

Disadvantages certainly are that such a concept only works with a small number of students, and skilled assistance is required with supervisors suited to non-routine courses where a high degree of flexibility is inevitable. Good research equipment should be made available and last not least good students are needed, students who are not going for a just a grade in the first place but who are interested in the subject they want to study because they do not want to be fed with facts but want to gain knowledge.

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SOFT MATTER: A PERSPECTIVE

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ABSTRACT

Soft Matter is a term used generally to describe materials that are held together by weak non-covalent interactions - with bond energy of the order of kT. Soft Matter obtains its identity largely from three categories of materials, *viz.* colloids, polymers and surfactants. It is common to have materials, which may belong to two of these categories simultaneously; in fact, there are some biological systems such as proteins, which have some features characteristic of all these three forms of Soft Matter. On the other hand, there are Soft Materials like liquid crystals, which may not fit strictly into the limits of these three categories, underlining that this classification is only 'broad'. Soft materials sit at the interface of Chemistry, Physics, Biology and Materials Science, thus forming an important focus in the interdisciplinary sciences. Today, traditional materials such as metals, ceramics and wood have partly been replaced by synthetic soft materials, which may be stronger, lighter, cheaper, and which, through scientific research, can be tailored to specific requirements. Hence, we are surrounded by products of daily use made from man-made Soft Matter: toiletries, gels, medicines, plastic containers, soft furnishings, cosmetics, etc. A variety of modern equipment and components in automobiles or in the workplace are often made of, or coated with, soft-composite materials. In spite of these facts, Soft Matter is rarely integrated in traditional instruction in Materials Science and Engineering. The present article is thus an attempt to remedy this situation. Some research done on soft materials recently in the laboratory of the author will also be presented briefly as illustrations. The emerging trends of using Soft Matter in health-related technologies will be highlighted.

Keywords: *Soft Matter, Colloids, Polymers, surfactants, Self-assembly, Applications*

1. INTRODUCTION

The term Soft Matter applies, generally, to materials that are held together by weak non-covalent interactions - with low bond energy of the order of kT, which is comparable to entropic forces. A chocolate is a typical example of 'Soft Matter' - it has a complex

structure and mechanical properties of solids at room temperature, but liquid-like in your mouth! A mere touch of our hand melts its surface, leaving a trace of the chocolate on our fingers. A significant change thus occurs in its mechanical properties due to an input of mild thermal energy - a typical characteristic of the

'soft' nature of the chocolate.

Soft Matter, even in its condensed state, can flow like liquids (has comparable viscosity), and at the same time it can bear stress (elastic deformation) like solids¹. In other words, it is viscoelastic (viscous + elastic). There are numerous examples of 'soft matter' from our daily lives such as rubbers, gels, pastes, creams, paints, soaps, liquid crystals, proteins, cells, enzymes, etc. that we shall discuss in this article. In spite of these facts, Soft Matter is hardly incorporated in instruction in Materials Science and Engineering. This was the motivation for writing the present article.

The term "soft matter" was coined by Pierre Gilles de Gennes as the title of his 1991 Nobel Prize acceptance speech², instead of the phrase 'Complex Forms of Matter' used in his Nobel Citation. Prior to that, the term 'Complex Fluids' was used for such materials in the USA. Two reasons provoked de Gennes to introduce the new term Soft Matter: (i) all the systems that qualify to be under this category are not necessarily fluid (like rubber, gels, etc.), and (ii) the usage of the word 'complex' may at times drive the young students away from these very fascinating materials. So, which materials should, by definition, be called Soft Matter? It is not easy to constrain the wide-ranging soft materials under a very strict definition, but one could define Soft Matter as what is not a simple liquid, not a hard solid and, of course, not a gas! Three broad categories known to us in Materials Science, viz.

Colloids,
Polymers, and
Surfactants

can broadly describe most of the known soft materials mentioned above, as well as elastomers, biological macromolecules, membranes, milk, blood, etc. Some biological systems such as proteins have all three characteristics of soft-matter, viz, polymeric, amphiphilic and colloidal. There are many systems in biology which have two of these three; prominent among them is DNA, e.g. calf thymus DNA³, and viruses⁴, e.g. tobacco

mosaic virus. The size of a large variety of biological aggregates falls in nano size regime. In fact, Nature went NANO millions of years ago, when it chose the size of a 'cell', the basic unit of life, to be in the nanometer (nm) regime. Why such tiny cells? A cell has to carry out all metabolism. All food and oxygen has to come in through the cell's surface. As size grows, surface area per unit volume falls. A 5-fold increase in diameter cuts the *surface area/volume* to 1/5 of the original: the cell starves. The cell is programmed to do 'energy in and garbage out' for its growth, adaptation, response to stimuli, and reproduction, and the surface-to-volume ratio of the cell needs to be optimum to do that most effectively. To respond to a change in the environment, the signal must travel from the surface of the cell *to and from* all parts of the cell. The bigger the cell, the longer it takes to respond to the environment. Hence, cells are limited to nm sizes.

The above three categories can be extended to include soft materials like liquid crystals. Unlike in "hard" condensed matter, such as Si or Cu, where strong covalent or metallic bonds give a crystal its strength and a high cohesive energy (*i.e.* the energy required to separate atoms), Soft Matter is characterized by weaker bonds - such as van der Waals, with bond energy being of the order of thermal energy kT , so that bonds are easily broken and re-formed. The nature of the bonding in Soft Matter is 'soft' (non-covalent) which could be electrostatic (charge-charge, dipole-dipole), van der Waals, H-bonding, amphiphilicity (*this combination of hydrophilicity and hydrophobicity is exploited extensively by Nature in its self-assembly processes*), dispersion forces, etc. Much of Soft Matter is of molecular origin - the bonding in which is governed by molecular interactions which decays with distance r and therefore, becomes significant at nm distances, the characteristic scale of the Soft Matter.

Four typical characteristics of Soft Matter are:

- i. the length scales in them (1 - 200 nm) lie

- between atomic and macroscopic;
- ii. they exhibit thermal fluctuations and Brownian motion;
- iii. a tendency to self-assemble into hierarchical structures (*i.e.* ordered on size scales larger than molecular); and
- iv. short-range forces and a variety of interfaces.

The multidisciplinary nature of the subject of Soft Matter implies that its investigation encompasses expertise from the subject areas of Chemistry, Physics, Biology, Materials Science and Engineering, Chemical Engineering, Computer Science, and above all the insights into the natural processes like self-assembly^{5,6}. Soft Matter is getting center-stage attention with the advent of powerful techniques, such as the use of synchrotron radiation, small angle neutron and x-ray diffraction or scattering (SANS and SAXS), confocal microscopy and scanning probe microscopes. It is not surprising, therefore, that research programs related to human health and environment are being strengthened in the twenty-first century by bringing different aspects of Soft Matter and its interdisciplinarity into focus. The Nobel 2009 laureate Venkatarman Ramakrishnan has a Ph.D. in Physics, works in a Molecular Biology lab and won the Nobel Prize in Chemistry for '*the protein producing ribosomes, which transform DNA into living matter – like skin and immune system and so on*' – a subject of Soft Matter!

To build interest in the subject of Soft Matter, de Gennes undertook extensive lecture tours, mostly in France, and delivered popular lectures in dozens of schools and often gave the example of how the Amazon Indians made their rubber boots by collecting the oozing sap from a rubber tree (natural rubber is a viscous white liquid called 'latex', which comes from the rubber tree, *Hevea brasiliensis*⁷) and spreading it around their bare feet. Their joy would know no bounds when, in a few minutes, the thick liquid solidified in the form of boots. What truly happened was that the oxygen from the air reacted with the long molecules of latex,

binding them together by linking them through an oxidation reaction, resulting in hardening of the thick latex liquid into the shape of solid boots. What is notable is that significant change occurred in the mechanical properties of latex due to a mild chemical action. This is the hallmark of Soft Matter, which comprises physicochemical systems that have *large response functions*, *i.e.* on which even a mild external influence has a big effect. However, the joy of Indians was short lived, since soon after, in a matter of a few hours their 'shoes' would crumble into powdery material. This was because oxygen is too severe an oxidant and after binding the large latex molecules, it continues the oxidation process and cuts the long chain molecules into much smaller units, and thereby the latex rubber lost all its characteristic properties. It was Charles Goodyear (1800-1860), who discovered in 1839 that by using sulfur, a milder oxidizing agent compared to oxygen, he could crosslink the isoprene monomer, successfully, without any breakage of long chains, to yield the gummy rubber, one of the most useful solid polymers of modern times. The process patented by Goodyear in 1844 is called vulcanization, where each of the adjacent isoprene monomers are crosslinked by 8 atoms of sulfur (S8 units), during the polymerization⁸. Quite similarly, a hair-dresser giving a lady a permanent wave exploits the curling iron's heat that creates links (because of the sulfur atoms in the hair's keratin) that 'freezes' the curls.

2. SELF-ASSEMBLY

Nature regularly (self)assembles large biological structures from families of small building blocks, *viz.* biomembranes from lipids, polysaccharides from sugars, RNA/DNA from nucleotides and proteins from peptides, all of which are Soft Matter. For this, Nature adopts a bottom-up approach – taking a molecular functional building block, and using non-covalent bonds (H-bonding, van der Waals, hydrophobicity, π -bonding, etc.), which consume an order of magnitude less energy than the covalent synthesis, for self-assembly.

Moreover, nature works largely at ambient conditions of temperature, pressure, or pH , unlike the energy-guzzlers and environment-unfriendly man-made processes adopted, say, for steel-making.

Nature has mastered the molecular self-assembly processes, using it to fabricate many useful materials, such as wood, bioceramics, bone, spider silk, etc. from simple building blocks. Besides DNA, proteins, etc. a classic example of complex coded self-assembly done by Nature for over a billion years is the assembly of *E. Coli* bacterium, a unicellular organism of about 10 microns size, which has sensors, memory, actuators, flagella (i.e. nanoscale molecular motors), all embedded in it to conduct jobs allotted to them. Another such example of Soft Matter is seen in the biomolecular aggregates which are important parameters to monitor our health, viz. the 8-11 nm sized HDL (the “good cholesterol” high-density lipoprotein), and the 18–25 nm sized LDL (the “bad cholesterol” low-density lipoprotein) both having cholesterol, phospholipids, proteins, etc.

Using the same self-assembly processes, interesting functional molecular materials can be prepared, one class of which is molecular magnets, which can have attributes of Soft Matter. For instance, single crystals of a new anisotropic Heisenberg chain compound Mn(III) tetra(*ortho*-fluorophenyl)porphyrin-tetracyanoethenide (Figure 1) prepared by our group, exhibit interesting magnetic behavior, including slow magnetic relaxations⁹.

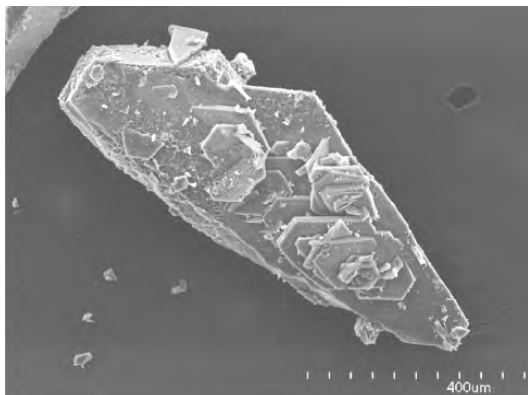


Figure 1. Single crystal of a linear-chain structure of Mn(III) tetra(*ortho*-fluorophenyl)-porphyrin-tetra-

cynoethenide with alternating Mn-porphinato and TCNE donor-acceptor ligands.

This material, assembled from ferrimagnetic chains composed of moment-bearing Mn-ion ($S=2$) and the radical tetracyanoethylene (TCNE, $S=1/2$), shows behavior typical of a ‘single-chain magnet’. A related compound, Mn(III) tetra(*meta*-fluorophenyl)porphyrin-tetracyanoethenide shows a different behaviour of slow magnetic relaxations, an interesting facet of magnetism exhibited by Soft materials at low temperatures¹⁰.

Self-assembly from a bifunctional building block, using a chiral ligand with an unpaired spin, led to the synthesis of a Soft Material which is chiral as well as a ferrimagnet below 53K (T_C), which we obtained in collaboration with the group of Inoue from Japan¹¹. However, the most interesting proof of the Soft nature of a Molecular Magnet was demonstrated by us when bulk magnetic behavior was obtained upon successive dehydrations of the building block (as shown in Figure 2); this process is reversible, viz. re-hydration destroyed long-range magnetism, splitting the ferrimagnetic chains back into non-magnetic building blocks. These CoCu-based molecular ferrimagnets exhibited high coercivities and at times even a color-change at the magnetic transition. We called them ‘Molecular Magnetic Sponges’ precisely since the process of dehydration-rehydration is reversible^{12,13}.

3. BROAD CATEGORIES of SOFT MATTER

3.1. Colloids

A colloid has sub-millimeter particles (not single molecules) of one phase dispersed in another continuous phase. Colloids lie between suspensions and solutions, the well-known examples being milk, blood, clay, paints, etc. An interesting example of a colloid is the ‘Indian ink’ (the black ink used by scribes of India and Egypt since ancient times, as long as 4000 years ago, for their writings). It is obtained by dissolving particles of carbon black in water. However, this simple act yields only a

suspension since the carbon particles quickly flocculate and form a sediment at the bottom of

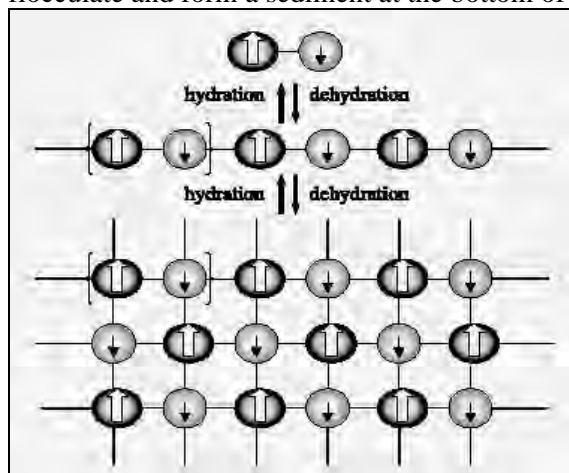


Figure 2. Dehydration Polymerization and Sponge-like Reversibility (typical of Soft Matter) in the molecular magnets $[MCu(obbz)] \cdot nH_2O$, where $M = Mn, Co$, and $obbz$ stands for 'oxamido bisbenzoato'. Upon dehydration, the spin-bearing precursors are linked through bonds (i.e. polymerization), viz. $n(S_M - S_{Cu})$. If n is infinite and the system is 3D, then long-range ferrimagnetic ordering occurs. This process is reversible. It should be noted that S_M denotes the large spin on Mn^{2+} or Co^{2+} and S_{Cu} denotes the small spin $\frac{1}{2}$ on Cu^{2+} .¹³

the container. One has to add a bit of Gum Arabic while dissolving carbon black in water, which stabilizes the nano-sized (≈ 100 nm) colloidal particles sterically, as a colloidal dispersion, producing the stable India Ink. It is interesting to note that most colloids are large nano-particles (1-200 nm) dispersed in a continuous phase, and we have been using them in our daily lives for ages, without the knowledge that Nature had provided these nano-phase materials, long before the recent breakout of the focus on 'nano' in modern science.

The process of dispersing a stable colloidal phase (nanoparticle) in a continuous phase can arise from a variety of situations: (i) a liquid-in-liquid dispersion, such as nanosized droplets of milk, mayonnaise, or a salad dressing; (ii) liquid clusters in a solid, like in a jelly/jam; (iii) liquid droplets suspended in a gas, like in mist, fog, hairspray or aerosols; (iv) gas bubbles in a solid/liquid, like in a whipped cream, shaving

cream or poly(urethane) foam; (v) solid particles dispersed in another solid, examples being a pearl, or a stained glass with metal particles suspended in it; (vi) solid particles suspended in a liquid phase, like in a sol, latex paint or a tooth paste; and (vii) solid particles suspended in a gas, viz. in smoke. 'Buckyballs'; i.e. Buckminsterfullerene, C_{60} nanoballs, were discovered in soot! Airborne solid dust particles (100 - 1000 nm) cause water to condense, which eventually form raindrops or snowflakes. It is worth noting that there cannot be an example of colloids based on gas bubbles in another gas phase, because it will never be a stable phase! What are the forces acting on colloidal particles? These are: (a) drag force arising from the movement of a colloidal particle through a viscous medium; (b) gravity, that leads to sedimentation or creaming; (c) random, "thermal" forces from neighboring molecules, which make a colloidal particle undergo Brownian motion; (d) Coulombic forces, attractive or repulsive, which are screened by the intervening medium; (e) van der Waals' forces which are attractive, though quite weak between isolated like molecules, but can exert significant pull between colloidal particles due to the additivity of those forces; and lastly (f) steric forces arising from intervening molecules which prevent a close approach.

Because colloidal particles are larger than molecules and have size comparable to the wavelength of light, they offer interesting optical characteristics. Au-colloid particles (< 100 nm) absorb green and blue parts of the visible optical spectrum, but *transmit* in the red, so a colloidal Au dispersion is red-colored. In 1857 Michael Faraday observed that colloidal gold turned blue if some NaCl was added to it. He concluded rightly that the change in color was due to a change in size of the dispersed particles. Au particles are negatively charged - thus repel each other; adding salt screens repulsion so that Au particles coagulate into larger aggregates - which scatter blue light^{14, 15}.

Natural opal consists of hydrated amorphous silica particles, containing water molecules, up

to 3% to 21% of the total weight. Though not strictly a mineral, it is deposited at low temperatures in the fissures of rocks. The size of silica particles (spherical, typically 250 - 400 nm in diameter) is about 1/2 the wavelength of light, leading to diffraction of the light. Thereby, opals can reflect various colours of light depending on the viewing angle, and are valued as precious gemstones¹⁶. Langmuir-Blodgett (LB) films grown from silica particles have been shown to yield artificial opals¹⁷. There is a possibility to diffract light from them, like X-rays diffract from ordinary crystals, owing to the existence of an optical band gap! This has potential for fabricating optoelectronic devices.

Soft condensed matter is not static but in constant motion at the level of molecules and particles. For each degree of freedom of a particle to move, there is $\frac{1}{2}$ kT of thermal energy. Colloids undergo Brownian motion, which is best described by random walk statistics¹⁸. The phenomenon was first reported by a Scottish botanist named Robert Brown (19th century), who observed spontaneous movements of pollen grains, though the pollen grains were not living entities. For a colloidal particle able to undergo translation in the x, y and z directions, thermal energy around (3/2) kT is needed. Now we understand that Brownian motion results from a slight imbalance of momentum being transferred between liquid molecules and a colloidal particle, which then execute random Brownian paths (Figure 3). Einstein predicted random particle motion in his work on molecular theory^{19, 20}.

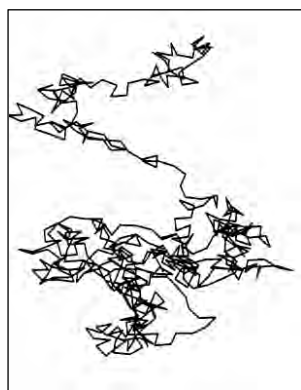


Figure 3. Schematic of a track of a colloidal particle exhibiting Brownian motion²¹.

Typical relaxation times for solids, t_{relax} is exceedingly large, $> 10^{12}$ s. For simple liquids, t_{relax} is very small, namely of the order of 10^{-12} s. For soft matter, t_{relax} takes intermediate values. For instance, for melted polymers, $t_{relax} \approx 1$ s. As a result of thermal motion, a liquid-liquid interface is never smooth at the molecular level. In fact, the liquid-liquid interface has been exploited as a simple template to grow some varieties of Soft Matter like polyindole nanofibers²², conducting polymers like polyaniline and polypyrrole²³, or even other technologically important materials like nanocrystalline Au and CdS²⁴. As the temperature increases, the liquid-liquid interface of course broadens.

Nano-sized colloidal particles, e.g. liposomes and polymeric micelles, preclude the introduction of a hydrophobic substance into the aqueous blood-stream, and can also protect their payloads (enclosed drugs) from degradation. The possibilities are: 1. *Polymeric micelles*: 60 - 100 nm aggregates with an inner core, where hydrophobic drugs may be contained and an outer hydrophilic shell made of PEG (polyethylene glycol, which is non-toxic), Pluronic (block co-polymers), poly(L-amino acid), for instance, for pH dependent release/delivery of poly(L-histidine) at tumour sites; 2. *Liposomes for drug delivery*: diameter ≈ 100 nm, spherical bilayers, made up of phospholipids and cholesterol; they can be coated with PEG and thus can avoid detection (providing stealth characteristics) by the immune system; 3. *Nanoparticles (polymer, lipid, ceramic, 200 -500 nm)*, which can be administered intravenously via subcutaneous, intramuscular, or intra-articular injections, and the biodegradable nanoparticles can release drug in a sustained manner at the target²⁵.

3.2. Polymers

Polymers are large chain-like molecules (like a string of 50 or more “pearls”), built from a structural repeat unit (called monomer), linked together by strong covalent bonds. Polymers are

obtained from monomers through polymerization, like large proteins (polymers) being assembled from amino acids (monomers)^{26, 27}. Polymers can be of different shapes: linear, branched, ladder, network, star, dendrimer, etc.,. There are many familiar examples of polymers, such as rubber, so called plastics (polystyrene, polyethylene) and biomolecules (proteins, DNA, starch)²⁸, all of which are Soft Matter. Polymers have many applications in industry and in our daily lives. For instance, pressure sensitive tapes used in medical applications have polymers as adhesives. Soft polymers can achieve intimate contact with a variety of rough surfaces, leading to mechanical interlocking, using simple van der Waals interactions, much like a gecko can stick to nearly any surface – ceilings or even under water – because of van der Waals attractive forces. Pads on the Gecko's feet have setae and spatulae (millions of them), to facilitate this^{29, 30}.

