[The article emphasizes how materials research must necessarily have an engineering objective and brings out the need for discretion in the choice of problems and funding. The article also underscores the importance of sophisticated facilities for carrying out worthwhile research in advanced technology materials, and points out that even materials research related to basic needs, requires considerable sophistication. Views and comments on the article are welcome—Ed]

MATERIALS SCIENCE FOR INDIAN NEEDS

J. B. GOODENOUGH* AND C. N. R. RAO

Materials Research Laboratory and Solid State and Structural Chemistry Unit,
Indian Institute of Science, Banglore 560 012, India.

*Raman Professor of the Indian Academy of Sciences;Permanent address: Inorganic Chemistry Laboratory, University of Oxford, South Parks Road, Oxford OX1 3 QR, UK.

INTRODUCTION

SOLID state physics and chemistry are transformed into materials science wherever they are motivated and coupled by an engineering objective. The nature of materials science can be represented by a tetrahedron (Figure 1) having, as its base, the fundamental sciences of experimental physics and chemistry, together with the theoretical framework that embraces them both; the tetrahedron is completed by the engineering design associated with a given technical target. At the centre, holding the disparate disciplines into an inter-disciplinary unit, is the monetary support provided by a potential customer for the technology.

Engineering design requires material specifications, which are generally formulated in terms of a set of engineering parameters that define the engineering function to be performed. Typical examples are efficiency, rate constants, specificity or signal-to-noise ratio, and the cost/benefit ratio. If the engineer turns to his handbook — or to the chemist, metallurgist or ceramist — to optimize his engineering parameters, he requires a theoretical framework by which to translate from the language of engineering design to the variables presented in his handbook or used by the scientist. These variables are the phenomenological parameters measured on a material of specific chemical composition, shape, size, and history. And if he wishes the chemist or metallurgist or ceramist to *design a material* that will satisfy the engineering requirements specified, the theoretical framework must embrace not only the phenomenological connections between the engineering and the phenomenological parameters, but also the fundamental understanding of how chemical composition — an intrinsic material property — and shape, size, history — extrinsic properties —combine to produce the particular properties (parameters) measured experimentally. Without a fundamental understanding of these relationships and the ability to formulate the phenomenological connections between engineering design and material parameters, the design of a material to perform a new or an improved function is left to empiricism.

In the past, industry has succeeded by an empiricism based on optimization of a set of parameters within a restricted range of variation; the "break throughs" to new structures or compositions having significantly different or improved properties appeared more by chance than by design. Industry therefore found it cost effective, to support only empiricism aimed at minor improvements in performance or major reduction in the cost of manufacture, and their research goals have been traditionally short-range and conservative. Today, our fundamental understanding of materials is such that this strategy is questioned, and those in charge of public funds for science and technology have a particular responsibility for the selection of engineering targets of national priority where concentrated support can lead to substantial public benefit.

In this brief presentation, we provide no history even of selected examples that illustrate how materials science (as presented in Figure 1) has led to such revolutionary technologies as digital computers, lasers and fibre optics, or plastics and composites. Rather, we attempt to identify some promising research goals and suggest that we could benefit from a more concentrated support of targeted research. The concentration would need to be confined to those few laboratories competent to bring together the disparate functions of engineering design and scientific measurement within a theoretical framework that is adequate for the development of new materials. But first, an observation on previous funding of such R & D efforts would be in order.

In general, materials science seems to have failed to provide technical results where the monetary support has come from two masters, an industrial sponsor for engineering development and a government sponsor for the basic science, unless these two masters worked cooperatively together to support research in the same laboratory. However, many success stories can be cited where either the government underwrote all the development costs because it was a prinicipal customer — as in defence or space exploration — or industry underwrote all because it had a guaranteed market. Where the interests of the two constituencies have converged, as in the multifaceted electronics industry, the mutual reinforcement of the two sources of support has produced a major technical revolution. The challenge, science planners and administrators face is in the identification of technical targets today that promise similar technical revolutions tomorrow.