The underlying structure of a polymer can make it strong for useful applications, like Kevlar used for making bullet-proof vests, which is a cross-linked polymer with strong intermolecular forces³¹. Another soft material with amazing properties is polyoxyethylene - a polymer called Polyox³²; just 1 g of which, if dissolved into 10 litres of water (1 part in 10,000), can facilitate the siphon action even if the end of the tube is raised 20 cm above the surface of the water, or increase the range of a fireman's hose by about 20 % against gravity! This is because Polyox molecules unwind when in water, and thereby pull the column of water like a stretched spring, and in doing so, counter-balance the weight of the water column to accomplish this feat.

Conjugated polymers (with alternating single and double bonds in the polymeric chain) show conducting behavior due to hopping of charge-carriers, provided by a π -electron cloud³³. Such polymers also have other interesting properties,

like they can contract in response to small electrical stimuli, and expand, i.e. come back to their original size, when the electrical stimulus is withdrawn. This raises the interesting possibility of fabrication of artificial muscles (electromechanical actuators) from them. We have demonstrated in our laboratory that microactuator action can be obtained if a small DC voltage is applied to a ribbon of the conducting polymer polypyrrole (PPy) doped with DBS (dodecylbenzene sulfonate, $C_{12}H_{25}C_6H_4SO_3^-$) anions (see Figure 4)³⁴.

Na^+ diffuses in and out of PPy during the application of voltage in an electrochemical cell. This causes a reduction in volume when the ions exit (during oxidation), and vice versa, causing the ribbon to bend almost 90 degrees to the left, or to right depending on the sign of the applied voltage, thus performing as an actuator³⁴. There is potential to develop artificial muscles using this concept, by fabricating bundles of such ribbons to simulate a skeletal muscle, which is made up of bundles of tiny parallel strands. The response time of a polypyrrole-based electromechanical actuator is estimated to be 0.01 - 0.1 s, which is reasonable when compared to that of the mammalian skeletal muscle. However, the strain that develops upon the applied electrical stress is only 2 – 7 % compared to almost 20 % in the case of the human muscles^{35, 36}.

Conducting polymers, particularly polyaniline (PANI) have some very useful properties. PANI's conductivity can be tuned by doping, it is stable in air, and has good optical and mechanical characteristics). However it was considered difficult to grow single crystals of PANI until a few years ago. We have demonstrated recently in our laboratory that micro-crystals of this soft material can be grown using a self-assembled monolayer (SAM) of aminosilane ({3-(2-aminoethyl)aminopropyl}trimethoxysilane) deposited on

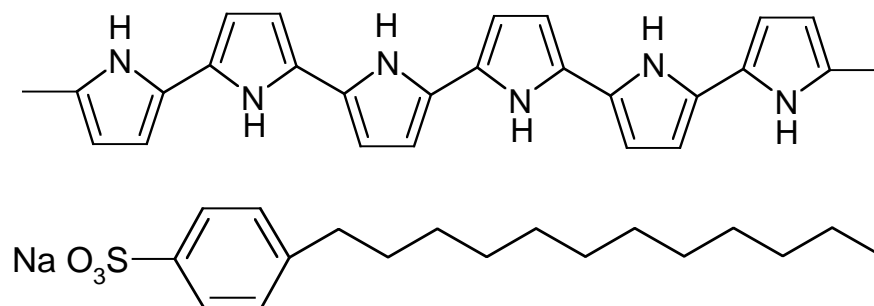


Figure 4. The structures of Polypyrrole and the dopant, Na-dodecylbenzene sulfonate³⁴.

hydroxylated silicon as a template^{37, 38}. In this method polyaniline (emeraldine hydrochloride) gets grafted on a silanized substrate, via polymerization of aniline (Figure 5).

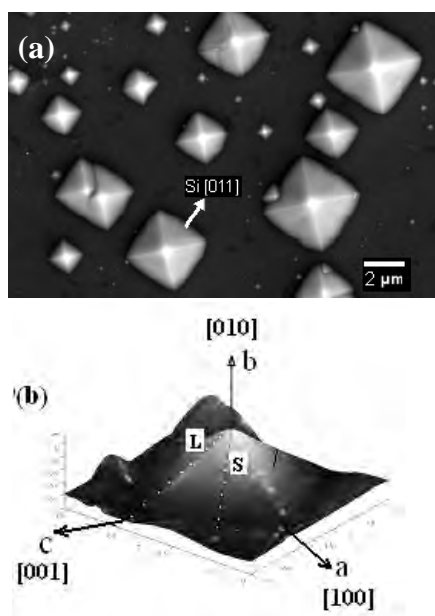


Figure 5 (a) SEM shows micron size fcc crystals of PANI on a substrate; (b) 3D-AFM image of one such single crystal pyramid, L and S denote lateral and slant heights³⁷.

We have shown that a thin film of such PANI crystals can sense very low concentrations (0.5 ppm) of NH_3 gas³⁹. Emeraldine (PANI) is an efficient sensor for NH_3 because N-atoms in both can bond with protons on the polymer chain. Sensitivity and reversibility of PANI to NH_3 comes through deprotonation–reprotonation mechanism (Figure 6).

Triblock copolymers such as $[(\text{EO})_{20}(\text{PO})_{70}(\text{EO})_{20}]$, where EO and PO denote ethylene oxide, and propylene oxide, respectively, form spherical or worm (rod-like) micelles in aqueous medium, under the influence of solvents or additions of salts⁴⁰. The self-assembly of such micellar aggregates has brought forth their use as containers for drugs. Drugs conjugated to polymers stay longer in circulation than just drugs alone, and cannot pass through normal blood vessels because of their large size. However, some tumours have leaky blood vessels, that can allow these large drug-conjugates to pass through and deliver drug directly to the tumour with minimal drug going to normal tissue⁴¹.

3.3. Surfactants

Soft Materials assembled from amphiphilic molecules (i.e. surface-active agents, or surfactants for short, e.g. phospholipids), which have a polar head (hydrophilic, or water-loving), and a long non-polar hydrocarbon (C-H) chain which is hydrophobic (water-repelling), exhibit interesting behavior of aggregation into regular ordered structures (like bilayers, micelles, vesicles, liposomes, etc.) at the air-water interface, via self-assembly^{42, 43}. Lipid molecules spontaneously form such structures in water, depending on their shape, the energetics, and entropic effects which determine the structure/dynamics of complex aggregates. As a rule-of-thumb, wedge-shaped lipid molecules form micelles; and cylindrical-shaped molecules (phospholipids) form bilayers^{44, 45}. Being

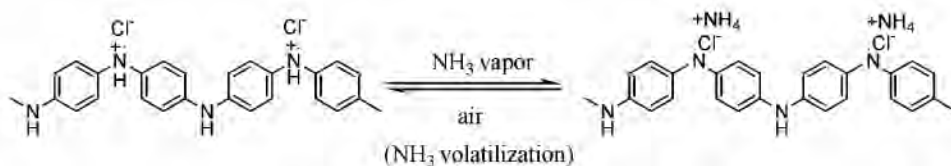
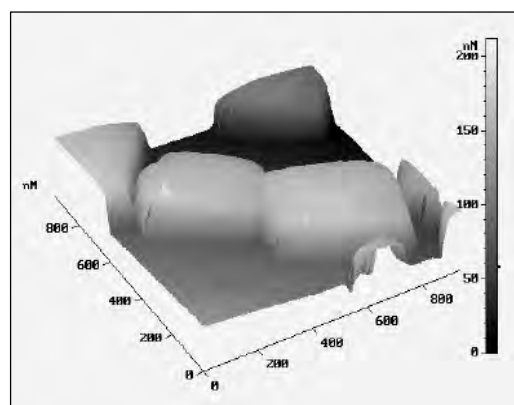


Figure 6. Deprotonation–reprotonation mechanism for sensing ammonia gas by PANI film³⁹.

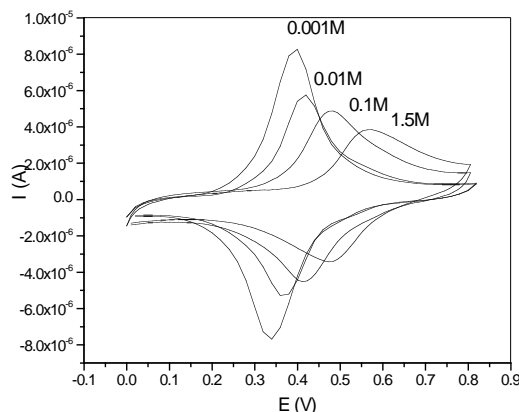
hydrophobic, lipids can form stable bilayers (basis for biological membranes). A cell membrane is a lipid bilayer 3–4 nm thick, embedded with proteins. It acts like a barrier that has selective permeability, viz. H₂O, CO can diffuse through it freely, but not Na⁺ / K⁺, which need hydrophilic channels or carriers to cross over^{46, 47}. Lipids also serve as a source of energy for the cell; lipids can produce twice more energy than sugar (by weight). Soap bubbles are, in fact bilayers of detergent molecules^{48, 49}.

We can use the air-water interface to grow functional materials. Use of a Langmuir-Blodgett (LB) trough enables preparation of ultrathin films (mono- and multi-layers) with controlled thickness and well-defined molecular orientation^{50, 51}. Crystals of useful materials (such as cholesterol) have been grown using an LB trough. Using this technique, we have grown fcc single crystals of a Prussian-Blue analogue Ni-hexacyanoferrate (Figure 7), by employing an octadecylamine monolayer on the water surface as a template⁵². We have used multilayers of such crystals as a K⁺ ion sensor⁵³.

Lungs are not hollow bags, but spongy tissue with many infoldings! Gas exchanged between air and blood in respiratory bronchioles and numerous tiny alveolar sacs (1.5 billion/lung providing a huge surface area for gas exchange). Each alveolus is coated by a monolayer of material made of proteins and surfactants, which helps it to expand/contract since it has the requisite surface tension. Puncture/destruction of this monolayer coating of pulmonary surfactant can lead to Respiratory Distress Syndrome, or even death. Simulation of the composition and other mechanical characteristics of the lung surfactant films provided by Nature is done by some research groups



(a)



(b)

Figure 7. (a) A three-dimensional AFM image of 900 x 900 nm² area, of Ni-hcf film on a mica substrate grown under the ODA monolayer over 3 days; and (b) cyclic voltammograms giving the response of 19 layers of DODA-NiHCF to different K⁺-ion concentrations using 0.001, 0.01, 0.1 and 1.5M KCl solutions^{52, 53}.

using the Langmuir-Blodgett technique^{54, 55}. Some studies have been also done in our laboratory to simulate the adhesion of blood platelets to the inner arterial surfaces (to address the formation of clots/blockages in arteries) by deposition of LB films of phospholipids, glycolipids and cholesterol in the

appropriate ratio (the cell mimetic composition) on polycarbonate (PC) membrane surfaces in collaboration with Sree Chithra Tirunal Institute for Medical Science and Technology at Thiruvananthapuram, India⁵⁶. Under this study, the contact angle behavior of these films was investigated in addition to their surface morphology using atomic force microscopy.

3.4. Liquid crystals

Whereas solid crystals possess orientational order as well as positional order of the building block in them, a liquid has neither orientational nor positional order, which is why the molecules in a liquid can move about freely. In between these states of matter is an important class of Soft Matter, known as liquid crystals, in the bulk of which rod-like molecules possess orientational order but have only limited positional order⁵⁷. This gives them anisotropic physical properties. A liquid crystal is called thermotropic or cholesteric depending on whether it undergoes phase transformations (like smectic, nematic or isotropic, etc.) upon heating/cooling, or upon the application of a concentration gradient⁵⁸. In thermotropics, van der Waals' forces of attraction are balanced by forces from thermal motion. A liquid crystal film can show useful features under application of applied electric fields, which can align the elongated molecules in it, blocking the passage of polarized light, which came through before the field was applied. This is the principle of liquid crystal displays - used extensively in many devices including digital watches^{59, 60}.

4. SOFT MATTER and HEALTH SECURITY

Soft matter is ubiquitous in living things. In fact, it can be said that *we* are soft matter, since the human body comprises a great deal of DNA, cells, membranes, proteins, etc. Again, when we fall sick our problems are created many a time by viruses, E-coli, pathogens, LDL, etc. Effective management of disease and aging (i.e. health security) has much to depend on potent drugs/pharmaceuticals. With ageing population,

the diseases of the central nervous system (CNS), *viz.* the brain, the spinal cord, and nerves (neurons) are spreading. These include Alzheimer's disease, Parkinson's disease, epilepsy, stroke, migraine, etc. To counter them, the Global CNS drugs market is projected to grow to > \$ 100B in 2015, and the challenge before the pharmaceutical industry is not only to design potent and safe drugs, but also to find ways to get drugs across the guardian of the brain - the blood-brain barrier (BBB). Other important issues for human health are the grafting/regeneration of human bones, muscles, cells, and skin. The subject of tissue engineering is fast gaining importance. All these health-related problems deal with Soft Matter, and their solutions need an interdisciplinary approach. For instance, the supermacroporous cryogels, produced by cryogelation of monomers or polymeric precursors, with adequate mechanical strength and osmotic stability, are potential scaffold material for various biomedical applications⁶¹. Similarly, the quest for energy security through photo-voltaics is related to mastering the nature's process of photosynthesis, which again deals with Soft Matter.

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HOW TO 'SURVIVE' AFTER GRADUATING IN MATERIALS SCIENCE - IV: WRITING COMPELLING PAPERS

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ABSTRACT

This article describes our view of how to write compelling papers for Materials Science journals (and hopefully for broader audiences). Most of this discussion also applies to both physics and chemistry journals. We will discuss the usual forms of written scientific communications, including short letters/communications, full papers, comments, perspectives, review articles, book chapters and even books. Besides the 'technical' or 'nuts-and-bolts' aspects of scientific writing, we once again emphasize a fundamental concept that we developed in the previous two articles, namely: *learn to play from the other side*. We remind the reader that anything that matters in the world of science is also peer-reviewed before it is seen by the ultimate readers; therefore, once again, we advise the reader to place him/herself in the mindset of those who are going to evaluate their written work to anticipate their reactions and forestall objections. As a matter of background, we remind the reader that this is the fourth article of a series. It follows the first (in which we described how the graduate course on 'Survival Skills for Scientists' was created at Institut National de la Recherche Scientifique (INRS) in Varennes (QC)), the second (in which we offered basic advice on how to apply the skills and knowledge acquired in graduate school to finding a job and developing a career in the 'real world' of science after graduating) and the third article (in which we described the Peer Review System and how it is used as a form of quality control in modern science).

INTRODUCTION

As pointed out by many illustrious authors before us, the best results that scientists are able to generate in the laboratory do not really 'exist' in any practically useful sense until they are published in a well-recognized venue, usually referred to as a "*peer-reviewed*" journal¹⁻⁶. In addition, due to increasing com-

petition for funds, for resources in general, and for positions/jobs, scientists are now constantly being made aware that they should "publish, or perish". (For general advice on scientific careers, we refer the reader to References 7-13. The total number of these scientific journals and consequently of papers published yearly worldwide has increased steadily over the last few decades (nor has the quality deteriorated

significantly), together with the number of journals and even the number of conferences. This increase means that it is more and more difficult for any individual paper to stand out from the others, and thus it is more and more important that you pay attention to what you have to do to produce publications that can indeed stand out from the others. Hence this paper.

To get to this desired state of refereed publication of a piece of work, the report you write must pass through the first gatekeepers (i.e. the editors), and then through the referees. Your report must sell on its quality and originality as well as on its clarity. Your chance of success will be better (not to mention the quality of the communication) if you take care to appeal to two classes of browsers or readers. At one level, to make the widest impact, you wish to reach people who may have only a superficial knowledge of the field (such as the editor and the browsing reader) and who therefore must, so to speak, be wooed. At the deepest technical level, however, you also need to convince the experts (the referees, the authorities in the field and your critics). They are the ones who know the field well, but they (or rather a subset of them) are also the ones who must first be convinced that your work is worthy (by the standards of the field) to be added to the canon of archived publications.

Before and after this archival peer-reviewed output there lie the more ephemeral but nonetheless vital communications delivered directly to the public in the form of oral presentations, invited talks, seminars and conference posters; these will be discussed in a forthcoming article of this series.

SCIENTIFIC WRITING: GENERALITIES

To be a successful scientist it is not enough to have original ideas, you must also be able to communicate your science and insights to others. You must therefore become a good communicator, and learn how to disseminate your ideas widely. You will have to

communicate your results and conclusions effectively in each publication, and to disseminate them broadly by arranging to publish in the journals with the best impact and which will agree to transmit your work to the world. This transmission will not only be most immediately apparent to the specialists in your community but also to a wider audience of scientists from different fields and eventually perhaps even to the layman. This ability to communicate effectively distinguishes at least partly, very good and good scientists from the average or below. The ability to do this can be learned and can always be improved.

Beyond this somewhat obvious view of the public communicator, there is the fact that the scientist who wishes to succeed widely (and don't we all) must be able to communicate on at least two levels. Besides communications to peers (initially through anonymous peer reviewers) via peer-reviewed publications, there are also more restricted (i.e., less public) communications to funding agencies and to various committees (again through peers) for funding and academic recognition. Since most of this communication is written, at arms' length, so to speak, without direct contact with the target audience, doing it effectively is obviously essential to success here.

The purpose of this article on written communication is not to help you to learn the basics of prose writing. (There are many excellent books for that. Our best advice to improve your prose is to read widely, and not just from the scientific literature¹⁴.) Rather, this is the place to discuss how to package and color the messages you want to send, to understand that you will always be sending more than one message at a time, and to understand and control all the messages (both explicit and implicit) that you will be sending.

Your most important underlying message, the one which you cannot avoid sending with each communication, is the one of *who you are*, or at least how you appear to the readership. To transmute a well-known aphorism of the Canadian communication guru Marshall

McLuhan (who famously said, “the medium is the message”), here you should understand that “the message is the messenger”, since the underlying message of your science communication is who and what you are. In fact, anything of any length that you write shows the reader to some extent who you are. However, like an actor in a play, if you pay attention, you can also learn to appear to be something more and perhaps rather better than harsh reality. Another aspect that you should learn to keep in mind is that usually you are engaged in *advocacy*. You are not just sending an objective message (“take an impartial look at this”), you are also putting forth your particular point of view (“and this is what it means”). Be aware that your voice will always be in your prose unless you make great effort to remove it. You should make the conscious effort to put on your “objective” spectacles and try to step back from the work and see what kind of a person you would seem to be.

Structuring the explicit text can be done much more effectively if you imagine a rather skeptical reader and then answer the questions, which such a reader might well, come up with. It is even better if, in the text, these questions can be answered before the reader even thinks of them. If successful the feeling will tend to arise naturally in the reader that this author is “really quite intelligent and someone to get to know”. This arises because the feeling also implies that “this author thinks like me”. (This is harder to do than one might think at first sight, because the most important unanswered questions, the ones that tend to block the reader out are often just those, which you are unlikely to invent for yourself. In lieu of this self-blindness, this is also another area where it is a very good idea to get help from others.)

Apart from the tactical aims in a given application, it is worth keeping in mind (for almost anything you write) that as indicated above you should try to impress two distinct levels of readers. One is class of reader is the eagle-eyed professional, someone who is perfectly at home in the discipline. It is invaluable if you can persuade a colleague to perform

this function — that of the Devil’s advocate — *before* your manuscript is submitted. You should also, however, try to communicate through the text with someone who is more like an informed layman, perhaps another scientist not at all in your specialty, or even further away. By the way, most of the top-ranked journals include this sort of intelligibility in publication in their criteria for acceptance. (This is because they are well aware that good scientists like to graze a bit outside their specialty and including this wider circle of readers will increase the journal’s citation record and overall impact. All too often, and most frequently for reasons of space, this requirement is often the first to be sacrificed to satisfy more technical requirements raised by referees, who as experts are not usually charged with paying attention to general intelligibility.)

By the way, this two-component audience aspect often applies to more restricted venues. In any specialized committee of your peers (such as those assembled for reviewing applications for funding) there should as a matter of course be an expert or two in your own field, but there will usually be many more who are experts in other fields but who are well qualified to easily understand your work, providing it (or at least the principal points) are simply and clearly explained. (Most members of such committees in any case would like to believe that they are not narrow specialists and can get the gist of most things that they are asked to evaluate.) If you can clearly explain the essentials to these scientists, such people will be much more inclined to accept that you know what you are talking about in the difficult and abstruse sections that they do not really follow. They will feel this that much better if they are finding themselves able to follow something noticeably outside their area of expertise, and thus their opinion of your work will likely be improved considerably. These people also vote on decisions and can sometimes counteract the excessively hostile expert(s). You may even find that the expert(s) will approve of the way that you can summarize the core of your work and infer that you are thinking clearly and are thus less likely to go

astray later in the research. (After all, this may even be true.)

Both for publication and for other texts, the resulting text may be a bit uneven, stylistically speaking. This is to some extent unavoidable, since dense and complicated technical paragraphs with long and complicated sentences (often so because of length limitations) and much technical verbiage are being interspersed from time to time with shorter paragraphs, with short, clear sentences with little technical jargon. If this lack of homogeneity is the price of clarity and of being able to address a wider public, then so be it.

We now turn to discussing some particular aspects of peer-reviewed publication. As we do so, we emphasize that the more senior you become, the larger the fraction of your time that you will spend writing. As your career progresses, you will spend less and less time in the laboratory, and more time directing those who do and more time advocating for the work thus done not only in peer-reviewed papers but also on many other levels. The effort in improving your writing skills for peer publication will be invaluable in the other areas as well, and we will be turning to these areas after we have dealt with peer-reviewed publication. It should also be recalled that the training of future scientists should include training them to communicate effectively.

PUBLICATION STRATEGY:

Where to publish? In letters or regular papers?

As we all know, the “normal” means of publication is via the peer-reviewed scientific paper. The shorter publications (Research Notes, Brief Communications and the like) are *either* for more limited topics which are not of the same weight as a regular paper (Brief Notes or the like) or for brief reports but on very important topics (so important as to be in the nature of “breakthroughs”) for which rapid publication before a wide audience is deemed essential (usually termed Letters or sometimes

Rapid Communications). It is the usual assumption that this urgent short publication will be followed by at least one full paper and one should hope several papers. (All too often, however, this is not the case. One then sees what are almost a series of short publications on a given topic, with few full papers, and often stigmatized as “serial publications”.) It is essential that the important short publications are clearly identified as such, and not confused with their humbler cousins. This is relatively easy because of the structure of the refereed literature.

It is worth pointing out that in some disciplines and sub-disciplines (e.g. biology and engineering) in which the authors of this paper are not directly active, short papers and communications are not considered prestigious at all. In fact several biologist and engineer colleagues frown on our appreciation of short publications, noting that in their field “*you either tell the whole story or you’re not taken seriously*”. Obviously you should use the strategy appropriate for your field.

For topics which are not extremely new, the work on these more established topics tends to be published in only a few major journals, which thus become the “normal” journals for the field. You should have a very good reason for publish a paper in a journal, which is not much used for the area in which you are working (as evidenced by the references you give). It may happen that the Editor may then say something along the lines of “We notice that only a very small fraction of the related papers to which you refer have appeared in our journal. We think that it would be better for you to submit to one of those other journals.”

Since we wish to discuss this hierarchy of journals in a field, we begin by recalling the unit of measure, which is commonly used to order the journals prestige, namely the “impact factor”. This term is applied to scientific journals (often by people who have not checked into their source or origin) and we will use it (or simply impact) in a general sense as the effective ranking or rating used to place

journals in a hierarchy of effectiveness in dissemination. For those readers who have not yet taken the trouble to look up “impact factors” of scientific journals, here are a few relevant gleanings from Wikipedia. “The impact factor, often abbreviated IF, is a measure reflecting the average number of citations to articles published in science and social science journals. It is frequently used as a proxy for the relative importance of a journal within its field, with journals with higher impact factors deemed more important than those with lower ones are. The impact factor was devised by Eugene Garfield¹⁵, the founder of the Institute for Scientific Information (ISI), now part of Thomson Reuters. Impact factors are calculated yearly for those journals that are indexed in Thomson Reuters Journal Citation Reports.” (It is worth reading the rest of the article for general background as well.)

Returning to our main topic, of the “normal” journals in which work in your field often appears, there will be some order of preference (other things being equal) and this is often given by the ranking of impact factor of those journals. Within this hierarchy, while no journal editor ever wants to publish papers with errors or with material, which is not, truly original, some of the higher-ranking journals may have an additional level of excellence required. In effect, although they find no errors in a particular submission, although it appears original and although the field is indeed one, which they frequently publish, that is not enough; in effect the journal may say, “This material is not quite of the high standards we set ourselves, so perhaps you should go elsewhere”. Of course, for the top journals the editor will find this easier to say this more directly, “While there’s nothing wrong with this work, it just does not have the wide impact for which this high-impact journal is being reserved.” Naturally, since the prestige of publishing in that journal with higher impact than another, is a key point, the authors often contest this assertion negative opinion rather vigorously. Of course, the discussion of this point then delays the eventual acceptance or rejection. However, as is often the case when

it is the higher-ranked journals which are involved, the speed of publication is really something to which only lip service is paid, since reaching the right public with maximum impact (plus the perceived publication prestige in the authors’ résumés) is what is really being sought by the authors. When the journal was first established, speed to publication was a primary objective of the authors, but later, when the journal has acquired sufficient prestige, publication as such and not speed becomes the dominant objective of the authors.

When the prestige of the journal is the dominant aspect, publication in one of the journals in the area of the research, becomes a game in which each set of authors aims at publishing in the highest-ranking of these journals. The game begins by making the initial choice of which journal in which to publish. This often comes down to estimating (1) the level of the work being submitted and (2) the level of the highest-level journal for which acceptance is probable. Aim too high and you may lose much time in the refereeing process and still not achieve publication in the high-status journal you have chosen; aim too low and you have an easy publication in a lower-ranking (and presumably less prestigious) journal than the work should have merited. Remember, however, that as far as eventual citations are concerned, if the work is sufficiently important the citations will come in the end (unless the journal is completely obscure). The citations may arrive more slowly if the work appears in a lower-ranking journal than might have otherwise been the case, but the work will usually be recognized by posterity. Merit will out, in time, particularly in today’s era of instant searches. In the end, the permanent difference in the choice of journal is mainly the perceived prestige of the journal as a citation in your curriculum vitae.

Of course there are also a few very high-status journals which publish exclusively letters or short contributions by other names of very high quality. Examples of these include, for physicists, *Applied Physics Letters* and *Physical Review Letters*; for chemists *Chem. Comm.*,

Nanometers and *Angewandte Chemie*; for materials scientists *Advanced Materials*. (Scientists from other fields are asked to kindly excuse our incomplete listing.) Some other journals publish both regular papers and communications in the same volume, examples being the *Journal of the American Chemical Society* (better known as *JACS*), and *Physical Review A* through *E*. (In these *Physical Review* journals the elite short papers are styled Rapid Communications, but some cynics cruelly term them “failed *Physical Review Letters*”.) Notable materials science journals that mostly publish full papers are *J. Mater. Res.*, *J. Mater. Sci.* and *Mater. Lett.*

Standing above and apart from these more specialized journals are *Nature* and *Science*, arguably the two most prestigious scientific journals in the world, and ones that cover most of science. These both have a section devoted to Letters (*Nature*) and to Reports (*Science*), and a shorter section devoted to Articles, which tend to be longer contributions that report major advances in a given field (each issue only contains one or two of them, on average). They also have a section on very short communications, *Briefs* (*Nature*) and *Brevia* (*Science*) which are one page in length or less. The latter are the most selective and prestigious sections in *Nature* and *Science*. The acceptance ratio for *Nature*'s Brief Communications section is in fact roughly 5%, much lower than the Letters section. While *Nature* used to be a single journal, it is now actually the flagship publication of the Nature Publishing Group, which includes other prestigious journals such as *Nature Materials*, *Nature Chemistry*, *Nature Physics*, *Nature Photonics* and *Nature Nanotechnology*, all of which may be of interest to a Materials Scientist.

Generally speaking, in many (but not all, see the remark above on biology and engineering) disciplines, Letter journals tend to be more selective, and therefore it is more difficult to publish in them. Precisely because it is more difficult, almost everybody would like to get published in a letter journal – the added difficulty and selectivity carry extra prestige

and are often associated with a higher quality. The necessity of rapid publication is now often slighted in the weighting of the likely impact and novelty of the publication. In fact, with appeals, corrections, and the like, it is not rare to have some publications in letter journals actually take longer to see the light of day than the average time for publication in the associated regular journals.

A prestigious Letter journal generally offers the advantage that your work, if published, will be read more broadly because of the valued *imprimatur* of a highly selective journal (and thus, one can hope, become one more frequently cited). In the scientific arena, everybody fights for exposure of this kind. Being in the spotlight is almost everybody's dream and peer recognition largely determines your success. (It is precisely because of this prestige that authors will contest unfavorable reviews more vigorously and it is this, which leads, as remarked above, to considerable increase in publication delay due to the time consumed in the back-and-forth salvos of a war with a referee.)

The tendency to write short contributions is not at all surprising, from another point of view than prestige alone. Most scientists, and especially important and famous ones, tend to be incredibly busy, and therefore, as consumers of science literature, are often unlikely to read long papers unless advised to do so by a colleague. Since many famous scientists also desperately want recognition from other famous scientists, they will often try to write short papers in the very best journals with the highest impact factors, so that a larger audience will read them; and so on.

The best approach to this in our opinion is likely to be to describe one sparkingly new idea in each Letter/Communication, and then to expand on it in a subsequent full paper with gorgeous detail and pithy expositions of the key points. After you have managed the arduous task of publishing a first Letter, the follow-up full paper has almost no chance of being actually rejected if the proper journal is chosen

as venue, although the details may be subject to considerable revision. This allows you to remind (in effect) everyone that you just published a Letter, and most importantly, to include all the experimental or theoretical details and background nuances that simply could not fit into the ultra-compact Letter format, but which are vital to publish if your work is to be thoroughly understood and appreciated. This is particularly true if someone wants to reproduce your data or perform calculations based on your experimental results. If you do not get the initial letter accepted in the best letter journal you may either recycle the letter for a somewhat lower-rank journal, or you may just absorb the letter material in the full journal paper. (A cynic might say that the top scientists read only Letters, while the full papers are read by the workers in the trenches, since they need to know the details.)

On the other hand, you may not want to go through the quasi-political hassle of writing a Letter and arguing its way past the best letter journals with their guard-dog referees. You may therefore decide to bypass the Letter-submission wars and publish directly in a long paper where the degree of hostility is usually lower. (However, this depends on the journal. As an example, *Advanced Functional Materials* and the Full Paper section in *JACS* are quite competitive).

Clearly, like the choice of journal in which to publish either the letter or the paper, the balance between the two is partly based on your own estimation of how important the work is and partly on your own taste for battle. It is a good idea to evaluate very carefully your personal motives in making those choices. You should also remember that, while you as an established researcher may feel detached about not pushing a particular piece of research to the Letter journal standard, by doing this, you may be denying your graduate student a legitimate shot at a good start in their publishing career. Ethically speaking, given work of equal merit, one should probably push more for the work in which a student is the first author.

CUMULATIVE PUBLICATION PROFILE

By the way, when you are on your way to accumulating papers in your profile, having gone through the process of where and how to publish several (or even many) times, some words on accumulating a profile with several or even many papers are now in order. As a general career strategy, it is best on the one hand, to publish as many glittering Letters as you can. For the rest, the regular papers, it is better to publish a few good meaty papers rather than many average papers of modest length. As a diagnostic for this symptom, if people tend say of your work, "Have you seen X's last paper on the "whatsit" effect?", you are publishing too many contributions so small that they risk being lost in the literature "noise". (A good analogy is maritime radar, where the noisy echo from the waves is called "sea clutter". If the boats you try to see are too small, they will be lost in the "sea clutter".)

(The tendency we are advocating is that of the famous German mathematician Gauss (who did not have to apply for research grant money), who had as his motto (on his seal): *Pauca sed matura* ("Few, but ripe"). Since you are not certain to be as talented as the legendary Gauss, you should not go to the extent he did. In fact, many of his results were found in his drawers after his death, because he felt that he had not yet polished them well enough. The real meaning of some of his Latin notes has not yet been decrypted.).

Publishing papers, which are each of impressive weight (in terms of contents, importance, originality and significance), will improve your signal-to-noise ratio, as well as your citation rate and your overall impact (of course it will also reduce somewhat the raw number of publications and might bring harassment from the strict publication counters). Psychologically it will also have a positive effect, since it will make you feel good about yourself and proud of your work. You would like to publish without having to say later (to yourself) something like, "This was a bit thin for a publication; it should have been tucked into another paper." In the

long run, you want to be able to look proudly at your publication list, rather than to view it as a collection of papers whose sole purpose was to advance your career. (However, to be realistic, your name may well be part of a group publication for a somewhat “political” reason, for a conference or some other occasion; a certain number of these are often an unavoidable aspect of working as a group or team.)

Graduate students often tend to fall into what we call the “short list” syndrome. It takes them a while to publish their papers, and they feel uneasy about having a short publication list, so they would, at least at the outset, publish more small papers. This is understandable, since the length of this list may be a determining factor in a student’s ability to find a job after graduation. This is especially true if you want to secure a place in basic research. However, students tend to forget that, in the long run, it is the quality of their work – even their very early work to some extent – which will largely determine their success in science. All in all, if someone has a few lightweight publications at the start of their career, it will not hurt them in the long run, if the lighter-weight “fluff” publications are phased out as the career gets up to cruising speed and you can better control your destiny.

Having settled the strategy for your paper in the sense of what form to use and where to submit the work, the actual writing still has to be done.

WRITING THE SCIENTIFIC PAPER: THE BASICS.

A full scientific paper should report new knowledge in a given area of science, typically in the form of data (collected either experimentally or through theoretical calculations or, occasionally, both, always accompanied by a thorough description of the methods used), their analysis and interpretation. (All this is also implicit in a Letter, but only the basics needed to understand the essential results are actually presented in the Letter.) This means that the authors should have studied the literature in depth and have made sure that their

data and/or interpretation is new with respect to what has been previously published, and all this should be done well before writing up the manuscript and submitting it for publication. (Of course, sometimes the writing process itself uncovers an area requiring additional investigation.)

The best way to start writing a paper, as pointed out by Whitesides (and others)² is to draft an extended and detailed outline. Besides helping you structure the manuscript itself, this can actually be very useful in planning your research. The outline should contain the key parts described hereafter in this section and should be progressively rewritten with an increasing level of detail, until it is quite easy to turn it into a “story”. (The concept is similar to writing a computer program by outlining the modules and their links and then filling the detailed items in each module.)

An essential point that most people tend to forget during the elaboration of the modules is that each paper as a whole should “*tell a story*”. In fact every type of scientific communication you engage in, whether written or oral, should tell a coherent story, though “how” you tell it obviously varies depending on the venue and other aspects.

The normal paper will typically follow the structure described below (although there may be variations depending on the journal, which also reflects the “culture” of the specific field of research).

An *introductory section* should provide a suitable context, describing what the paper is about and why the topic is important, what has been done before and how the authors propose to address one or more of the remaining problems of the field. This includes performing a thorough literature search on prior art, with an appropriate reference list.¹ The literature search is in fact the starting point of any scientific project (not just its write up once the data are collected and analyzed).

A *methodology section* should describe all the theoretical and experimental techniques that

were used to perform this work. This should contain enough details on the novelties in approach and in apparatus, together with the parameters used, so that a reader who has access to similar techniques and equipment would be able to reproduce the work without too much difficulty. None of the useful results should be presented in this section, since, in order to avoid confusion they should be only in their proper section. In a real sense, this is more like the documentation of the details required by the reader to accept that the methodology is sound. If there are novel aspects here then they are naturally given in useful detail for those who might wish to emulate the work. (Sometimes this aspect is to be placed by the journal in a separated section on "Methods" or the like.)

The *Results and Discussion* forms the intellectual core of the paper. (A minor variant is that some journals require you to keep the "Results" and "Discussion" sections separate.) The best way to present results and to discuss them is to prepare excellent figures and then to use them as the 'core' of the story you are telling, in a manner, which might well resemble the presentation, one would give as a talk or a poster. (Poster presentations are very useful trial runs to help you tailor the presentation by practicing various presentation approaches on one or two "clients" at a time and checking their reactions.)

The *Conclusions* are naturally the last part (of the main paper, i.e., except for appendices). Actually, we prefer to call it *Conclusions and Perspectives* to make clear distinctions between present summary conclusions and the possibilities for future work. The *Conclusions* are redundant in that what they will have been said piecemeal in the Results, the real function here is to summarize for the browser who has not read the *results* what the results actually mean. As to future work, you should weigh carefully the choices between (a) revealing some of your research plans prematurely and exposing them to rapid competitors and (b) in effect putting your intellectual stamp on concepts, which you will not be able to attack yourself in the near future.

"PLAY FROM THE OTHER SIDE" (like a hostile referee) while writing the paper

Now that the order of presentation is determined, the next thing to consider is how to do the actual writing. To reduce the amount of re-writing you will have to do, you need to pay close attention to what you are doing. When writing a paper you should be very critical about your work, your approach, your results and the way you are presenting them. The best way to do this is to do what we have repeatedly denoted by the phrase "Play from the other side". First, ask yourself all the time, how would you rate this paper if you were to review it as an anonymous and ruthless referee? Would it meet the standards of the journal where you wish to submit it? Would it have a fair chance of being accepted? You need to answer these questions honestly and objectively and then make the appropriate changes to your paper. It is even a good idea to pose the questions as they would be put by a hostile referee. As we have already remarked, many small points of clarification in a paper are actually inserted to forestall pointed questions by a referee. (In effect, you answer the question before it is asked.) Of course, being objective about your own work as if you were a referee is the tricky part here, but doing this is a lot easier if you have done some refereeing yourself.

Any of the scientists who have been even modestly successful will admit that their ability to write papers improved tremendously after the first few chores of difficult refereeing have been done. After that it is much easier to put on your "referee's hat" to see the flaws in your own work and in its presentation. For this reason you should be generous about acting as a referee; you will get as much benefit as the service you render to the journal and to the scientific community. (Besides, it looks good on your CV.) Thus, if you are a student or post-doc and your supervisor is doing a lot of refereeing, offer to help. Most will be grateful for the offer; but once you are experienced enough to contribute usefully, it is a good idea to make sure if feasible that it is you who sends the report in to the journal (or is at least given

credit to the journal for assistance) and thus gets added to their list of referees. (If you do a sufficiently good job of refereeing, you may eventually be asked to become an Editorial Board member or Associate Editor and this is a very useful addition to your CV.)

If you do this exercise of serious self-evaluation each time you write a paper, it will generally save you a lot of time and frustration later (and even more so for the toughest journals). A good paper has to be thought through exhaustively and should convince you more than 100% when you submit it. One measure of when you have done enough self-evaluation is how you feel when you contemplate another re-write. If you are exhausted and cannot stand the sight of it any more, you are probably incapable of improving it and further work may well make it worse¹. At that point, you are definitely ready to submit, because it is unlikely that you can make any more useful contributions. As we have said above, another important piece of advice is to ask some colleagues (e.g. your mentor if you have one) to read the final manuscript critically for you before submission. (If you are good, enough terms you may do this even if you have had them look at an early draft. Do not wear your friends out!) This “internal” review is important, and since it is informal and usually constructive, it is likely to save you a lot of time and frustration. If you can, you should also try to have a final review by a friendly expert (for content) and by someone less than expert (for clarity).

When junior colleagues are first authors, one should try to have them produce at least the first draft of the paper; after all they will have to learn eventually, so you are not doing them a favor by doing too much of the “spade work”. A strategy, which often works, is to sit down together and write the outline, and then send the student to write the paper from that. Of course, this approach will not be as efficient as if you wrote it all yourself, especially while they are learning, but a very important part of the education to which the student (or a post-doc) is entitled is some training in writing good papers.

CHECK THE BROWSING SEQUENCE: Title, abstract, introduction, conclusions and references

The remarks here apply to both a letter and to a full-length paper, since in terms of overall structure, there is not a huge basic difference between them, except in the length and the degree of detail. The sequence given in the title above is important because it gives the *browsing sequence*, by which we mean the sequence in which a paper is usually scanned by a browsing scientist to be flagged for possible detailed reading. Since a very busy scientist nowadays may not be able to go through the literature more than once or twice a month, and sometimes even less (sad, but all too true), to be flagged for reading your paper will have to elicit a “yes” at each browsing step or the browser will move on to the next paper.

In more detail, then, in browsing through journals, the reader will first skim through the titles. If the *title* attracts enough attention to warrant going further, the next step is to read the *abstract*, then the *introduction*, then the *conclusions*, and (perhaps) finally one checks the *references*. (The references are often checked before the body of the paper to see if you have cited the reader’s work, and to see if your knowledge of the literature is adequate.) The body of the paper will only be attacked if these preliminary indications are promising enough to make the reader think that it is worthwhile. (However if there is a particularly striking *picture*, one that may “leap off the page” even for the casual browser, you should give it a chance to do its work by making sure that all the essential information is inside the frame of the picture and not buried in the caption or in a distant part of the text.) Although you are not writing your papers exclusively to captivate and please super-busy scientists, if you do not pass this browsing sequence of checkpoints, your paper will be read only by the small set of people who read everything on the particular topics they care about. You should want to do better than that.

The situation resembles that of a store window full of merchandise trying to lure a customer inside. This includes the name of the store and what it sells, any indication of a special sale, window displays, perhaps a display inside the store and finally the merchandise itself. Another way to look at is from the point of view of the literature browser. In effect, the title should answer the implicit question in the browser's mind for each component of the *browsing sequence*: "Should I stop to look at this paper in more detail?" Unless most of the *browsing sequence* "boxes" (*title, abstract, introduction, conclusions*) look as if they are ticked "yes", your paper may not be looked at further in depth.

The *first* lesson from all this is that, when you submit a paper for publication, you should make sure that the *title* you choose is appropriate and captivating. It should be as short as you can make it, since longer titles are somewhat of a turn-off. (A superb title for review of some work on how frogs' eyes automatically track motion was "What the Frog's Eye Tells the Frog's Brain." That is a title that is difficult to beat.) Remember that your title does not have to have too much detail, because that you can put into your abstract.