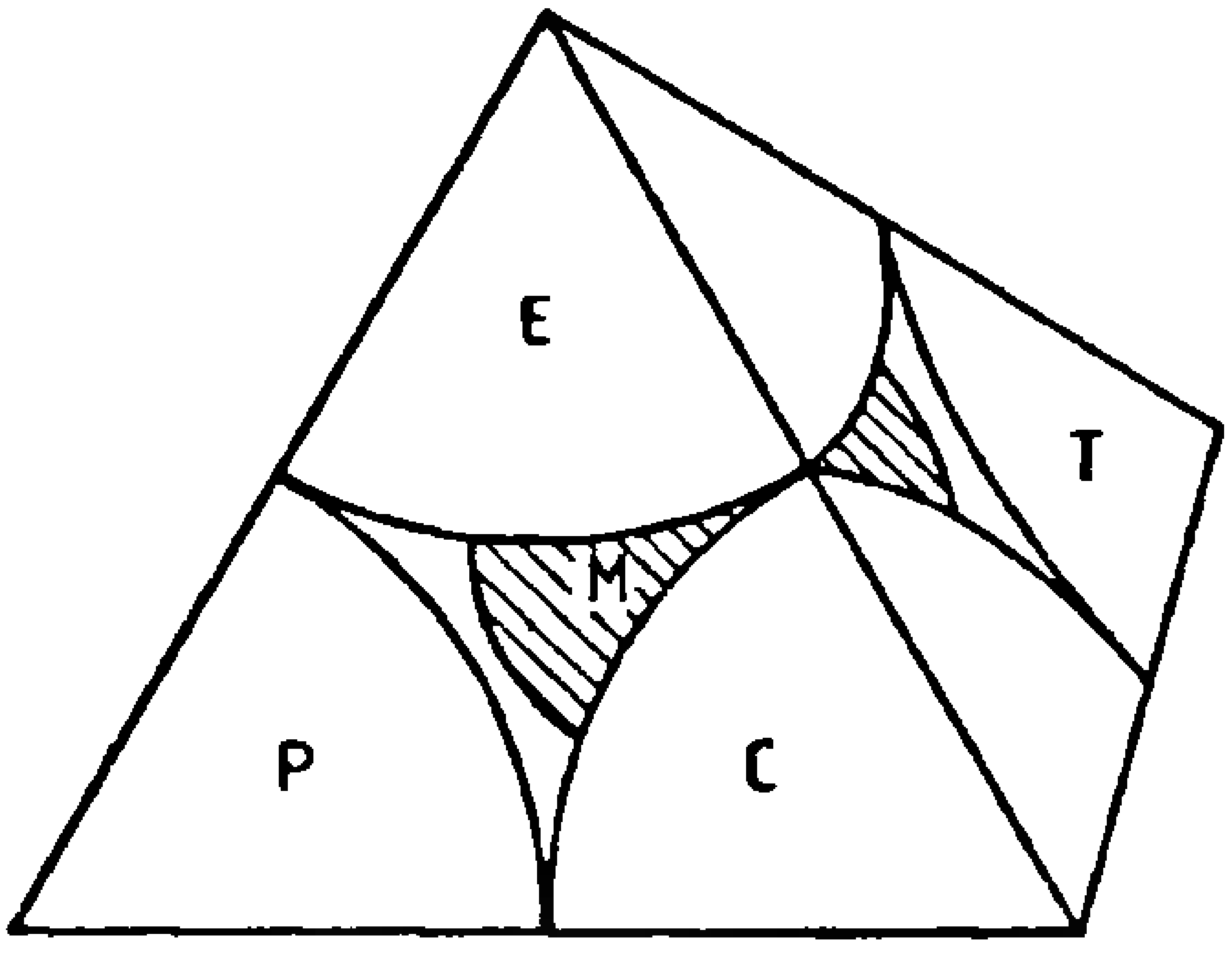

Figure 1. Materials Science as a tetrahedron: P, Experimental physics; C, Experimental chemistry; T, Theory; M, Money (funding).

THE INDIAN SCENE

India is a pluralistic democracy with a vast population. Her most important socio-economic commitment is to the alleviation of poverty and human suffering. There is an implicit faith in the country in the use of science and technology as vehicles for development. To this end, India has created a large infrastructure for science and technology. A number of sophisticated industries are now in operation in the country. Yet, fruits of this investment in science, technology and industrialization seem to have fallen below expectations. The present is therefore, a critical moment for a political act that will elicit a conscious civic faith in the national capacity to excel. Given the political will, can we identify, within the field of materials science, *targets of need* that correspond to a national urgency requiring centres of excellence for their resolution?

Two categories of need can be distinguished: materials for basic needs and materials for advanced technology. For example, wood is a traditional natural resource that has been depleted to the point where substitutes for wood are urgently required; and oil is an international resource that is too expensive to import in adequate supply which raises the issues of alternate energy sources. These are basic needs, and the adaptation to scarcities in these two commodities alone will require imaginative development of alternate technologies, only some of which may be simple; the development of adequate substitutes will require advanced materials technology as well. Development of an indigenous advanced materials technology is imperative if the material aspirations of the people are to be realised within the possibilites of a balanced international trade.