Your *abstract* should also be short, clearly written, and should contain the main points of your paper. Your *introduction* (really the first paragraph if you can manage it) should place your work in its proper context, and give a broad view of why this field is important, and where it is leading. It should not repeat information known to the reader from the title. Your *conclusions* are also important, because they may be the only thing most of your readers will remember. The *conclusions* may make the difference as to whether the paper is marked for a high-priority read, as something to come back to when there is more time, or is merely to be copied into a running bibliography for the next paper the browser may be writing. Ideally, the concluding / summary section as well as the actual conclusions, should also point to new perspectives and directions of research. Finally, of course, in the references, you should make

sure that you are citing all the relevant literature, and if possible, even more. Remember, being generous in citing other people's work is very unlikely to do you any harm. (After all, some people may look at your paper simply to see "what it says about my work".)

Remember again that you are "telling a story". After reading your Introduction (and perhaps Methods section), the reader, if properly engaged now wants to come to the "juicy core" of your story. This is where your most important Figures come in. You need to "package" your data in well prepared, easy-to-read and captivating Figures. If your work revolves around some kind of microscopy technique, which produces colorful images that are easy to understand, you are obviously at an advantage with respect to someone who plots a graph that is not simple to read for a non-expert. Either way, you need to prepare those figures in the best possible way, then to tell your story around them. Many figures are crippled by the fact that some essential detail (such as usefully clear labels (not just A, B or C) for curves or objects) are hidden in the captions or buried in text, which is not right next to the Figure. Often this is done because it is "easy", such as coloring the curves and having no useful labels in the frame. A good figure is worst place to be lazy and the best place to add some showmanship.

Letters are so short that, paradoxically, they require a lot of re-writing to get it right and yet keep it compact. The actual effort can easily exceed that of a full-length paper where space requirements are not as restrictive. The tricky micro-decisions for letters are often whether or not to drop a detail because keeping it might mean compressing it to incomprehensibility. With full papers one can readily arrange to have dense patches for the expert and simple elucidating paragraphs to bring the less specialized reader up to speed on what is going on; doing this in a Letter is much harder.

Full papers should include all the follow-up details, figures, data and in-depth discussions

that cannot fit into a Letter. You have not really told the whole story until you publish the full paper, so it is something to be taken seriously at least once for each major line of research, rather than publishing many skimpy letters without the necessary follow-up details. There often is a separate section for Methods, for an exhaustive description of the experimental and/or theoretical methodology used to obtain the results. This is partly for those who just want to verify that you did it correctly, and partly for those who want to pay you the compliment of using your methods. (Of course, people who use your method(s) should provide more citations to your work for the bean counters who check these things.) Usually there is no page limit for a full paper (well, sometimes you may be asked to split it into two parts); this however should not be taken as an indication not to write concisely. There is no need for being as concise as to confuse the reader, however, it is important not to overdo compactness in a paper.

THE ORDER IN WHICH YOU WRITE

After this discussion on the structure, here are a few tips on the order in which you should write your manuscript (which is not the order in which the sections appear in the paper):

- (i). The *introduction*. You should really start writing the introduction before you even start working on the project. This may sound unusual, nevertheless it is very important. When you choose (or are assigned a project), you should already know what is likely to be important and significant about it, what has been done before you begin the work and what you are setting out to do. This is essentially the real reason for your introduction, and, if you write it before starting the actual work, it can guide you later. (In effect, your initial summary, which is essentially, "Why I am doing this work", later becomes "Why you should read this paper".) This also means that you can already write down the essential bibliography of what the patent office would call "prior art". If your results eventually take you in a different direction, all you have to do is go back to rewrite a bit of the *introduction* once you have finished collecting all the data.
- (ii). You should write the *methodology*, in extensive detail (to be edited and shortened later if needed) *while you are carrying out the project*. This is the best way to ensure that you record properly *all* your experimental and/or theoretical parameters, approaches and subtleties. It is easy to forget some details on the way to doing a project of several years, and writing this section up as you go will save you time and frustration later.
- (iii). For the *results*, once your experiments and/or calculations are done, you need to thoroughly analyze and interpret your data, then package it into Figures in such a way as to *tell your story* around them (see discussion above). (Sometimes you may even find that there is something missing, and if you are prudent (and perhaps lucky), you may be able to fill this lack yourself. If not, address this as a topic for future work, but do not just sweep it under the rug or ignore it. You do not want to leave it for a hostile referee!) This section is called Results, or sometimes Results and Discussion depending on the journal guidelines. The results section is really, what you need to set the stage for discussing your pretty pictures. Remember to make the key figures leap off the page at the reader they are often your real crescendos.
- (iv). After preparing the sections above you now write the *conclusions* and *perspectives*, then the *abstract* and, finally, the *title*. (After having done all this you may well have to re-write the *introduction*.) Recalling the discussion above, remember above all to write and structure all these elements of the paper in a captivating way, so as to draw the reader in.
- (v). You then write the *acknowledgements* (see below), then the cover letter (further down below) and finally submit.

ACKNOWLEDGEMENTS

This section serves at minimum to express gratitude to all the funding sources that sponsored the work. (It can actually be useful, sometimes, to read the acknowledgements in other people's papers as they occasionally report new funding opportunities) This same section is where you also thank anyone who contributed something, which was not yet quite enough to be listed as an author. Both are a must. Funding agencies usually state clearly in their guidelines that their support must be acknowledged. The authorship / acknowledgement issue can be delicate because of potential ethical abuses. (It often happens that people who did not contribute much are listed as authors (perhaps for political/economic reasons), and it sometimes happens that people who contributed quite a lot find themselves slighted (in their opinion) because they are only thanked but do not appear as co-authors.) Welcome to the political process!

THE COVER LETTER

Once the publication is properly written and has been approved of by all co-authors, it is time to submit. While we have already discussed the general factors, which influence the choice of journal, to go further here, would require considerable detail for each field, so we leave this "as an exercise for the reader".

There is one crucial document, which must still be produced and sent: the cover letter. For most journals this is just a formality – a couple of paragraphs indicating who the authors are (including of course the corresponding author), what is the title and the text guaranteeing that the manuscript is being submitted on an exclusive basis.

However, this document should be taken a little more seriously for the medium-level journals and especially for upper-tier journals. In such cases it is important to describe why the authors are choosing this specific journal and to spend time to highlight the originality, significance

and importance of the work itself. If the journal is one of the select few where this work is usually published (easily checked via the reference list), this should be emphasized. Very often the cover letter is the very first document that the editor reads upon opening your submission, and it may therefore play a very important role in determining its ultimate acceptance or rejection so its importance is not to be underestimated (For instance it may make it more difficult for the editor to use the response that "your work is not really suitable for our journal" or "we note that our journal is rarely cited in this work").

In addition to the basics just discussed, some journals encourage authors to suggest a list of possible reviewers¹⁶ and this list is generally attached to the cover letter. Whenever possible, you should try to use this to your advantage, by suggesting people who are well known in the field and who are likely to provide a fair assessment of your work, but who, of course, are not among those with whom you have had a relation (collaboration or the like) which would provide a conflict of interest. (Since it based on your interactions with them to date; the choice can be a bit tricky, of course. As peer review is anonymous, you will probably never know if someone you think is fair and friendly may be unexpectedly severe in your absence.)

This is also the document in which you may request the exclusion of specific reviewers whom you think might have a specific conflict of interest (such as being in direct competition) in assessing your work. In general you do not have to be very detailed here, since the editor really does not want to know the details and is in any case very unlikely to overrule your expressed wishes in this context.

REVIEW ARTICLES

While at the outset of one's career one is very unlikely to be asked to provide a review article, eventually that day may well come. Invitations to write reviews are usually issued to senior scientists who have an established reputation in

the field. These people are however usually very busy, so they often turn down such invitations or ask their younger collaborators to co-author the review with them. This state of affairs often opens opportunities for younger scientists to write or at least participate in writing a review, if only to compile and organize the list of references. If a review is done properly this is an excellent scientific exercise which will make you intimately familiar with the literature and hopefully draw attention to your ideas and perspectives as well as attract many citations. In addition, if you have a good idea for a review article you can always write a proposal and submit it to an editor, hoping that they will agree for you to write the review.

A good review article should of course give a broad overview of a field, or at least part of a field. Shorter review articles are often referred to as Feature Articles or Mini Reviews. Normally a review does not contain original results, however it reports an original viewpoint on the main discoveries of the field and where it is heading (or should be heading) according to its authors. If done well, it is a fairly monumental task, and a useful contribution to the literature and may hence garner a respectable number of citations. It is best pursued, in our view, coupled with writing another significant piece of work such as a PhD dissertation or a grant proposal so as to take advantage of the common bibliography, introductory paragraphs and several discussions. (Not many of us can expect to follow the illustrious example of Nobel Laureate astrophysicist Subrahmanyan Chandrasekhar as recalled in a special number of *Physics Today* (December 2010, pp 38 – 53. He would make titanic contributions in a field for a few years, write a landmark monograph book and then go on to something else, repeating whole cycle eight times in his life! The first cycle was the one for which the Nobel prize was awarded.)

A review should not be simply a list of what has been done presumably in a usefully

organized manner (although many bad ones do merely that), but rather should help draw broader conclusions by comparing and cross-referencing the key results of the literature, trying to point the reader towards new directions and opportunities. This last is never easy and usually requires considerable experience (more than you are likely to have in the early years). However as a junior author, the discussions on this with the senior author may be invaluable (particularly the undiplomatic parts, which may well, not make the final cut).

HIGHLIGHTS AND PERSPECTIVES

Some journals (e.g. *Science*, *Nature* journals, *Small*, *Angewandte Chemie*, etc.) also publish fairly short commentary papers whose purpose is to highlight an emerging new field. These are usually called “Highlights”, or “Perspectives” and are only a few pages in length. In some sense they are like mini-reviews, since they describe the key results and future potential of an emerging field where little has been published so far. They are usually written upon invitation from the editor, however if you have a good idea on a Highlight you can always propose it to the editor in the form of a synopsis and hope that they will consider it for publication.

In some cases the “Perspective” is a direct (positive) comment intended to highlight another paper that appears in the same issue of the journal, which was chosen by the editorial team for the spotlight. The author of this Perspective, in most instances, is one of the referees of the journal itself who participated in reviewing said paper. For the two papers to come out together in the same issue/volume, the timing has to be perfect. Therefore, from the point of view of editor it makes sense to ask one of the referees of the manuscript (who should be a well known and respected scientist in the same field) to write the Perspective as this person is already intimately familiar with the paper itself and is in a unique position to describe its importance to the community.

RESPONDING TO REFEREES.

Several weeks after submission (hopefully weeks rather than months although this can happen too!) you will receive a message from the editor with an acceptance or rejection notice, also including comments from one or more referees (see our previous article on the peer review system). In a good majority of cases, the referees will request some revision, either minor (if you are lucky and have done a good job to begin with) or major. In some cases they will recommend outright rejection (in which case you are unlikely to win publication), but more often you will get mixed reviews (often the case when you receive two or three reports) with comments and requests that might even to some extent contradict each other. At this point then you can either withdraw your paper (if it is rejected you do not really need to formally withdraw) and submit it elsewhere or revise it and prepare a response to the referees.

Responding to negative comments from referees is a delicate matter, especially when their comments were not only substantially negative but also somewhat hostile. If the comments are entirely hostile it is actually possible to discredit the referee in the eyes of the editor by diplomatically pointing it out in a separate letter, and asking to have an additional opinion by a different referee. If the hostility is more veiled, it is much harder to respond effectively.

The best response in any case should always be cool and diplomatic, avoiding vehemence, which may become shrillness. One should freely acknowledge any valid points the referee has made (even going so far as to thank the referee for the help in improving the paper) and show that you are making an effort to improve your manuscript based on his/her comments, yet still defending your ideas where this is required. An ultimate tactic for specific points of disagreement is to summarize both positions and leave it to the reader to judge. (This has the advantage of getting your point of view into print in spite of the referee, and of making you look very fair-minded, yet confident, in leaving the final judgment to history.)

We cannot say too often that if the referee proves obdurate, you should maintain a polite tone always. If the editor thinks that you are being reasonable and conciliatory and the referee a little shrill, you may well win in the end. (After all, the final decision is the editor's, the referees being really advisors, without the direct powers of actual judges.) In the same vein, if the referee says something particularly unpleasant, the very best advice is to not fire off a joyously hostile response in the heat of the moment. Do nothing at all for several days and let yourself cool down. Heated answers will never help. Have an arms-length colleague look at your response for excesses before you sent it in. If this is done properly, the editor might in the end side with you as an open-minded and reasonable person (perhaps being afflicted by a vociferous extremist), and either invite an additional reviewer or just discard the negative reviewer's views.

COMMENTS AND REPLIES.

Certain journals make space for a comment-rebuttal exchange on previously published papers. These consist of a "Comment" on the original paper from some critics, usually followed by a "Reply" from the authors of the original paper, who usually wish to defend their viewpoint. Comments and Replies can be useful additions to the literature, especially if they are constructive and bring new insights. It is wise to write both of them diplomatically rather than use a confrontational tone because typical readers will not be interested in a petty dispute – they will want to learn something new. Writing a Comment once in a while is a useful exercise, however we encourage you to take this initiative with caution. (It is more likely to win you enemies rather than friends. Tudor: 'As an exception to this, one of my longest collaborations arose from a Comment and Reply, which led to a useful new result.')

BOOK CHAPTERS AND BOOKS.

Publishers nowadays are continuously on the hunt to sign up scientists for the arduous task of

writing a book (especially on new “hot” topics). One of us (Tudor) has co-authored a very successful book on Plasma Physics a while back. The other (Federico) has been frequently solicited to write books on “Nano” (broadly speaking) by a number of publishers and has (so far) resisted the temptation. (Tudor: 'This sort of thing is much better done with two authors, each of whom is prepared to take on the work when the other is temporarily saturated with the effort of the detailed corrections and re-writing. However increasing the number of authors may bring one into the domain of the instabilities of games with more than two players.')

Writing a book (including *Survival Skills for Scientists*, which we co-authored and which turned out to be a great success) is a monumental task, which takes up a huge amount of time, energy and effort. While it may be financially justified in certain cases (for example if you are the main instructor of a large undergraduate course and there is no adequate textbook to cover the course’s material) it is usually not worth the effort it requires. It rarely brings much “glory” (in the form of scientific impact, e.g. citations) and usually does not yield a substantial financial return either. (The exception being a book for a large undergraduate course, in which case, if there is no credible alternative, you might actually make a lot of money from it.)

Writing book chapters represents a similar endeavor, although the effort is much smaller and thus may be justified on occasion. Similarly to the exercise of writing a book, it is to be considered as a service to the community. In some ways it is akin to writing a review article, although the purpose of the book and its book chapters will be mostly educational, whereas the audience and readership of review articles consists mostly of your peers.

Forthcoming article in this series.

The next article in this series will deal specifically with how to give an oral presentation

(including short conference talks, poster presentations, invited talks, plenary talks, as well as departmental seminars and colloquia and even public lectures).

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DIFFUSION IN A GEL: AN UNDERGRADUATE PHYSICAL CHEMISTRY EXPERIMENT

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ABSTRACT

A simple laboratory experiment to measure diffusion coefficients in a gel is presented. It involves a particular solution of Fick's second law as well as the Einstein-Smoluchowski equation. The measurements allow a discussion of the meaning of both expressions.

Keywords: *diffusion, gel, Fick's second law, Einstein-Smoluchowski equation.*

INTRODUCTION

Diffusion is an irreversible molecular transport process which occurs when concentration differences arise inside a phase. In that case, the associated gradient of chemical potential is the force which drives the particles (discharged atoms, ions or molecules) to move so as to restore the concentration homogeneity in the system.

This spontaneous phenomenon arises when the molecular distribution inside the phase is not homogeneous, i.e. if there exists a chemical potential gradient. It is customary, however, to use instead the concentration gradient, which is allowed in the case of dealing with dilute solutions. That is, a chemical potential gradient induces a particle flux along the gradient's direction, in the same way that an electrical potential gradient causes a flow of charged particles.

It is a very common physical chemistry phenomenon playing an important role as a necessary step in heterogeneous processes such as reactions at electrodes, corrosion of metals, transport through biological membranes, and the like¹.

It is not easy to deal with at the undergraduate level, particularly in the laboratory, due to the long time needed for making sound measurements. One serious drawback when working with liquid media is presented by the almost inevitable presence of the parallel process of spontaneous convection which can be difficult to control and evaluate. An elegant way to get rid of this trouble is to use a gel as diffusion medium; the gel suppresses convection due to mechanical and thermal disturbances². It has been established that the diffusion coefficient measured in this way is about 10% lower than in aqueous solution³. On the other hand, the use of gels as reaction media has created much interest in recent years⁴.

Thus, in the following a technique for measuring diffusion coefficients of inorganic salts dissolved in an agar gel which can be carried on in relatively short times, is presented. The method has an acceptable accuracy and also allows the student to deal directly with some fundamentals relationships, namely the Einstein-Smoluchowski equation and a particular solution of Fick's second law.

FUNDAMENTALS

The main empirical expression for diffusion is the well known Fick's first law, which states that the rate of transport per unit area or mass flux, J , in a certain direction, x , is proportional to the concentration gradient in the flux direction:

$$J_x = -D \frac{\partial c}{\partial x} \quad (1)$$

The proportionality constant, D , is of course, the diffusion coefficient. The concentration may be expressed as mole or grams per unit volume, the flux in mole or grams per unit area and time. Thus D is always given in units of area / time, $\text{cm}^2 \text{s}^{-1}$ or $\text{m}^2 \text{s}^{-1}$. It is worth noting that D is taken as no function of concentration, this assumption being valid at relatively low concentrations. Eq.1 gives the instant mass flux at a certain point on the curve describing the course of concentration along the diffusion distance (concentration profile). In the case of a linear profile, the gradient can be taken as constant (stationary state) and Eq. 1 transforms in:

$$J_x = -D \frac{\Delta c}{\Delta x} \quad (2)$$

In this way, determination of D is possible, if the increments ratio is known⁵.

In general, the concentration profile of the diffusing entities changes not only with position, but also with time. This situation is described, in one dimension, by Fick's second law, a second order partial differential equation:

$$\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2} \quad (3)$$

The solution of this equation gives $c = f(x,t)$ and depends upon the initial and boundary conditions defining the diffusion system.

Almost all the possible solutions may be found in the classical book by J. Crank⁶. A common case, which will be the basis of the experimental determinations described later in this paper, is that of one dimensional diffusion of solute in an infinite solvent medium from an extended source of constant concentration, c_0 , which at $t = 0$ extends from $x = -\infty$ to $x = 0$. That is, initially all diffusing particles are located between $x = 0$ and $x = -\infty$. Thus, at $t = 0$, $c = c_0$ for $x < 0$ and $c = 0$ for $x > 0$. At $t > 0$, $c = c_0$ for $x = -\infty$ and $c = 0$ for $x = +\infty$, (Figure. 1). As the total amount of particles must be the same, independent of time, a symmetrical profile is established, with $c = c_0/2$ in $x = 0$. The solution of Eq. 3 reads:

$$c(x,t) = \frac{c_0}{2} (1 - \text{erf}(z)) \quad (4)$$

where $\text{erf}(z)$ is the error function, defined by:

$$\text{erf}(z) = \left[\frac{2}{\sqrt{\pi}} \right] \int_0^z \exp(-\eta^2) d\eta \quad (5)$$

where $\eta = x/2(Dt)^{1/2}$ is an auxiliary variable. This function is closely related to the Gaussian distribution $\Phi(z)$, well known from the kinetic theory of gases, through the expression⁷:

$$\text{erf}(z) = 2\Phi(\sqrt{2}z) - 1 \quad (6)$$

where $\Phi(\infty) = 1$ and $\Phi(0) = 0.5$. The value of $\text{erf}(z)$ depends only on the limits of the integral, i.e. on z (the argument). This integral has the properties: $\text{erf}[-z] = -\text{erf}[z]$, $\text{erf}[\infty] = 1$, $\text{erf}[0] = 0$, and its values are available in tabular form⁶. In turn, $(1 - \text{erf}[z])$ is known as the error function complement, erfc .

For the present case, the argument is given by:

$$z = \frac{x}{2(Dt)^{1/2}} \quad (7)$$

Eq. 4 can be used for determining D , but it involves obtaining at least one concentration profile which implies making a great number of measurements. In the following a simplified form for some particular diffusion systems is proposed, noting that Eq. 4 may be rearranged to

$$\frac{c(x,t)}{c_0/2} = (1 - \text{erf}[z]) \quad (8)$$

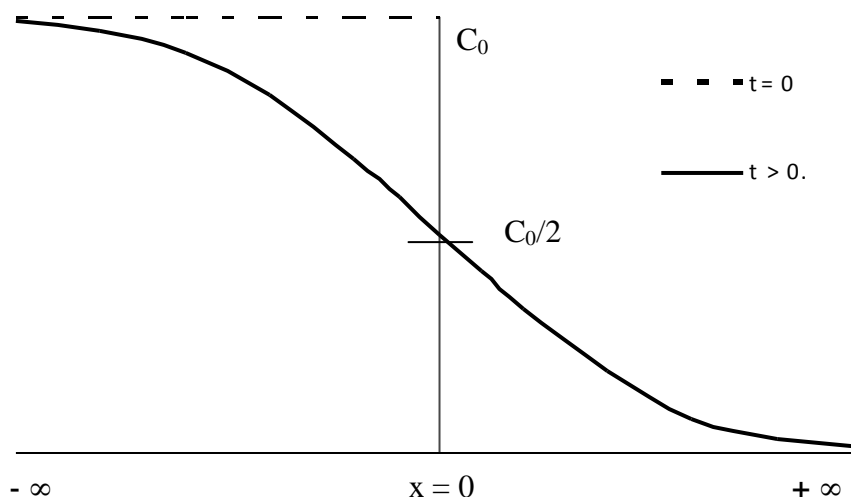


Figure 1. Concentration-distance curve for an extended source of semi-infinite extent.

In that way, if the ratio between the concentration at a certain diffusion time, t and length, x and the initial concentration, c_0 are known, it is possible to determine the value of the argument z from the tabulated values. After that, from Eq. 7:

$$D = \frac{x^2}{4z^2t} \quad (9)$$

and the calculation of D is straightforward.

Another useful expression is found from the molecular point of view, where diffusion is related to the inherent movement of the particles in the phase due to its kinetic energy. This so called Brownian movement, occurs with the same probability and speed for each direction, provided that the medium is an isotropic one (random walk)¹. The statistical treatment of the one-dimensional random walk leads to a direct relationship between the mean square distance travelled, $\langle x^2 \rangle$ and the diffusion time, t :

$$\langle x^2 \rangle = 2Dt \quad (10)$$

and similar equations for the y and z axis. Eq. 10 is known as the Einstein-Smoluchowski (E-S) equation, and offers a simple way to obtain the diffusion coefficient. However, it must be

noted that this equation refers to the average distance travelled by a statistically valid number of particles.

EXPERIMENTAL PROCEDURE

Two different ways for obtaining D are proposed, on the basis of Eqs. 9 and 10. Both of them involve the measuring of a diffusion distance and the associated time. In the first method two soluble salts, namely potassium iodide and lead nitrate, each one diffusing from reservoirs attached at the opposing ends of a cylinder containing agar gel, till they meet forming a visible spot of reddish lead iodide precipitate. This spot marks the diffusion length and elapsed time of diffusion for both salts. Furthermore, the onset of precipitation allows determination of the concentration values at the meeting point, which can be calculated from the known solubility product, K_s of PbI_2 :

$$K_s = a_{Pb^{2+}} a_{I^-}^2$$

To meet the conditions implied in Eq. 10 the distance available for diffusion along the cylinder and at both ends was chosen as $L > x / (2Dt)^{1/2}$. By taking an approximate value of $D = 10^{-5} \text{ cm}^2 \text{ s}^{-1}$ and a maximal value of $t = 10^4 \text{ s}$,

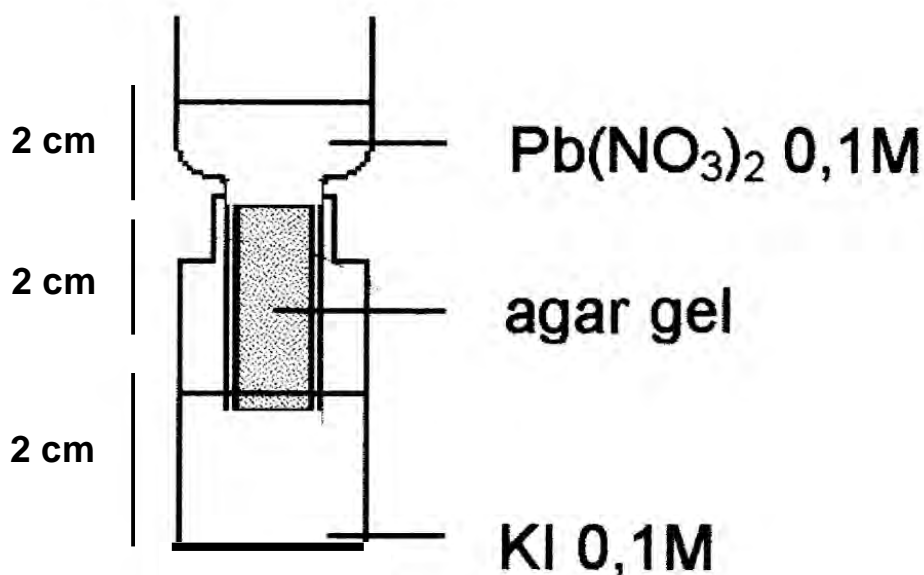


Figure 2. Diffusion cell

L is approximately 0.4 cm. Thus, the length of each one of the three compartments was about 2 cm. Figure 2 shows the employed diffusion cell.

The second type of measurement involves following the advancement of the diffusion front of an acid (HCl), which is marked by the boundary between the acid and neutral forms generated using an indicator dissolved in the agar gel. This is carried out with the same cell, without the upper solution reservoir. Some measurements were made using a micropipette of about 20 cm in length, in order to allow for longer diffusion times (Figure 3).

The solutions were prepared with ultra-pure water and reagent grade chemicals. The gel was formed by dissolving 3 % purified agar in water. The solution was slowly warmed and gently stirred until the powder was completely dissolved. The warm solution was transferred to the diffusion cell and was allowed to gel at room temperature. The agar gel was chosen as diffusive medium because it is easy to handle and a common laboratory staple. For the HCl diffusion bromophenol blue was used as indicator. Distances were measured with a

resolution of ± 0.05 cm by means of a vernier caliper and time with a laboratory chronometer.

In the case of KI and $\text{Pb}(\text{NO}_3)_2$ diffusion, the ratio $2[c(x,t)/c_0]$ used in Eq. 9 was calculated by taking $c(x,t)$ as given by the PbI_2 solubility, which in turn was obtained from the corresponding solubility product⁸, namely 7.1×10^{-9} at 20 °C. Thus for $\text{Pb}(\text{NO}_3)_2$ the value was 1.21×10^{-3} whereas for KI twice that figure was used, according to the stoichiometry of the

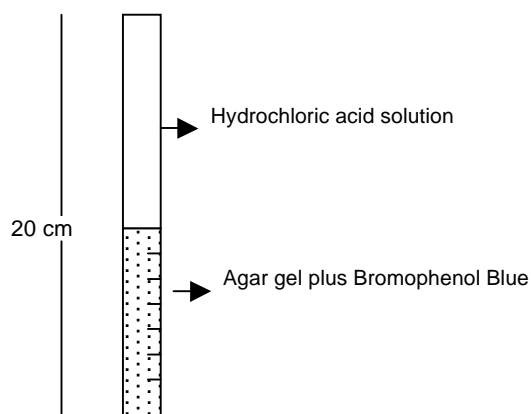
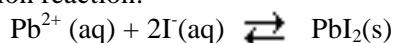


Figure 3. Diffusion cell using bromophenol blue as indicator.

formation reaction:



As the experiments were conducted with 0.1 M solutions, the ratio $2[c(x,t)/c_0]$ was 0.0242 giving $\text{erf}[z] = 0.9758$ and $z = 1.60$ for the $\text{Pb}(\text{NO}_3)_2$ side and $\text{erf}[z] = 0.9516$ and $z = 1.40$ for the KI side. For the HCl diffusion two solutions of 0.01M and 0.05 M were employed. In this case, $c(x,t)$ was defined by the turning point of the indicator, namely $10^{-4} \text{ mol L}^{-1}$, thus giving $\text{erf}[z] = 0.9800$, $z = 1.65$ and $\text{erf}[z] = 0.9960$ and $z = 2.04$, respectively. For instance, the ratio $2[c(x,t)/c_0]$ was 0.02 giving $\text{erf}[z] = 0.9800$ for the experiment conducted with the 0.01 M solution.

RESULTS

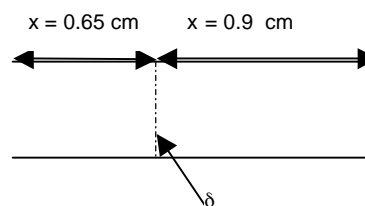
On tables 1 to 6 the obtained data of time and length are shown, together with the calculated values of the diffusion coefficients using both the (E-S) equation, Eq. 10, and the one derived from Fick's second law, Eq. 9.

Measurements with KI and $\text{Pb}(\text{NO}_3)_2$

After some preliminary experiences, two different end times were taken: 1) when the first visible points of precipitate appears, t_1 and 2) when a thin layer of precipitate was formed, t_2 , (Figure 4). Thus, Tables 1 to 4 show the diffusion coefficients calculated with Eq. 9, D_F , and Eq. 10, D_{E-S} at those different diffusion times.

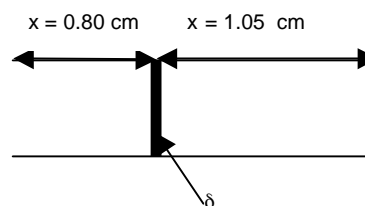
These data are to be compared to the literature values⁹ at the same concentrations, namely, $D = 1.86 \times 10^{-5} \text{ cm}^2\text{s}^{-1}$ for KI and $D = 1.10 \times 10^{-5} \text{ cm}^2\text{s}^{-1}$ for $\text{Pb}(\text{NO}_3)_2$, both at 25 °C. It should be noted that these values are affected by an estimated error of about 10 %, as mentioned in the introduction.

It is noted, that at longer times the best values are those obtained using the (E-S) equation, whereas at shorter times Eq. 9 is better. The experimental error may be relatively high, in particular due to determination of the diffusion



Line of precipitation.

Example: tables 1 and 3, run 1,
 $t_1 = 7200 \text{ s}$. $\delta < 0.05 \text{ mm}$, first visible points of precipitate appear.



Line of precipitation.

Example: tables 2 and 4, run 2,
 $t_2 = 28800 \text{ s}$. $\delta \sim 1 \text{ mm}$, a thin line of precipitate is formed.

Figure 4. Two different end times for measurements with KI and $\text{Pb}(\text{NO}_3)_2$.

time, which involves obviously a certain amount of subjectivity on the part of the observer. However, the obtained average values are quite reproducible within a range of about 15 %, which may be regarded as acceptable, in the context of the educational purpose of the experiments.

Measurements with HCl

The obtained results are shown in Tables 5 and 6, for short and long times. i.e. for short and long diffusing distances, respectively. The corresponding values from literature¹⁰ at 25 °C are $D = 3.07 \times 10^{-5} \pm 0.002 \text{ cm}^2\text{s}^{-1}$ and $D = 3.05 \times 10^{-5} \pm 0.002 \text{ cm}^2\text{s}^{-1}$ for HCl 0.05M and HCl 0.01 M, respectively. In this case, the D values calculated with the E-S equation are consistently low, whereas Eq. 9 gives fairly good values at all times.

Table 1. Potassium iodide solution, $c(x,t) = 2.42 \times 10^{-3} \text{ mol L}^{-1}$, $c_0 = 0.1 \text{ mol L}^{-1}$
 $\text{erf}[z] = 0.9516$, $z = 1.40$

run	$t_1 / (\text{s})$	$x / (\text{cm})$	$10^5 D_F / (\text{cm}^2 \text{s}^{-1})$	$10^5 D_{E-S} / (\text{cm}^2 \text{s}^{-1})$
1	7200	0.90	1.5	5.6
2	11000	1.10	1.4	5.5
3	9800	0.94	1.2	4.5
4	7200	0.95	1.6	6.3
Averages →			1.4 ± 0.2	5.5 ± 1

Table 2. Potassium iodide solution, $c(x,t) = 2.42 \times 10^{-3} \text{ mol L}^{-1}$, $c_0 = 0.1 \text{ mol L}^{-1}$
 $\text{erf}[z] = 0.9516$, $z = 1.40$

run	$t_2 / (\text{s})$	$x / (\text{cm})$	$10^5 D_F / (\text{cm}^2 \text{s}^{-1})$	$10^5 D_{E-S} / (\text{cm}^2 \text{s}^{-1})$
1	21800	0.85	0.43	1.7
2	28800	1.05	0.50	1.9
3	21600	0.84	0.42	1.6
4	21600	0.90	0.49	1.9
5	23400	0.95	0.50	1.9
Averages →			0.47 ± 0.04	1.8 ± 0.2

Table 3. Lead(II) nitrate solution, $c(x,t) = 1.21 \times 10^{-3} \text{ mol L}^{-1}$, $c_0 = 0.1 \text{ mol L}^{-1}$
 $\text{erf}[z] = 0.9758$ y $z = 1.60$

run	$t_1 / (\text{s})$	$x / (\text{cm})$	$10^5 D_F / (\text{cm}^2 \text{s}^{-1})$	$10^5 D_{E-S} / (\text{cm}^2 \text{s}^{-1})$
1	7200	0.65	0.57	2.9
2	11000	0.85	0.64	3.3
3	9800	0.80	0.64	3.3
4	7200	0.80	0.87	4.4
Averages →			0.68 ± 0.2	3.5 ± 0.9

Table 4. Lead(II) nitrate solution, $c(x,t) = 1.21 \times 10^{-3} \text{ mol L}^{-1}$, $c_0 = 0.1 \text{ mol L}^{-1}$
 $\text{erf}[z] = 0.9758$ $y = z = 1.60$

run	$t_2 / (\text{s})$	$x / (\text{cm})$	$10^5 D_F / (\text{cm}^2 \text{s}^{-1})$	$10^5 D_{E-S} / (\text{cm}^2 \text{s}^{-1})$
1	21800	0.65	0.19	1.0
2	28800	0.80	0.22	1.1
3	21600	0.74	0.25	1.3
4	21600	0.75	0.26	1.3
5	23400	0.81	0.28	1.4
Averages \rightarrow			0.24 ± 0.5	1.2 ± 0.2

Table 5. Hydrochloric acid solution, $c(x,t) = 1 \times 10^{-4} \text{ mol L}^{-1}$, $c_0 = 0.01 \text{ mol L}^{-1}$,
 $\text{erf}[z] = 0.9800$, $z = 1.65$

$t / (\text{s})$	900	1200	1620	2820	2880	3480	3540
$x / (\text{cm})$	0.55	0.63	0.69	0.80	0.90	0.96	1.00
$x^2 / (\text{cm}^2)$	0.300	0.40	0.48	0.64	0.81	0.92	1.00
$10^5 D_F / (\text{cm}^2 \text{s}^{-1})$	3.1	3.0	2.7	2.1	2.6	2.4	2.6
$10^5 D_{E-S} / (\text{cm}^2 \text{s}^{-1})$	17	17	15	11	14	13	14
Average $\rightarrow D_F = (2.6 \pm 0.5) \times 10^{-5} \text{ cm}^2 \text{ s}^{-1}$							

Table 6. Hydrochloric acid solution, $c(x,t) = 1 \times 10^{-4} \text{ mol L}^{-1}$, $c_0 = 0.05 \text{ mol L}^{-1}$
 $\text{erf}[z] = 0.9960$, $z = 2.04$

$t / (\text{s})$	900	3000	6180	9960	14220	19140	24580
$x / (\text{cm})$	0.58	0.96	1.43	1.80	2.15	2.45	2.70
$x^2 / (\text{cm}^2)$	0.34	0.96	2.04	3.24	4.62	6.00	7.29
$10^5 D_F / (\text{cm}^2 \text{s}^{-1})$	2.2	1.9	2.0	1.9	1.9	1.9	1.8
$10^5 D_{E-S} / (\text{cm}^2 \text{s}^{-1})$	0.2	0.2	0.2	0.2	0.2	0.2	0.1
Average $\rightarrow D_F = (1.9 \pm 0.3) \times 10^{-5} \text{ cm}^2 \text{ s}^{-1}$							

DISCUSSION

An important point comes out from these measurements, namely, why for the PbI_2 precipitation the (E-S) equation gives better results at longer times, whereas at shorter periods the Fick equation yields more satisfactory data. Besides, there is also to consider why the measurements with HCl give sound results only with the Fick equation, whereas the (E-S) fails at all times. This can be explained on the basis of the different meanings of each one of these equations. The E-S analysis represents an average over a very high number of diffusing particles, whereas the Fick analysis expresses the distribution of all particles along the concentration profile. In fact, the (E-S) equation cannot be interpreted as stating that each diffusing particle travels over the sq. root of the mean quadratic distance in time t . It states that, during time t , some particles jump a distance x_1 , other x_2 ...and so on giving an average quadratic displacement of:

$$\frac{x_1^2 + x_2^2 + x_3^2 + \dots + x_n^2}{n} = \langle x^2 \rangle = 2Dt$$

where n is the number of jumps. (11)

In the present context, it is relevant to consider at which point along the concentration profile is the equality resulting from (E-S) equation valid, i.e.:

$$\sqrt{\langle x^2 \rangle} = \sqrt{(2Dt)}. \quad (12)$$

Taking the value from tables of $\text{erf}[z]$ when $x = (2Dt)^{1/2}$ i.e. $z = (1/2)^{1/2}$, the concentration ratio from Eq. 8 results:

$$\frac{c(x, t)}{c_0/2} = 0.32 \quad (13)$$

That means that most of the diffusing particles are located between 0 and $x = (2Dt)^{1/2}$ but a sizable number had already crossed that distance. It is clear then, that the Einstein-Smoluchowski analysis will be valid only when a definite layer of product is visible, i.e., when a large number of particles have diffused to that point. On the other hand, the first precipitate

particles to be seen pertain to the tail of the concentration profile given by Fick's second law. This is made visible in Figure 5 where calculated concentration profiles are shown for some of the experimental conditions of Tables 1 and 2 including those corresponding to average diffusion distances, calculated from Eq. 10. As expected, by the measurements at short diffusion times, when the better D values are obtained from Eq. 9 the experimental diffusion lengths lie well under the statistical value, on the tail of the concentration profile. However, the opposite is found by the measurements involving longer times. It is to be noted that the need for waiting for a relatively high amount of diffusing particles in order to apply (E-S) introduces a limitation to the precision of the method. Effectively, if the thickness of the precipitate layer is too wide, the time involved is too long and the resulting D value too low. By the calculations involving Eq. 9 there is also an error source related to the concentration of the diffusing particles needed to satisfy the solubility product; the former being of the order of 10^{-3} moles L^{-1} . That means that a relatively high number of particles should be present at the meeting point of the diffusing molecules coming from the ends of the diffusion medium. Thus, the time values are likely to be too long and the diffusion coefficients tend to be too low. It is then clear that using a system of lower solubility product would improve the precision of the method.

As for the experiments made with the HCl solution, it is clear that only Eq. 9 is relevant for, due to the sensitivity of the indicator, only a relatively low number of particles are needed to change its colour. Thus, all measured distances will fall on the profile tail. In this case, the uncertainty will be lower than in the case of precipitate formation.

The obtained values may be considered as acceptable, bearing in mind the fact that the reference values are approximate, as mentioned above. To get better values, it should be necessary to know quantitatively the effect of the gel in interfering with the particles movement.

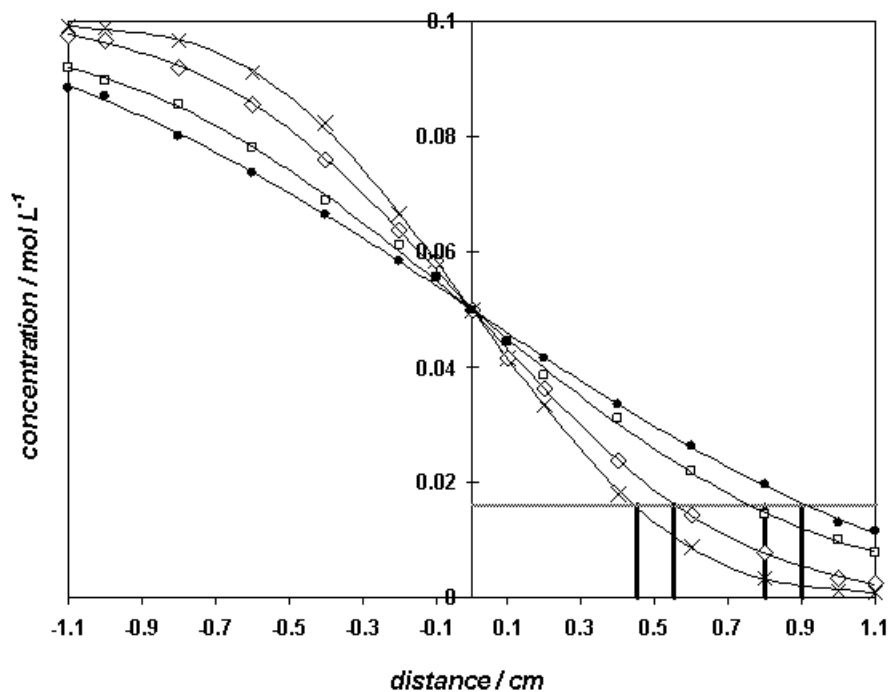


Figure 5. Calculated concentration profile. Potassium iodide solution, $C_0 = 0,1 \text{ M}$; $D = 1.4 \times 10^{-5} \text{ cm}^2 \text{ s}^{-1}$. Black bars show the corresponding average diffusion distances.
 $\times t = 7200 \text{ s}$, $\diamond t = 11000 \text{ s}$, $t = 21600 \text{ s}$, $\bullet t = 28800 \text{ s}$

CONCLUSIONS

The indicated determinations are easy to carry out in the undergraduate laboratory. However, the experimental/analytical process is not trivial since it allows for discussion of the basic characteristics of fundamental expressions of diffusion. It also introduces an opportunity to illustrate the problems associated with apparently simple measurements of distance and time in the reaction system and how those parameters are implicit in the interpretation of the analytical methods employed.

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PSYCHOMETRIC PROPERTIES OF THE SCIENCE ESTEEM INVENTORY

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ABSTRACT

The purpose of this study was to investigate the psychometric properties of the Science Esteem Inventory (SEI). The SEI was designed to assess the level of esteem that secondary students related to three aspects of science esteem: Passion for Science (PS), Processes of Scientific Inquiry (PSI), and Processes of Technological Design (PTD). A sample of 1,104 students in the Midwest United States attending science classes in four public high schools was used to evaluate the reliability and validity of the 21-item SEI. A correlated three-factor model consisting of the latent constructs of PS, PSI, and PTD was fit using confirmatory factor analysis and found to be adequate. Potential applications for the SEI and future research are discussed.