MATERIALS FOR BASIC NEEDS

Wood: We shall take wood as a typical example of a material related to basic needs. Wood has traditionally supplied paper, lumber, and fuel as well as chemical resins. Forests represent great reserviors of water that moderate the climate, minimize flooding and erosion, and conserve moisture for the dry season. With a growing population, the short-term demands for paper, for lumber in construction and for furniture, and for firewood and charcoal have denuded the Indian landscape of forests, and there is now an urgent target of need to find wood substitutes and to restore the forests.

Conservation of wood used for paper can be accomplished on two fronts: (a) wood substitutes in the paper industry and (b) substitutes for paper itself. The latter is especially important since it is predicted that the world will soon face a severe shortage of paper. Typical of the wood substitutes in the paper industry are paper recycling, rice papers, and the use of water hyacinth and bagasse. Examples of paper substitutes (besides the telephone and the radio) are computer displays and magnetic-tape storage. The inability of libraries to cope with the ever increasing flow of learned journals and books is forcing consideration of radically new methods of electronic publication and retrieval. The electronic means to accomplish this revolution must be based on an indegenous production of semiconductor materials, microcircuitry, storage, and software. Thus, a combination of advanced technologies that can replace paper usage and of alternate raw materials for the paper industry itself can sharply reduce the use of wood in this important industry.

Reinforced concrete, fibre glass, plastics, aluminium and steel have displaced wood from much of the lumber and furniture market. Wallboard from water hyacinth and composite materials can compete with wood favourably.

Wood, coal and cowdung are still the dominant fuels used for cooking and heating in large parts of India. Considerable conservation can be achieved by the design of a grate for use with a clay furnace that will allow more efficient combustion. The importance of biogas for the energy economy in India has been pointed out repeatedly. The use of bagasse from sugarcane and the conversion of agricultural wastes into methanol are two other possible substitutes.

Methanol, whether obtained from agricultural wastes or coal is a convenient liquid fuel that can be either blended with petrol or burnt directly in a conventional internal combustion engine. More efficient and cleaner utilization can be envisaged for automotive transport, should a cheap, reliable, long-lived methanol-air fuel cell be developed. Two principal materials problems must be overcome before such a cell can be realised in the market place: a proton electrolyte capable of cheap manufacture and stable to about 300° C and a catalytic anode for the conversion of methanol and water *via* the reaction,

$$CH_3OH + H_2O \rightarrow CO_2\uparrow + 6e^- + 6H^+$$

Imaginative fuel-cell designs must be coupled with this materials effort. Some encouraging news has come out of Canada in the area of proton electrolytes, but lack of a fundamental understanding of the catalytic processes operative in a suitable anode is hampering the design of this component.

Energy: The affluence of the developed countries rests in a large measure on their ability to convert the energy stored in fossil fuels (coal, gas and oil). As the century of oil draws to close, alternate sources of liquid fuels are needed for transport, and the problems of converting coal into the feedstocks of the chemical industry are being intensively reinvestigated. The technology required for proper processing of coal depends, at the least, on the development of new or improved catalysts.

The available energy sources are very few. In addition to biomass, which is renewable but of limited supply, the traditional sources are hydropower and fossil fuels. Of the remaining ones (geothermal, solar, lunar (tides), and nuclear), nuclear power and solar power are the only viable alternate long term energy sources. Power from nuclear fission represents a point source of heat and electric power; it cannot alone satisfy the varied energy demands of the country. Power from nuclear fusion would also be from a point source; it remains an unproven and uncertain option. Therefore we have to take the solar option seriously. Sunlight represents a distributed power source available throughout a large part o the year. It could be supplemented with local combusters for converting agricultural wastes into methanol; such combusters are now under development by the Solar Energy Research Institute (SERI) in Colorado.

Efficient, low-cost conversion of solar energy remains an important technical challenge. Two targets of particular interest would seem to be: (i) refrigeration and hot-water generation with low-temperature ($\lesssim 100°$ C) heat from a flat-plate collector, a technology of demonstrated feasibility and (ii) photovoltaic cells coupled to electrochemical cells for the generation of fuels or for storage in secondary batteries of high specific energy and power. For this latter purpose, cheaper photovoltaic cells of indigenous manufacture and approaching 15% conversion efficiency need to be coupled with advanced electrochemical cells.