KEYWORDS: *science esteem; scientific inquiry; engineering design; technological design; STEM; measurement; reliability; validity*

INTRODUCTION

The processes of scientific inquiry and those of technological design or engineering design have much in common. Both demand that students venture through unfamiliar modes of risk-taking and cognition, thus challenging their sense of personal confidence or esteem. Analysis of any

gains in student self esteem achieved by participating in scientific inquiry and technological design activities in the high school classroom has eluded teachers and researchers. To date this area of research has been left largely untouched, even though most science teachers would agree that young people will readily self-identify as being good or not good

at “doing science.” The self appraisal connects closely with the course decisions they make in high school and college, and eventually influences whether they can see themselves choosing careers in an area of science and technology.

The use of design projects as a correlate to science instruction has been slow to emerge as a focus of interest despite the fact that technological design was included as one of the core components of the National Science Education Standards¹. Design projects, unlike typical canonical units of science instruction, engage each student at his or her unique level of readiness². For example, when students are called on to develop their own designs, the lessons start automatically at developmentally appropriate points for each student, and motivation becomes naturally intrinsic. More traditional science instruction centers on the teacher’s starting point irrespective of the likelihood that each individual student is at a different level of sophistication. Over time, this has led educators to assess motivation using quantifiable, extrinsic (grades) rather than more intrinsic (awe and wonderment) methods. By adding design projects to science instruction, knowledge and applied skills that are typically taught in separate secondary education departments, are naturally woven together to create a compelling awareness of how science is applied to create the products and services that serve human and societal needs. Further, self-directed design projects provide students with authentic skills and experiences to address problems outside of formal instruction.

To advance research in the areas of science, technology, engineering, and mathematics (STEM), the education community needs a simple instrument that can assess students’ level of esteem as they attempt and/or complete design projects as part of science instruction. Such an instrument could also be used as a diagnostic tool, to assess students’ level of skill acquisition before undertaking specific projects demanding scientific inquiry and technological design. Thus, the *Science Esteem Inventory* (SEI) was constructed to reflect three domains

of interest: (1) students’ interest in or passion for science; (2) students’ confidence in being able to employ the inquiry processes of typical scientific investigation; and (3) students’ confidence in being able to employ the processes of technological design.

Those three domains of interest often have been treated separately in the literature because of the organizational separation of academic disciplines at secondary and post-secondary levels. Student interest inventories were usually the work of the guidance department, for example, rather than academic departments, and scientific processes were the work of the science department. The processes of technological design were the work of the technology education or pre-engineering departments. Logically, there has to be an overlap, but to date no inventory has attempted to capture whether these three domains are truly distinct. Further, no research to date has identified or investigated unique subscales within the three domains that might inform classroom educators and researchers.

A Passion for Science

A common question often asked of students is “Do you *like* science?” This is an important question, but liking something can mean different things, at different times, in different degrees, to different students. *Liking* is semantically too broad for wording an assessment item although it often has been used in the creation of questions for other high school interest inventories. Therefore, the authors of this article elected to describe in operational terms what it means to “like” science, and identified relevant intrinsic behaviors that suggest a genuine passion for science apart from simply liking a particular class or teacher. Furthermore, it is recognized that actual work in the science classroom is not the sole source of esteem building. Self-initiated activities such as reading, watching TV, conferring with family members, and informal learning experiences often captivate and satisfy a sense of wonderment³. Another important source of esteem building is the influence of peers who

can set a pace, establish standards, and cultivate confidence. For example, Usher⁴ found that students with high efficacy in mathematics interacted more with peers about math than with adults asking such questions as: Did you get that stuff? How did you do that?

Krapp^{5,6} claimed that student interest is a dual regulation system that includes a cognitive component of values and goals and an affective component of emotion-related experiences. Bandura⁷ posited that successful experiences nurtured over time tended to result in internal standards or expectations for success. Thus, the passion to achieve followed by the reward of esteem appears to result in a progressive and deepening interest in a subject area that is often followed by a sense of pride and higher achievement. If one experiences early success in a subject area, then, there is a greater likelihood of following through with a career in that field. Thus, items 1-6 of the SEI reflect the previously mentioned ideas.

Processes of Scientific Inquiry

In 1985, the American Association for the Advancement of Science³, commissioned a long-term policy project titled, *Science for All Americans*, often referred to as *Project 2061*. The goal of this work was to identify what constitutes literacy in science, mathematics, and technology at various grade levels. Besides identifying the components of a core curriculum, the authors proposed that the teaching of science should be consistent with the nature of scientific inquiry. Further, the teaching of science should build on classroom success in an effort to counteract learning anxieties and fear of failure.

The processes of scientific investigation were subsequently articulated in two major reports published in 1996: *The National Science Education Standards*¹ and *A Framework for High School Science Education*⁸. The science processes advocated for both are similar, as can be noted from Table 1.

Table 1

A Comparison of Scientific Processes as Articulated by the National Research Council and the National Science Teachers Association

Fundamental Abilities to do Scientific Inquiry <i>National Science Education Standards</i> ¹ (NRC, 1996)	Science as Inquiry <i>Framework for High School Science Education</i> ⁷ (NSTA, 1996)
a. Identify questions that can be answered through scientific investigation.	a. Identify questions and concepts that guide scientific investigation.
b. Design and conduct scientific investigation	b. Design and conduct scientific investigations
c. Use appropriate tools and techniques to gather, analyze, and interpret data	c. Use technology and mathematics to improve investigations and communications
d. Develop descriptions, explanations, predictions, and models using evidence	d. Formulate and revise scientific explanations and models using logic and evidence.
e. Think critically and logically to make the relationships between evidence and explanations.	e. Recognize and analyze alternative explanations and models
	f. Communicate and defend a scientific argument.

The abilities mentioned above are stated in general terms. To be made operational, they need to be translated into observable actions that are familiar to both teachers and students. Thus, for assessment purposes, items 7-13 of this inventory are worded to identify easily recognizable processes in most science classrooms.

Processes of Technological Design

There has been general agreement on the abilities of technological design. Any differences would reflect the level of detail to which students are expected to perform. Underlying all aspects of technological design are two realities: (1) design is a creative process and (2) advances are the result of trial and error. Therefore, novices engaging in technological design will need to develop a high tolerance for failure as well as a tenacity to persevere until a solution, or a best solution is found⁹.

The National Science Education Standards¹ summarized the abilities of technological design as: (1) identify a problem or design an opportunity; (2) propose designs and choose between alternative solutions; (3) implement a proposed solution; (4) evaluate a solution and its consequences, and (5) communicate the problem, process, and solution (p. 192). Likewise, the National Science Teachers Association⁸ called upon science educators to assure that all students in grades 9-12 develop the abilities of technological design and understandings about the relationship between science and technology (p.190). The International Technology Education Association¹⁰ expanded on the abilities or attributes cited above, noting that the design process:

“...includes defining a problem, brainstorming, researching, and generating ideas, identifying criteria and specifying constraints, exploring possibilities, selecting an approach, developing a design proposal, making a model or prototype, testing and evaluating the design using specifications, refining the design, creating or making it, and communicating processes and results (p. 97).”

Thus, items 14-21 of the SEI reflect the general processes of technological design. The wording

of the SEI items went through three stages of development over a period of eight years. In brief, the wording of SEI items is a continuation of the word-smithing pattern used to develop a similar instrument that was used to evaluate the classroom effects of Materials World Modules (MWM), a series of 20 secondary modules developed under the direction of R.P.H. Chang, Materials Research Center, Northwestern University, Evanston, IL. The objective of the original 25 item MWM science esteem survey was to craft items that reflect the natural first person syntax students use to make their feelings known about science and design projects. For example, “I feel sure that I could deal with lab failures.”

Starting with the MWM evaluation (Pellegrini, 2010), the wording of items was suggested and affirmed first by a panel of eight experienced high school science teachers who piloted the instrument with 720 students resulting in a Cronbach alpha of 0.90. After piloting and editing, the survey was used successfully with a nationally-representative sample of 2,026 students in 118 classrooms across 42 states, resulting in a Cronbach alpha of 0.92, and no indication of wording problems¹¹. Finally, from the results of that sample and additional factor analysis, we regrouped the items into three subscales, and discarded items with low correlation to classroom gains. For consistency, we made slight edits to the syntax of some items. Thus, the wording of the SEI took its final form of 21 items.

Relationship of Scientific Inquiry with Technological Design

Several researchers and policy proponents have discussed the close relationship, and in many instances the interdependence, between scientific inquiry and technological design^{9, 12, 13, 14, 15, 16}. It seems unfortunate that this interdependence, which has been so prevalent for decades in research laboratories, has taken so long to reach a level of acceptance in secondary science teaching.

Table 2 presents the similarities and differences of the scientific process, often referred to as inquiry, with that of technological design.

Table 2
A Comparison of Scientific Processes with Technological Design Processes

Steps of the Scientific Process (Inquiry)	Steps of Technological Design (Problem Solving)
<ul style="list-style-type: none"> ▪ Observe/question/wonder about a phenomenon ▪ Develop a researchable question ▪ Conduct a literature search ▪ Propose a hypothesis ▪ Select a research design ▪ Identify independent variables, dependent variables and controls as applicable ▪ Plan the methodological details (e.g., sample size, treatment plan, equipment set-up, etc.) ▪ Conduct the investigation and collect data ▪ Analyze and display data ▪ Interpret findings ▪ Draw conclusions to support/not support the hypothesis. ▪ Discuss findings and state implications for future research. ▪ Write the report and publish as appropriate 	<ul style="list-style-type: none"> ▪ Recognize a need ▪ Create an initial definition of the problem. ▪ Articulate the design constraints ▪ Gather information from a literature search or from pilot observations ▪ Revise the problem statement based on the new information ▪ Brainstorm possible solutions or iterations (trials) ▪ Create a prototype(s) or model(s) ▪ Test and assess each solution/prototype/model ▪ Evaluate the possible solutions and select the most feasible given the design constraints ▪ Communicate the results (oral or written) to an audience of stakeholders

Bybee¹⁴ argued for the inclusion of technological design as a component of science instruction. In an effort to build a bridge between the formerly separated areas, Bybee differentiated between the processes of science and technology, and explained how each can contribute to students' cognitive and problem solving abilities when used together. He further articulated what students should know and what students should be able to do after engaging in a combined experience. According to Bybee, students should be able to:

- Identify a problem or design an opportunity
- Propose designs and choose between alternative solutions
- Implement a proposed solution
- Evaluate the solution and its consequences
- Communicate the problem, process, and solutions

Bybee's appeal was echoed by Lewis¹⁶ in a lengthy retrospective that constructed a convincing argument for the inclusion of technological design as an important component of science instruction. Lewis advocated more instruction in the sciences as a worthy component of technology classes. Lewis further proposed joint professional development between science teachers and technology teachers plus a convergence of research aimed at answering questions in the realms of student cognition, instructional pedagogy, student assessment and professional development.

Since 1998, there has been a modest stream of research and scholarship aimed at examining the benefits of integrating technological design with science^{2, 12, 15, 16, 17, 18, 19, 20, 21, 22, 23, 24}. The results are encouraging, yet indicate the need for additional studies.

METHOD

Instrumentation

The SEI is a self-report instrument, consisting of 21 items anchored by five response options from 1 = *never true of me* to 5 = *always true of me*. The SEI was designed to tap into three aspects of science esteem: Passion for Science (PS), Processes of Scientific Inquiry (PSI), and Processes of Technological Design (PTD). Additional items used in the questionnaire included current grade point average (GPA), gender, racial/ethnic identity, and grade-level (e.g., 9th, 10th, 11th, 12th).

Sample

The sample used to evaluate the properties of the SEI was a nonprobability sample; that is a cross-sectional sample of students in the Midwest attending science classes in four public high schools located in two metropolitan suburbs, one rural small town, and one small city. More than 1,000 ($N = 1,104$) students completed the instrument. Over half (56.9%) of the sample was male and 43.1% was female. Less than 20% self-identified their race/ethnicity as African American/Black (16.6%), 5.0% as Asian, 0.7% as American Indian/Alaska Native, 68.8% as White/Caucasian, 1.5% as East Asian/Middle Eastern, 3.8% as Hispanic/Latino, 0.6% as Pacific Islander, and 3.0% as Other. One-third (33.3%) of respondents reported that they had a GPA from A+ to A-, 47.0% from B+ to B-, 16.2% from C+ to C-, 2.5% from D+ to D-, and 0.9% of F. Less than 20% of respondents were in 9th grade (16.9%), whereas 42.4% were in 10th grade, 24.3% in 11th grade, and 16.4% in 12th grade.

RESULTS

Confirmatory Factor Analysis

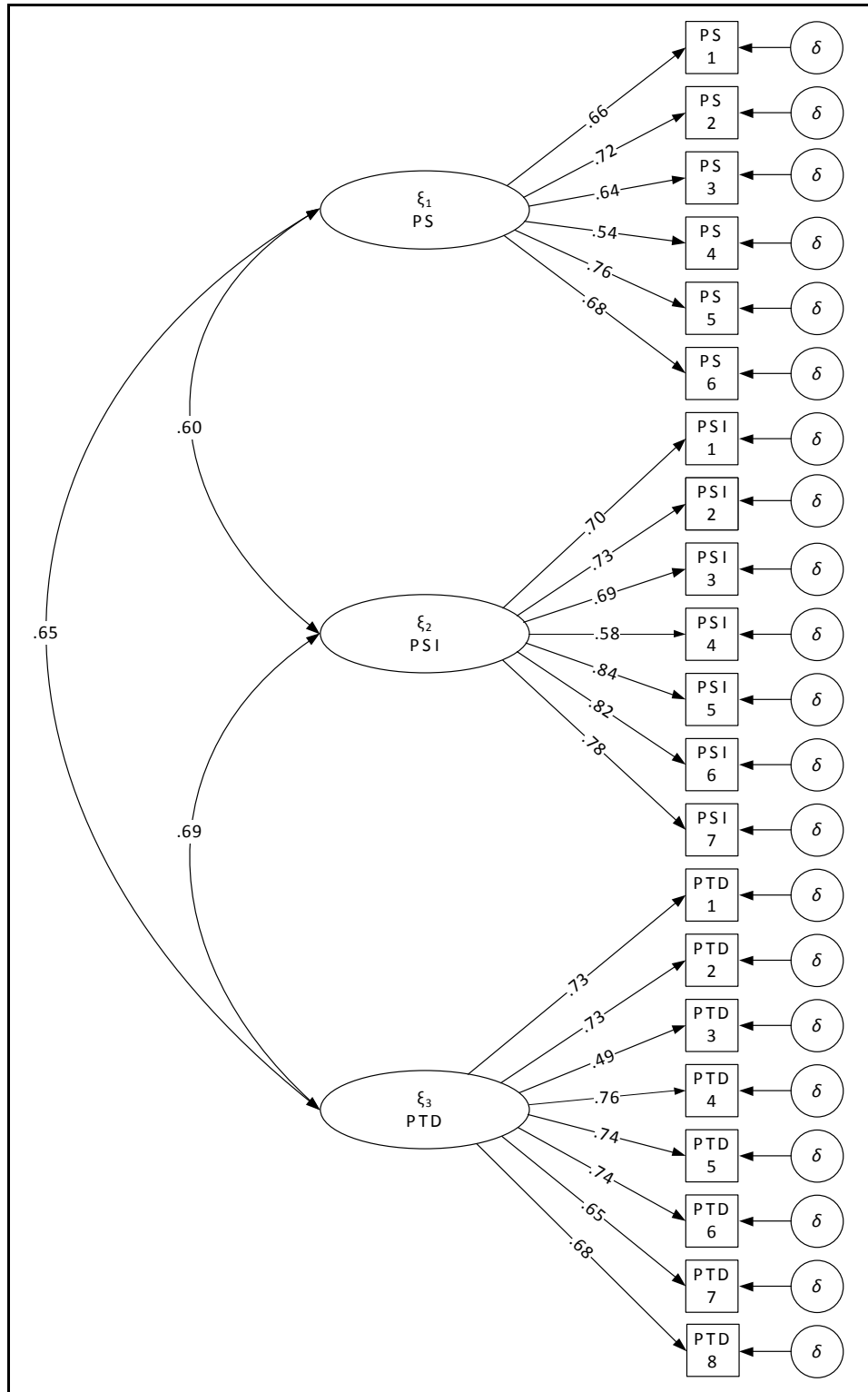
Confirmatory factor analysis (CFA) was used to test the hypothesized factorial structure of the SEI. In the hypothesized model, the three latent constructs (i.e., variables that cannot be directly

observed) PS, PSI, and PTD are assumed to be correlated and were allowed to co-vary in the model. The parameters and fit of the CFA models were estimated from the raw data and sample variance-covariance matrices using mean- and variance-adjusted weighted least squares method of estimation (WLSMV; see Beauducel and Herzberg²⁵) in Mplus 5.1²⁶. The model contained no double-loading indicators and all measurement error was assumed to be independent.

Model fit was evaluated using the χ^2 goodness-of-fit test, the χ^2 to degrees of freedom ratio (χ^2/df), the adjusted goodness of fit index (AGFI), the comparative fit index (CFI), goodness of fit index (GFI), normed fit index (NFI), and the root-mean-square error of approximation (RMSEA) and its 90% confidence interval (90% CI). Multiple indices were selected because they provide different information for evaluating model fit (e.g., absolute fit, fit adjusting for model parsimony, fit relative to a null model). Used together, these indices provide a conservative and reliable estimate of model fit²⁷. Overall, the model adequately reproduced the data [$\chi^2 = 1416.127$, $df = 186$; (χ^2/df) = 7.616; AGFI = 0.900; CFI = 0.901; GFI = 0.920; NFI = 0.900; and RMSEA = 0.054 (confidence interval = 0.048 - 0.060)]. Although model fit was evaluated as adequate, the null hypothesis of no difference between the model-implied population covariance and the observed sample covariance could not be rejected based on the χ^2 goodness of fit test, in part, because of the large size of the sample used to evaluate the model²⁸.

The standardized solution and parameter estimates for the model are shown in Figure 1. In the model, each ξ represents a latent construct (i.e., ξ_1 represents PS)—or factor—and is indicated by an ellipse, each SEI item (i.e., indicator or manifest variable) is represented by a square, and each δ represents an error term (i.e., measurement error) and is indicated by a circle. As shown in Figure 1, all standardized factor loadings (i.e., PS \rightarrow P1) were relatively large in magnitude (i.e., ~ 0.70). Standardized factor loadings are estimated correlations

Figure 1.
Factor Structure of the Science Esteem Inventory



Note: Standardized solution with error terms omitted for presentation purposes.

Table 3
Science Esteem Inventory Item Means and Standard Deviations

Item	Stem	<i>M</i>	<i>SD</i>
PS 1	I like to talk about science with my friends.	2.20	1.14
PS 2	I find it enjoyable to read science information on my own.	2.38	1.20
PS 3	I think about a career in some type of scientific field.	2.59	1.43
PS 4	I like to wonder why things happen.	3.78	1.13
PS 5	I feel confident when I'm learning science concepts.	3.13	1.13
PS 6	I take pride in my science work.	3.20	1.16
PSI 1	I feel sure that I could draft a hypothesis statement.	3.44	1.21
PSI 2	I feel sure that I could write a research question.	3.34	1.20
PSI 3	I feel sure that I could design a science experiment.	3.23	1.22
PSI 4	I feel sure that I could collect lab data.	3.85	1.67
PSI 5	I feel sure that I could analyze lab data.	3.57	1.13
PSI 6	I feel sure that I could prepare a lab report.	3.43	1.17
PSI 7	I feel sure that I could draw conclusions about an experiment.	3.62	1.11
PTD 1	I feel sure that I could draft a design problem statement.	3.06	1.13
PTD 2	I feel sure that I could brainstorm solutions to a design problem.	3.44	1.17
PTD 3	I feel sure that I could work as a team member.	4.23	1.02
PTD 4	I feel sure that I could test whether my solutions work or not.	3.67	1.11
PTD 5	I feel sure that I could redesign something that didn't work very well.	3.30	1.15
PTD 6	I feel sure that I could deal with confusing results.	3.06	1.16
PTD 7	I feel sure that I could deal with lab failures.	3.30	1.22
PTD 8	I feel sure that I could prepare materials for presentations to others.	3.61	1.18

between an indicator and its latent factor²⁹. Squared standardized factor loadings are proportions of explained variance, or R^2_{smc} . The standardized factor loading for indicator, or item, PR6 is 0.82, for example, therefore, the latent factor PSI explains $0.82^2 = 0.672$, or 67.2%, of the variance of indicator PR6.

In the model, the estimated inter-factor correlations ($\Phi = 0.65, 0.60, \text{ and } 0.69$) between PS, PSI, and PTD are large enough to suggest that the three latent constructs may not be clearly distinct and imply the existence of a second-order factor structure^{30,31}. Cronbach's α values for the 6-item PS, the 7-item PSI, and 8-item PTD constructs were 0.824, 0.880, and 0.879, respectively. Means and standard

deviations from the sample for the 21-item SEI are shown in Table 3.

Subgroup Differences

Subgroup differences for the sample by GPA, gender, and grade-level for PS, PSI, and PTD were investigated using multivariate analysis of variance (MANOVA). Means and standard deviations for each of the three SEI constructs by GPA, gender, and grade-level are given in Table 4. Although these analyses between GPA, gender, and grade-level groups explore differences of mean SEI, they do not suggest whether the SEI is factorially invariant across these groups. Therefore, these analyses are exploratory.