The technology associated with dry photovoltaic cells is now capable of approaching this target with polycrystalline materials. Silicon has been the material of industrial choice because of the large investment and know-how in this material. However, silicon has an indirect bandgap that is somewhat smaller than optimum; so it will be difficult to achieve conversion efficiencies greater than about 12 percent with production units. Nevertheless, the manufacturing of silicon solar cells would seem to be a suitable technical target to obtain relevant experience in this emerging field. Attention should be given to the coupling of dry photovoltaic cells with wet electrolysis cells for the conversion of sun-light to hydrogen gas by the photoelectrolysis of water. Hydrogen is an important chemical feedstock that is now obtained primarily from fossil fuels. Improved catalytic electrodes would be useful in the wel cell, which again calls attention to the need for a better understanding of surface properties.

Besides solar-energy related devices, there is much to be done in developing new types of batteries. For example, sodium or lithium ion batteries which are promising, require the development of ideal superionic conductors. If we have to develop metal-air batteries, we need good and cheap oxygen electrodes. It is obvious that R&D in energy devices involve a major materials component.

ADVANCED TECHNOLOGY MATERIALS

The two examples discussed above illustrate how advanced R&D at the very frontiers become necessary to solve problems related to materials for basic needs. Then there are several advanced technology materials which are crucial to innovations that will make India energy efficient, promote its industrial growth and render it capable of competing internationally in the future. Important among these groups of materials are: (i) electronic materials, especially semiconductors, (ii) metals, alloys, silicates and ceramics, (iii) polymers and (iv) catalysts. Major R&D programmes have to be initiated in these areas and there is little time to lose. In some of the advanced countries, major break-throughs in materials research occur in industrial research establishments. In India, however, much of materials research is carried out in academic institutions and national laboratories. Proper links have therefore to be established to transform research results to industrial production. We list below the important classes of advanced technology materials in relation to the industries they serve.

- Electronic materials for communication and data processing
- Electro-optical materials for display and communications
- Conducting, insulating and magnetic materials for electrical transmission
- Construction materials—from improved cements to polymers and composites, from adhesives to speciality alloys (e.g., high strength, low-alloy steels and turbine super alloys)
- Superhard materials for machine tools
- High-temperature structural ceramics for high temperature engineering systems, vehicular engines and other applications
- Electrochemical materials for stationary and portable energy conversion
- Heterogeneous catalysts for chemical processing
- Surface coatings for solar energy conversion and corrosion resistance.
- Glasses for optical communication and other applications.
- Nuclear materials—from reprocessed fuels to ion exchangers for nuclear wastes, from fuel-rod cladding to avoidance of hydrogen embrittlement.

Materials science is thus an all-pervasive underpinning of a technological society. Indeed, the development of a technological society depends on the identification of new or improved materials. Even the medical industry is turning to materials scientists for new prosthetic materials for artificial organs and limbs.

Although we have listed broad areas of materials science relevant to the different industries, it is important to identify specific materials that are critical to each industry before embarking on a major programme of R & D.

SUPPORT FOR MATERIALS RESEARCH

As indicated earlier in the introduction, a soundly based effort in materials science is an interdisciplinary affair containing a well defined engineering objective with theoretical and experimental grounding in solid-state physics and chemistry. It is encouraging that a few of the educational institutions are developing supportive interactions between chemistry, physics, and engineering departments in impotant areas of solid state and surface science. Groups that have demonstrated the capacity for excellence should be encouraged by the provision of adequate facilities as well as by opportunities to consult with industry and national laboratories charged with mission-oriented responsibilities.

In order to carry out materials research competently, several experimental facilities are necessary especially those related to the preparation and characterization of materials. Preparation and characterization form the essential first step in materials research. Preparation includes not only the making of a wide variety of materials in crystalline, microcrystalline or amorphous forms, but also purification of materials, selective doping and crystal growth. It may involve the use of extreme conditions of temperature and pressure.

Characterization requires at the least, measurement of the physical property of interest; but even with an empirical approach, it is essential to correlate the physical property with the chemical composition, shape and thermal history during preparation. Ultimately, what is required is the correlation of the physical property with the chemistry, configuration, and structure of the material. The chemical characterization involves not only the purity and stoichiometry, if it is a single-phase, but also the chemical homogeneity of constituents and/or distribution of dopants. In the ferrospinel used in the magnetic memory of a digital computer, for example, it was necessary to establish not only the manganese concentration, but also the annealing time required to introduce the chemical inhomogeneities responsible for giving the square B-M hysteresis loop required by the engineer. In the manufacture of the $p-n$ homojunction of a dry photovoltaic cell, the introduction of dopants must be controlled not only as to concentration, but also as to distribution on moving in from the surface of the material. If a material is two-phase, as in a composite, the shape and interpenetrations of the two phases must be controlled. Moreover, where surface properties are critical, as in catalytic electrodes, characterization of the surface must be distinguished from characterization of the bulk Structural characterization of a given phase can also prove to be subtle, especially if it contains two-phase intergrowth or extended defects. The new revolution in high resolution electron microscopy wherein the ultrastructure and compositional analysis of solids can be examined with hardly 10^{-20}g of a sample (~10-100 Å diameter) promises tremendous possibilities. Higher resolution NMR spectroscopy of solids with magic-angle spinning may unravel many complex problems as it has already done in the case of zeolites. Thus, the techniques employed for the preparation and characterization of materials are becoming increasingly sophisticated, and even the definitions of purity, perfection, or composition of materials are changing with time. These two activities therefore require high investment initially.

Preparation:

* High-temperature furnaces of various kinds (including SiC, Pt, W, graphite furnaces, induction furnaces, skull melter and diffusion furnaces)
* Various types of crystal-growth equipment
* High-pressure facilities, including anvil and belt systems, autoclaves.
* Sputtering equipment, evaporation units.
* Low-temperature facilities (preferably going down to liquid helium temperatures).
* Clean room for solid state electronics and related research.

Basic Characterization

* X-ray diffractometer and related x-ray facilities with access to neutron diffraction where required.
* Electron microscopes (SEM, TEM, STEM)
* X-ray fluorescence
* Electron microprobe analyzer
* Atomic absorption spectrometer
* Mass spectrometer.

Measurement of properties for finer characterization

* IR/Raman spectrometers
* UV-Vis/Luminescence spectrometers
* Surface analysis instruments (XPS/UPS, Auger, LEED)
* ESR spectrometer
* NMR spectrometer for study of solids
* Electrochemical instrumentation
* Instruments for transport measurements
* Facilities for magnetic measurements, including a magnetometer
* Instruments for measuring mechanical properties.

Facilities of the kind listed above could be made available to a large body of materials scientists by establishing viable centers for materials research in the academic sector as well as under the aegis of scientific agencies. Materials research centres in the academic sector would also be required to train young people in the most up-to-date techniques and in devising materials strategies. In the absence of such facilities, it will be difficult to take up any challenging tasks related to advanced technology materials. Science planners and administrators should note that they cannot expect or demand much out of materials scientists in the country until these critical inputs are made.

In order to encourage excellence in mission-oriented laboratories supported by government or industry, it is necessary to establish some form of accountability with, perhaps fixed-term contracts associated with levels of support, further renewals depending on performance. Special financial incentives could also be provided to encourage success. Without an appropriate punishment/reward structure, the mind is inadequately focussed and the enterprise is too rarely in the hands of the adventurous.

CONCLUDING REMARKS

In conclusion, we would like to stress again that all research on condensed matter is not materials research; the latter must necessarily have an engineering objective. We find it necessary to stress this point since many scientists seem to classify their research under solid state physics, chemistry, solid state electronics or materials science purely based on personal preference and convenience. This may hurt the interest of materials research in the long run. It is also necessary to use discretion while funding research projects. There appears to be a tendency in recent years to support any passable project that is even remotely connected to an area that is fashionable or of supposed national relevance. This is particularly common in materials research, and investigators often pick a minor problem related to an age-old material or work on a trivial modification of a known material. It is most essential to be selective if we want materials research to yield worthwhile results. Not all materials can be equally significant in terms of the quantity needed or their strategic importance; neither can all of them offer equally exciting research possibilities.

Unlike the situation in basic condensed matter science, the following important factors have to be kept in mind before taking up or funding a research project in materials science: (i) What exactly is the engineering objective (mission) where the material is to be used? (ii) How crucial is the material to be investigated for the concerned industry or how important is the material strategically? (iii) What is the quantity of material required and what would be the approximate financial benefit if the material is produced in the country? (iv) Is the material a substitute for an important natural resource (that is fast diminishing) or for an imported material? (v) Is there any possible spin-off from the effort that could benefit the industry or the country at large?

Materials research requires a number of sophisticated facilities and involves heavy initial investments. It is suggested that several good centres be started in the country with definitive objectives and critical inputs so that they may provide the proper infrastructure for effective research in this area of vital importance.

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