Table 4
Means and Standard Deviations for PS, PSI, and PTD
by GPA, Gender, and Grade-Level

	Passion		Process		Design	
	<i>M</i>	<i>SD</i>	<i>M</i>	<i>SD</i>	<i>M</i>	<i>SD</i>
GPA						
A+ to A-	3.167	0.841	3.740	0.886	3.681	0.770
B+ to B-	2.793	0.856	3.507	0.946	3.458	0.825
C+ to C-	2.608	0.812	3.097	0.904	3.112	0.806
D+ to D-	2.458	0.857	1.157	1.157	2.857	1.140
F	2.733	1.464	2.886	1.423	3.325	1.074
Gender						
Male	2.944	0.894	3.512	0.999	3.483	0.871
Female	2.792	0.846	3.480	0.902	3.428	0.799
Grade-Level						
9 th	2.811	0.877	3.569	0.950	3.602	0.822
10 th	2.922	0.806	3.455	0.919	3.417	0.812
11 th	3.004	0.914	3.609	0.965	3.536	0.817
12 th	2.651	0.955	3.376	1.041	3.311	0.940

For GPA, the omnibus test (i.e., a test of the multivariate hypothesis of no statistical difference across all dependent variables simultaneously) indicated a statistically significant multivariate effect across the three constructs [Wilk's $\Lambda = 0.902$, $F(12, 2902.681) = 9.579$, $p < 0.000$, $\eta^2 = 0.034$]. Univariate ANOVAs were used to investigate the locus of the multivariate effect for PS [$F(4, 1099) = 18.205$, $p < 0.000$], PSI [$F(4, 1099) = 17.833$, $p < 0.000$], and PTD [$F(4, 1099) = 18.806$, $p < 0.000$]. Post hoc pairwise comparisons using the Scheffé test (a conservative test with less statistical power and fewer chances of making a Type I error) indicated that statistically significant differences existed between GPAs of A+ to A- and B+ to B- ($p < 0.000$), A+ to A- and C+ to C- ($p < 0.000$), A+ to A- and D+ to D- ($p = 0.001$) for the PS construct. For the PSI construct, statistically significant pairwise differences were found between GPAs of A+ to A- and B+ to B- ($p = 0.009$), A+ to A- and C+ to C- ($p < 0.000$), A+ to A- and D+ to D- ($p =$

0.002), and B+ to B- and C+ to C- ($p < 0.000$). For the PTD construct, statistically significant pairwise differences were found between GPAs of A+ to A- and B+ to B- ($p = 0.003$), A+ to A- and C+ to C- ($p < 0.000$), A+ to A- and D+ to D- ($p < 0.000$), B+ to B- and C+ to C- ($p < 0.000$), and B+ to B- and D+ to D- ($p = 0.006$).

For gender, the omnibus test indicated a statistically significant multivariate effect across the three constructs [Wilk's $\Lambda = 0.990$, $F(3, 1100) = 3.115$, $p = 0.025$, $\eta^2 = 0.008$]. For the PS construct, a univariate ANOVA [$F(1, 1102) = 8.191$, $p = 0.004$] indicated that males ($M = 2.944$, $SD = 0.894$) reported significantly higher levels of PS than females ($M = 2.792$, $SD = 0.846$). However, neither the PSI or PTD constructs statistically differed across gender ($p = 0.584$ and 0.277 , respectively).

For grade-levels, the omnibus test indicated a statistically significant multivariate effect across the three constructs [Wilk's $\Lambda = 0.966$, F

(9, 2672.394) = 4.305, $p < 0.000$, $\eta^2 = 0.012$]. Univariate ANOVAs were used to investigate the locus of the multivariate effect for PS [$F(3, 1100) = 6.731$, $p < 0.000$], PSI [$F(3, 1100) = 2.838$, $p = 0.037$], and PTD [$F(3, 1100) = 4.848$, $p = 0.002$]. Post hoc pairwise comparisons using the Scheffé test indicated that statistically significant differences existed between 10th and 12th graders ($p = 0.006$) and 11th and 12th ($p = 0.001$) graders for PS. For the PTD construct, statistically significant pairwise differences were found only between 9th and 12th ($p = 0.011$) graders. No statistically significant pairwise differences were found for the PSI construct.

DISCUSSION

Purpose of the SEI

The purpose of this study was to determine the psychometric properties of an inventory to assess the level of esteem that secondary students bring to either science experiments or technological design projects. The study also fulfills a research need for a short, quickly administered instrument to be used by those conducting research in science education. Future users need to be assured that the SEI is valid and can be used to reliably draw inferences about the readiness of a class or experimental group to successfully undertake authentic science experiments or original design projects that demand more than the typically prepared set of instructions or templates that accompany secondary lab manuals.

In some instances, students' confidence, attitudes, or esteem may be observable, such as in classroom presentations or extra-curricular activities related to science where students are more willing to display high self-esteem. However, low science esteem is more difficult to observe; in fact adolescents are particularly sensitive and prone to hide any inadequacies or uncertainties they may experience. Additionally, because esteem is not only elusive in a qualitative sense, it is difficult to quantify, and therefore has not been taken into account as a

covariate of classroom learning or research outcomes.

The first construct, Passion for Science (PS), describes an overall natural attraction to science and problem solving and is the product of inferences regarding intrinsic behaviors of interest and motivation cited in the literature. The other two constructs of the SEI, Processes of Scientific Inquiry (PSI), and Processes of Technological Design (PTD), were identified and articulated from the National Science Education Standards¹ and related literature. Taken together, the three constructs create a comprehensive behavioral profile that can be used to define and measure science esteem.

Future Research Possibilities

The initial psychometric properties of the SEI as reported in this study have the potential for several future research possibilities. For example:

- Standardize or norm reference (i.e., relative to other test takers) the SEI for use as a diagnostic tool.
- Investigate the utility of the SEI for action research projects in classrooms, science departments, and for district curriculum decision-making (e.g., curriculum reform).
- Investigate the SEI for use in quantifying student understanding of the relationship of science to technology as articulated in the present National Science Education Standards¹, and in the forthcoming *A Framework for Science Education*³².
- Further investigate the influence and factorial-invariance of racial/ethnic identity on science esteem by using randomized blocked samples of major ethnic groups.
- Investigate the utility of the SEI as an outcome measure of professional development for science teachers.
- Investigate the relationship of low SEI scores with student achievement in order to determine the minimum level of esteem

required to undertake materials design projects. For example, if a class should score high on the subtest of technological design (PTD), then that class may have a high level of affective readiness to attempt more advanced design projects. The opposite situation would signal the teacher to be aware that the class might have difficulty dealing with design constraints and especially with the necessity and frustration of “returning to the drawing board.”

The Promise of the SEI

As this research finds its niche in the larger picture of educational research, it may result in science educators gaining a better understanding of how to teach science and technology. For example: (1) teachers can use the SEI to determine the readiness of a class to venture into projects involving risk-taking and experimentation; (2) the SEI yields values for three constructs as well as for individual items thus informing a teacher or researcher about specific target areas needing emphasis and/or instruction, and (3) the SEI, and its further refinements, can diagnose the process difficulties students are having in the still often misunderstood areas of inquiry and technological design. Furthermore, if the inventory helps to pinpoint student apprehensions, then the teacher is better informed as to how to redirect, and structure curricular activities.

For most teachers, their primary career motivator is to make a positive difference. And most would agree that making a difference goes beyond student success on standardized tests. Secondary science teachers are drawn into their field by the compelling advancements of scientific content, scientific inquiry and technological design. Many science teachers search for methods that awaken the awe and wonderment of science. The success that comes when students weave together knowledge and applied skills can establish patterns of higher level thinking that last a lifetime.

From the data obtained in determining the psychometric properties of the SEI, we conclude that the instrument can be a reliable and valid tool to use in assessing secondary students' affective readiness to venture into materials science design projects.

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EDUCATION AND RESEARCH IN POLYMER MATERIALS AT THE DEPARTMENT OF MATERIALS SCIENCE OF THE UNIVERSITY ERLANGEN-NÜRNBERG

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ABSTRACT

A short description of the Friedrich-Alexander-Universität Erlangen-Nürnberg, its Technical Faculty and the Department of Materials Science is given and the study courses in materials science are introduced. Two examples are presented for the research within the field of polymer materials which offers students possibilities to perform their bachelor or master theses.

Keywords: *University Erlangen-Nürnberg, materials science education, research in materials science, rheology, nanoparticle filled polymer melts, antimicrobial polymers*

UNIVERSITY AND TECHNICAL FACULTY

The Friedrich-Alexander-Universität Erlangen-Nürnberg is the largest university in Northern Bavaria. Some figures and facts are given in Figure 1. The university is divided into five faculties. Besides classical subjects like arts, law, economics, medicine, and natural sciences it houses a faculty of engineering. This broad spectrum makes the Friedrich-Alexander-Universität the institution with the greatest variety of subjects offered to students in Bavaria. The number of students approaches 30,000. The Technical Faculty consists of five departments which are listed in Fig. 1. Counting nearly 6,000 students now, the Technical

Faculty compares to some Technical Universities in Germany by size. A great number of technical subjects are offered, as Figure 1 demonstrates.

DEPARTMENT OF MATERIALS SCIENCE

Figure 2 shows the organisation scheme of the Department of Materials Science. It covers the most important material classes, namely, metals, glass and ceramics, polymer materials, materials for electrical engineering, and biomaterials by independent institutes which offer lectures for all students of materials science. In addition, the institutes “Corrosion

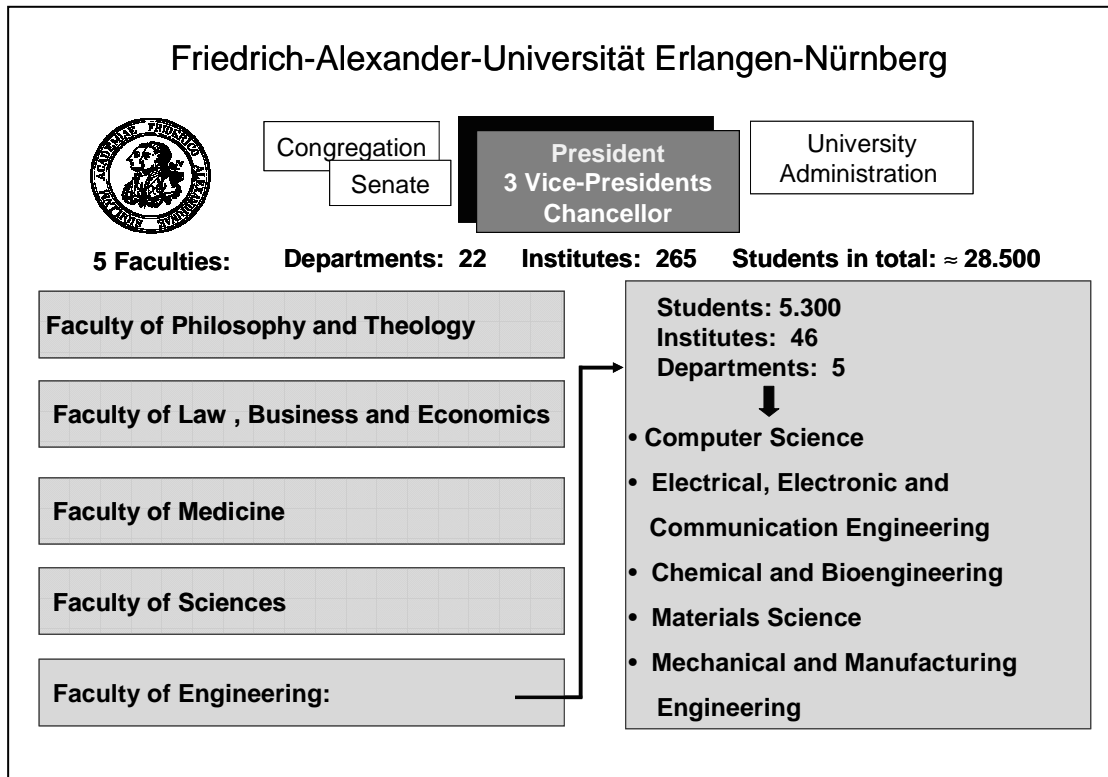


Figure 1. Organisation chart of the Friedrich-Alexander-Universität Erlangen-Nürnberg and its Technical Faculty

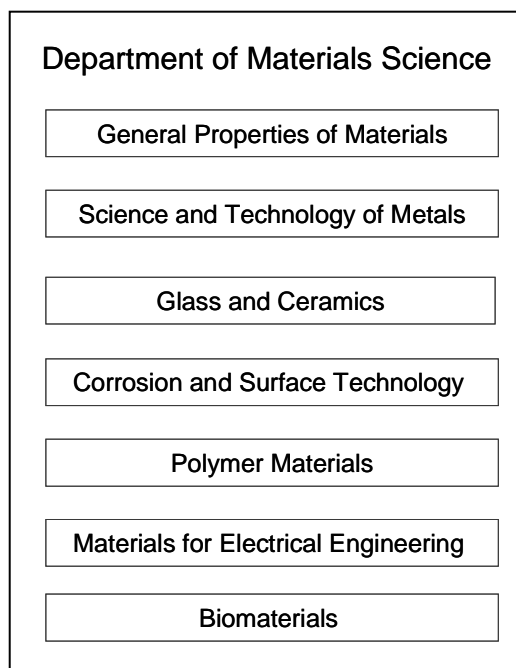


Figure 2. Institutes within the Department of Materials Science

and Surface Technology” and “General Properties of Materials” work on research topics which are not strictly related to one class of materials, but address questions of a more general aspect in the field of materials science.

Five study courses are offered. They are listed in Figure 3. Materials Science and Technology is the topic the department started with. It still has a strong position, but nanotechnology has become a competitor which was started only some few years ago. Both study courses educate bachelor and master students. Owing to the image of the highly appreciated degree “Dipl.-Ing.” (diploma engineer), which is not available any longer, the bachelor as the final degree has not been in much demand from the students up to now, resulting in the fact that nearly all the students in materials science at Erlangen want to finish their studies with a master degree. The courses “Energy Technology”, “Medical Technology”, and

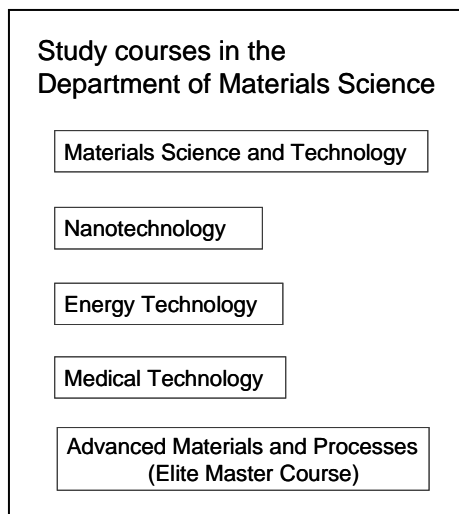


Figure 3. Study courses of Material Science at the University Erlangen-Nürnberg

“Advanced Materials and Processes” are jointly executed with various other departments. They offer the students an education which spreads over several subjects. According to the great variety of courses the curricula differ from each other and, therefore, are beyond the scope of this presentation. An actual overview can be found in the internet ¹.

Special attention should be paid to “Advanced Materials and Processes” as it is an internationally oriented elite master course which is open for application to gifted students from all over the world. More detailed information can be obtained from Ref. 2.

The role of research for the education of students

Although the time frame for studying engineering subjects has been tightened over the years, particularly, by the introduction of the bachelor studies, care is taken within the curricula that the students get at least some insight into more practical aspects of their profession they have to work for. An internship of some weeks within a company is obligatory for many studies of engineering subjects and for the study of materials science as well. Besides that, laboratory courses at the department are part of the education at the University

Erlangen-Nürnberg. For the bachelor degree and the master degree, as well, the student has to deliver a thesis which comprises work on a special project going on at the Institute. The student learns to solve a problem on his own and often gets a feeling for the first time what research looks like. In many cases experiences of such kind have been the base for a student’s decision to start a doctoral work later on. The time for performing a bachelor thesis is limited to five months, that for a master thesis to six.

Examples of recent research projects

In the following, two research projects are briefly described which amongst many others have been carried out at the Institute of Polymer Materials. Special tasks arising from them became the topic of bachelor and master theses.

1. Rheological experiments on polymer melts filled with nanoparticles

Within the expanding fields of nanoparticles the question is of interest in which way their addition influences rheological properties of the melts of polymers which play an important role in the field of modern engineering materials. Creep and creep-recovery tests were applied as they are a very effective method to measure the elastic and viscous properties of a polymer melt. The principle of this method is presented in Figure 4 and it is described in detail in Ref. 3, for example. For the students, the performance of the sophisticated measurements is a challenging task. Surprising are the results shown in Figure 5 that the viscous part of the deformation mirrored by the creep compliance J is much less influenced by the added nanoparticles than the elastic part J_r (for details see Ref. 4). As published in Ref. 4, the effect of the particles on the elasticity is reflected by the retardation spectra which are presented in Figure 6. Calculating spectra, the student can exercise his mathematical skills and the model shown in Figure 7 offers him the opportunity to refresh his basic knowledge on polymers. For a student who is more application oriented, the findings presented in Figures 8 and 9 are

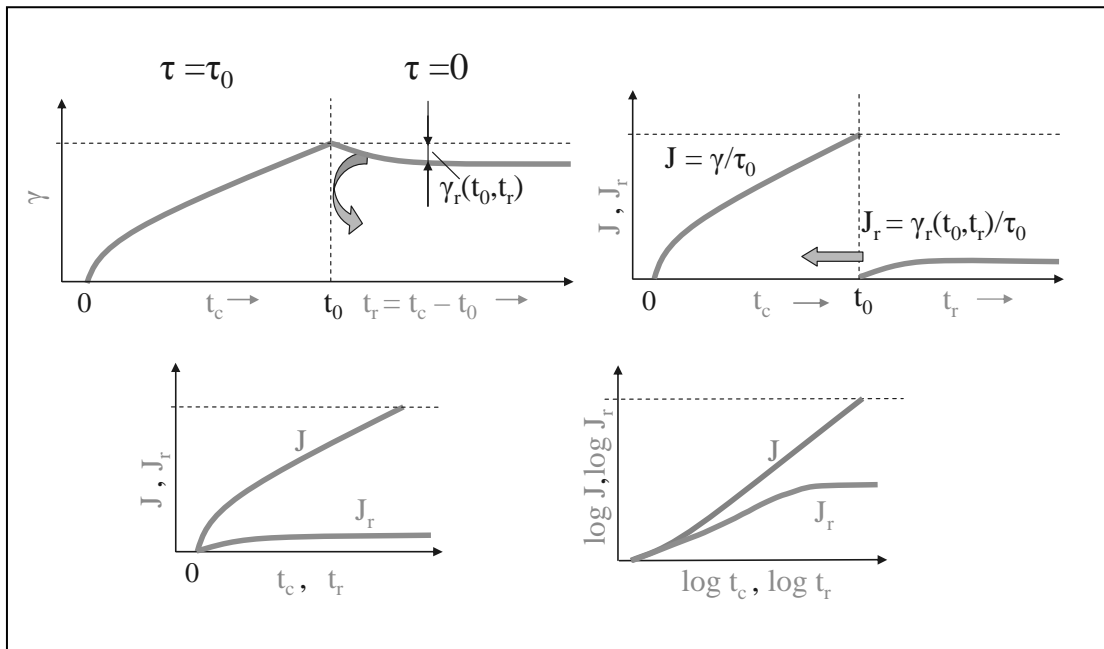


Figure 4. Principle of a creep-recovery test

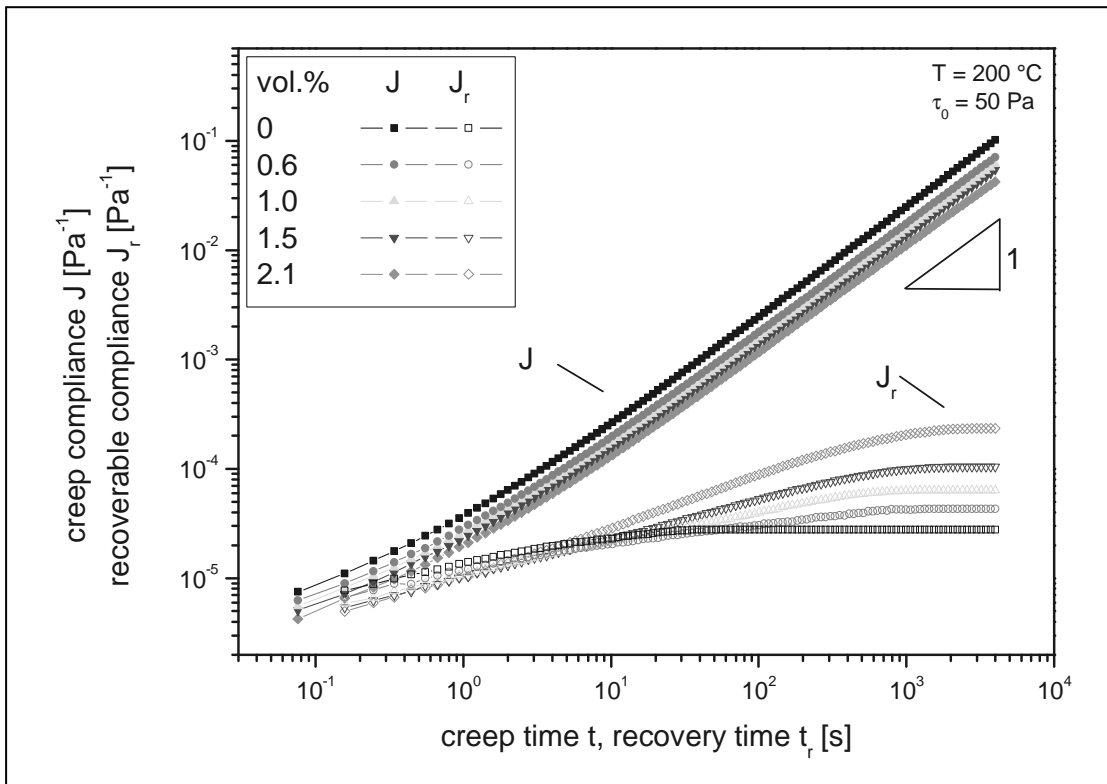


Figure 5. Creep and recoverable creep compliance of a polymethylmethacrylate filled with silica nanoparticles of various concentrations

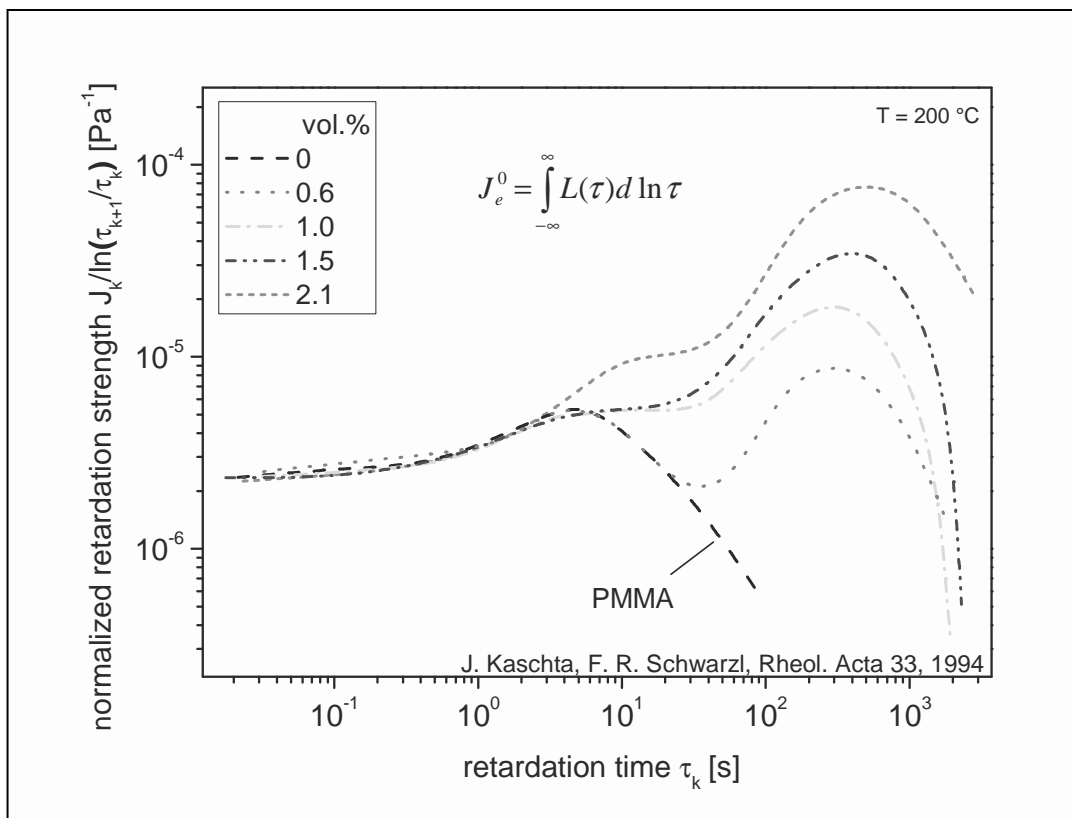


Figure 6. Retardation spectra of polymethylmethacrylate filled with silica nanoparticles of various concentrations

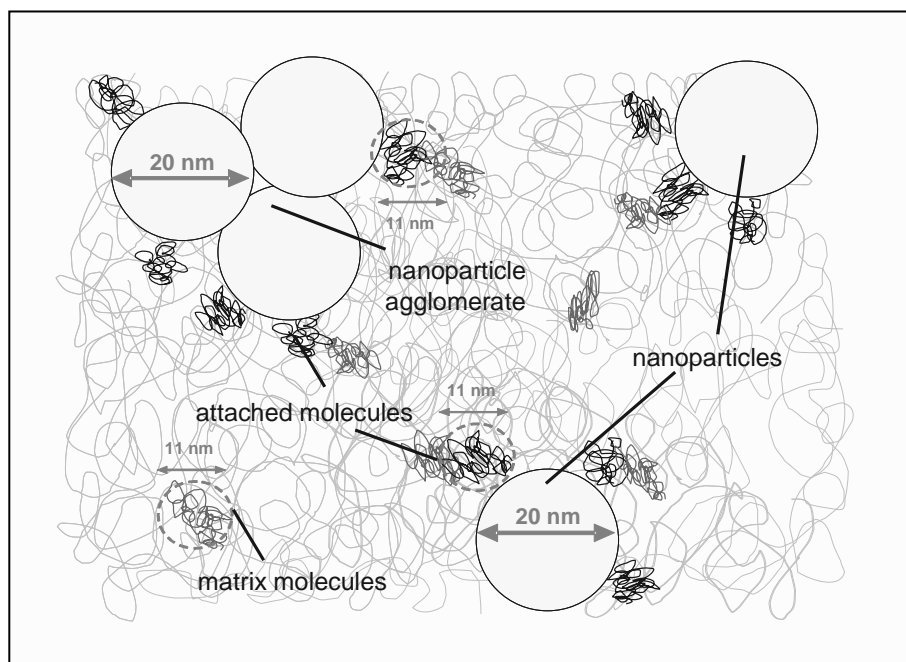


Figure 7. Model for the interaction between filler particles and matrix molecules

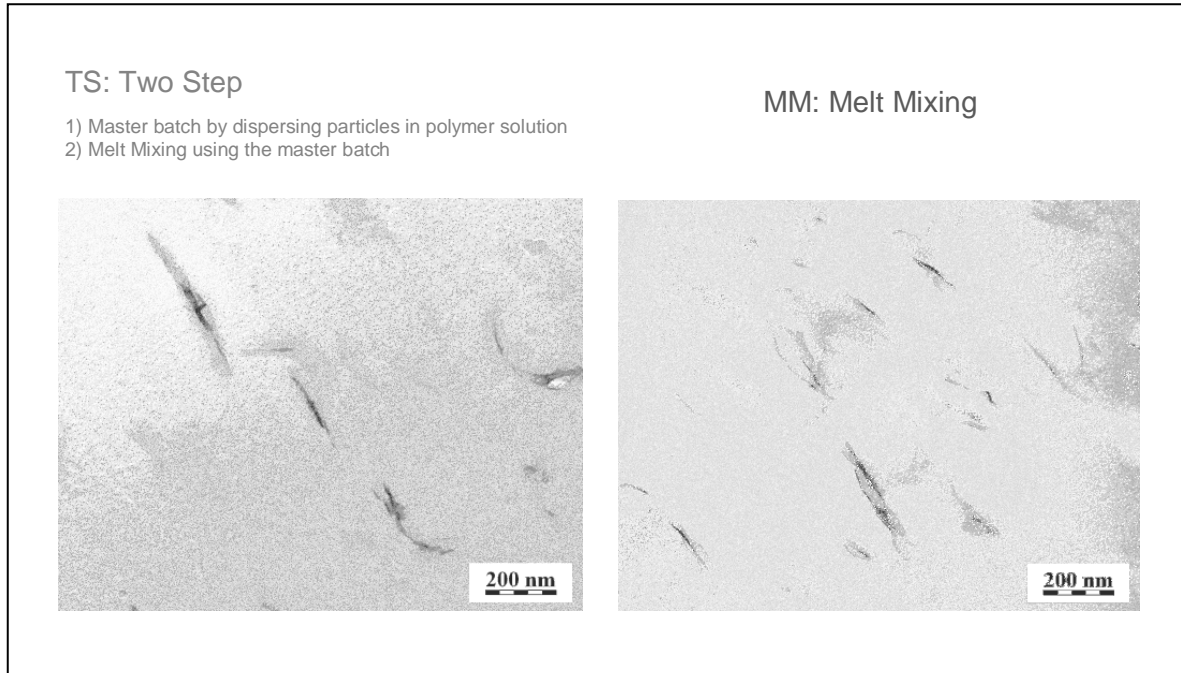


Figure 8. Electron micrographs of polymethylmethacrylate filled with nanoclay by two different processes

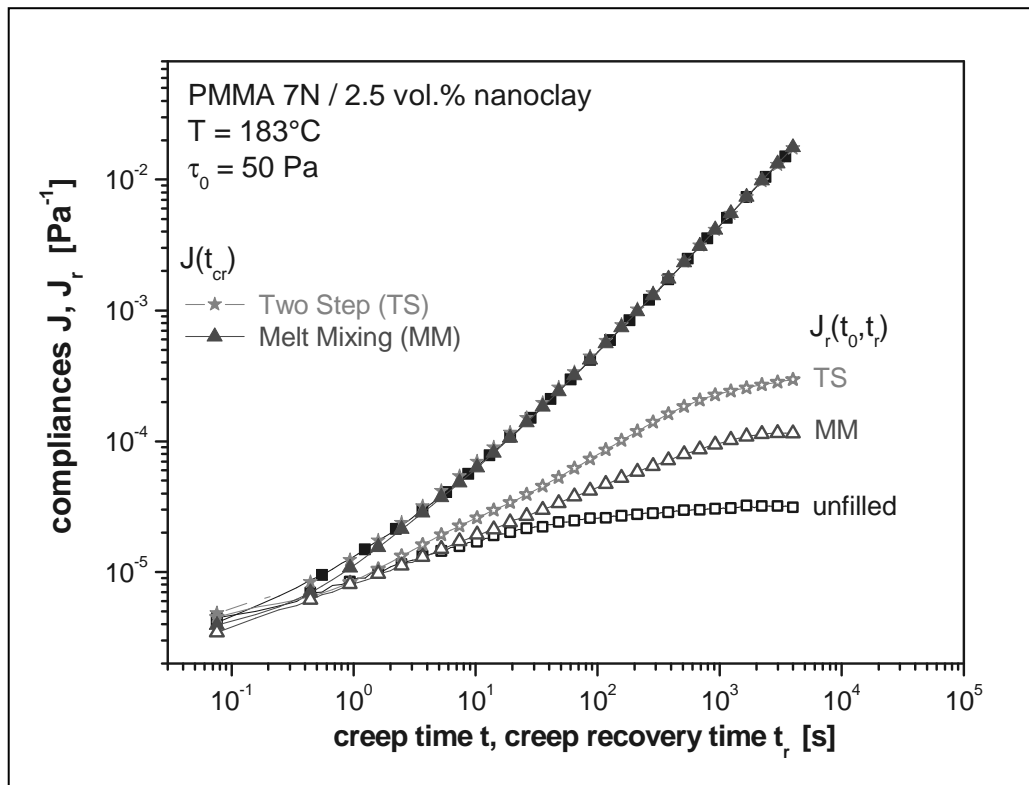


Figure 9. Creep and creep recovery of the samples shown in Fig. 8

interesting. They are related to investigations on the assessment of the degree of dispersion of nanoclay in a polymethylmethacrylate (PMMA) matrix obtained by the two different processes indicated in the electron micrographs of Fig. 8. The particle distribution on the right picture was achieved by simple melt mixing in a kneader, that one on the left by a two-step process. In the first step, a master batch was made by dispersing the nanoclay particles in a PMMA solution and in the second, the dried master batch was used then to get different samples of various concentrations. Obviously, from the two micrographs it cannot be decided whether there are differences between the two methods with respect to the degree of dispersion obtained. The recoverable compliances of the two samples plotted in Figure 9 reveal clear differences, however. J_r of the material prepared in two steps is higher indicating a better dispersion of the particles (for details see Ref. 5). This finding is interesting as it opens a way to contribute to the determination of a dispersion quality. Investigations of this kind are a good example how fundamental research can be used to answer questions of practical interest. Theses in such a field are very suitable to educate engineers of materials science who should be able later on to find answers to technical questions related to the development of new products and their processing.

2. Antimicrobial polymers based on silver particles

Rendering polymer materials antimicrobial is a very actual topic of research and development today. Its obvious connections with the medical area, with hygiene matters and the well-being of people attract students of these days and, therefore, theses on this subject are highly requested.

As it is well established and sketched in Figure 10, silver ions which are released from a polymer surface can interact with bacteria and kill them. To assess the efficacy of a silver modification and to optimise the ion release the silver ion concentration is measured using the method of anode stripping voltammetry, the principle of which is presented in Figure 11. A description of its function is given, for example, in Ref. 6. Many questions have to be tackled in order to establish a base for the development of effective materials. In one project the release of silver ions from different polymer materials was investigated using a distinct silver powder. Polyamide was found to be a very suitable material for a high release rate⁶. For polypropylene, however, only a very low release rate could be measured⁷. From detailed experiments the conclusion could be drawn that water plays an essential role for the generation and diffusion of silver ions.

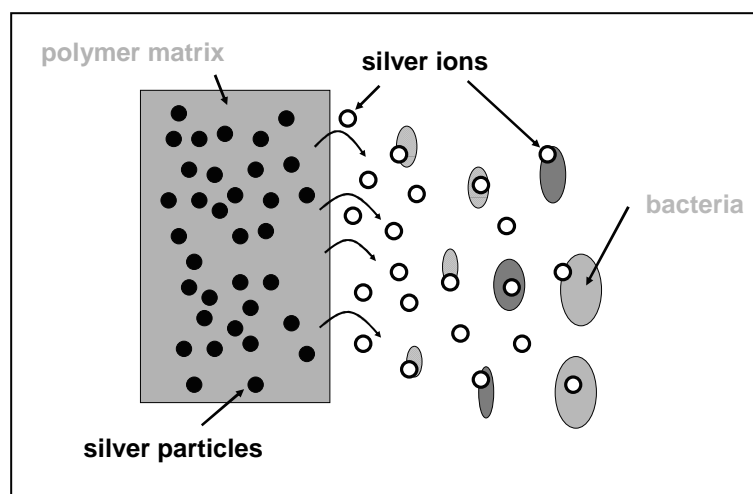


Figure 10. Way of interaction between silver ions and bacteria

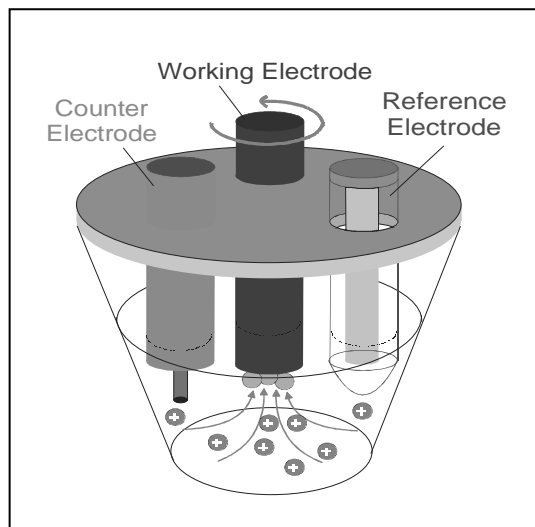


Figure 11. Principle of the anode stripping voltammetry

Another question addressed the influence of the specific surface area of the silver particles on the release. Not unexpected, nanoparticles were more effective than those of micro sizes⁸. A research project interesting from a fundamental and a practical point of view was the ion release of nanoparticles of different sizes from a thermoplastic polyurethane for applications in the medical field. Figure 12 shows the distributions of the two kinds of nanoparticles generated by different routes as described in Ref. 9. The nanoparticles prepared by a special process and then mixed into the polymer are smaller and their distribution is narrower than obtained by a chemical reaction of silver salts within the polymer matrix. The influence of these geometrical differences on the silver ion release is striking as Figure 13 demonstrates. At a comparable concentration, the release from the smaller particles of about 5 nm is higher by nearly two decades in comparison to the larger ones with an average diameter of around 40 nm.

This short description of some few results from the field of silver filled antimicrobial polymers makes it easy to imagine how many topics for bachelor and master theses could be derived from the ongoing research. All of them are either building blocks within projects related to

fundamental questions or they contribute to the development or optimisation of materials for companies.

Students who are interested in the generation of nanoparticles and the preparation of polymers filled with them, those who favour the measurement of the ion release as a function of polymer composition and water content find their special fields they would like to work in.

SUMMARY

These two examples from the Institute of Polymer Materials demonstrate that bachelor and master theses can be chosen in such a way that they become a part of the actual research work going on at the Institute. This education of students in materials science has the advantage that they learn by doing work just at the front of new developments. They very often experience that, at least for a limited period of time, they are members of a team devoted to reaching a special goal. Their contribution to this aim is obvious and, therefore, in most cases the level of motivation is rather high, which is a prerequisite for successful work.

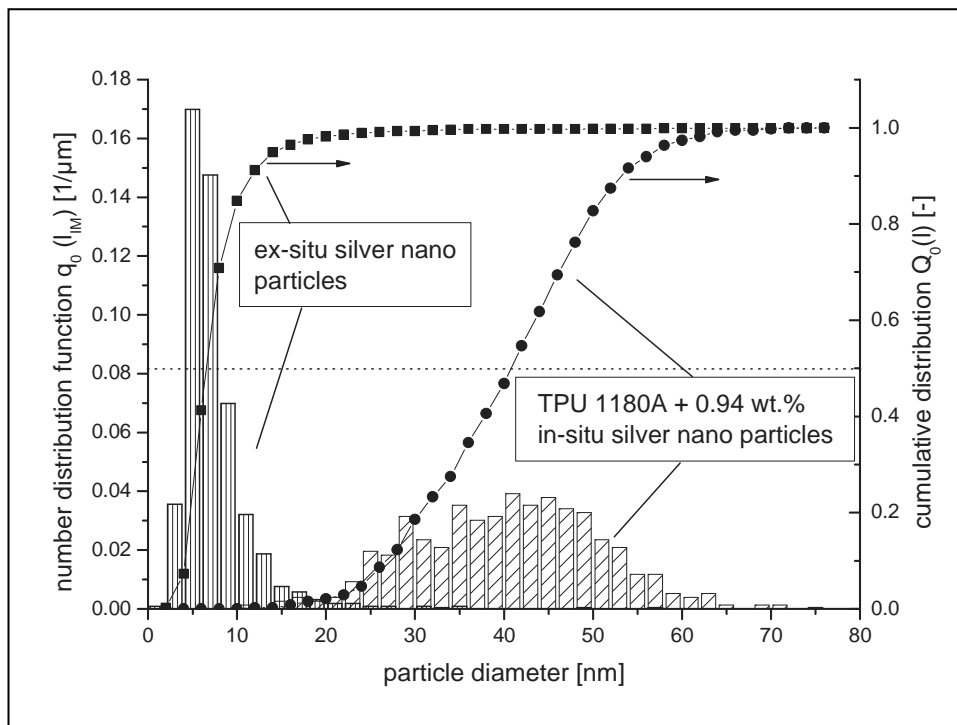


Figure 12. Distribution curves of two kinds of silver nanoparticles

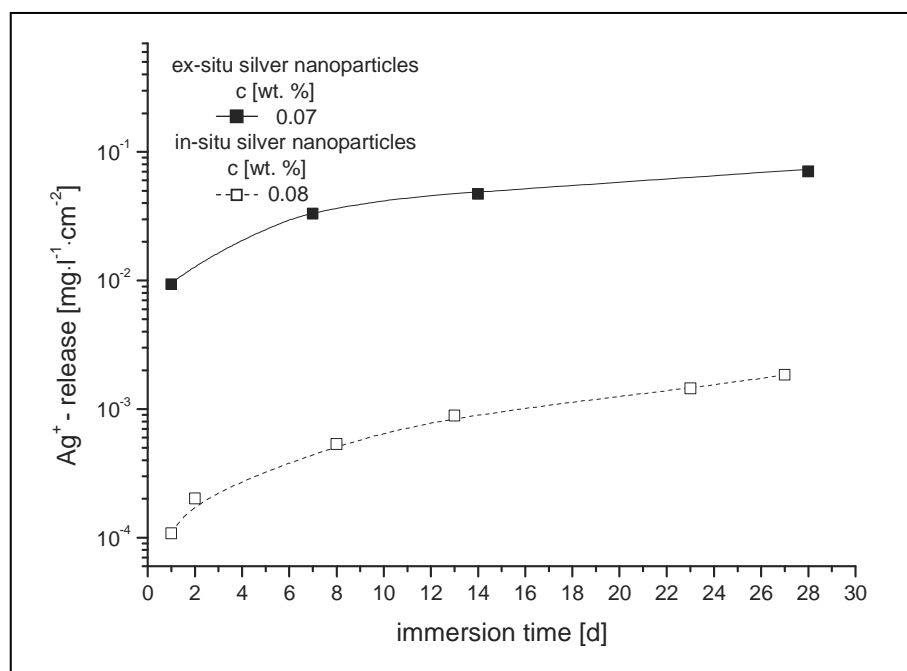


Figure 13. Silver ion release from a matrix of thermoplastic polyurethane filled with the two different kinds of nanoparticles shown in Fig. 12

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