Recent progress in the development of materials

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Progress in materials research and development during the recent times has been phenomenal. The article aims at presenting a perspective on the noticeable trends in the following aspects: (a) extending the limits of capability of selected structural and functional materials, (b) resorting to multicomponent compositions, (c) exploiting the benefits of fine-scale microstructure and (d) employing extreme temperature, pressure and strain rate for materials processing. Recent developments in energy efficient materials processing and integrated computational materials engineering (ICME) have also been outlined.

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Introduction

Materials science was first recognized as a discipline in the late 1950s at Northwestern University, USA [1] and has since grown multifariously. The number of research papers and reviews relating to materials science published annually has increased spectacularly since 1980 to be over a million now [2]. The present essay presents a perspect- ive on the trends discernible during this phenomenal progress. Materials science is interdisciplinary, being grounded in the fundamentals of chemistry, physics and, more recently, biology. Ellingham's diagram [3] during the early 20th century provided a scientific method to deter- mine reduction temperatures for metal oxides, which formed the basis for metal extraction processes. While chemistry evolved into the modern field of chemistry of materials [4] the celebrated room at the bottom Feynman lecture stimulated worldwide involvement in research based on nano concepts. Jean-Marie Lehn propounded the room at the top thesis, which led to materials synthesis and processing via supramolecular chemistry involving non-covalent inter-molecular bonding. The other major foundation of materials science was based on physics, with the development of electron theory of solids. Subsequently, the density function theory (DFT) [5*] contributed in several ways to the understanding of the material behavior. In recent years, significant impetus from biological sciences has led to rapid developments in areas of biomaterials, biomimetic or bio-inspired materials and bioleaching [6].

The grand march of materials science is manifested in the over 40 Nobel prizes awarded for pioneering work in various aspects of the field. The representative list of accomplishments recognized by Nobel awards in recent times includes: (i) new materials: ceramic superconductors (1987), fullerenes (1996), conductive polymers (2000), semiconductor heterostructures (2000), optical fiber leading to optical communication and CCD sensor

(2009), graphene (2010) and quasicrystals (2011); (ii) materials- related phenomena: Bose–Einstein condensate (2001) and giant magneto-resistance (2007); (iii) theory of materials: physics of liquid crystals and polymers (1991) and density functional theory (1998); and (iv) techniques to character- ize materials: scanning tunneling electron microscopy and transmission electron microscopy (1986), high resolution nuclear magnetic resonance (1991), neutron diffraction (1994), femtosecond spectroscopy (1999) and laser-based precision spectroscopy (2005). Clearly, the pedestal on which the field of materials stands majestically aloft is supported by two pillars: one representing experimental techniques for comprehensive material characterization and the second is centered on theory anchored by a hard scientific approach. The third leg of materials tripod, though not reflected in the Nobel awards but emerging as an important tool, is based on computational techniques involving predictions.

Trends in the advancement of materials

Extending the limits of capability of structural and functional materials, crafting multi-component compositions, ensuring fine-scale microstructure, and employing extreme temperature and pressure are recent trends in materials and their processing.

Extending the limits of materials capability

Increasing strength, stiffness of engineering polymers and fracture resistance of high strength ceramics, as well as unique combination of properties of composites and hybrids of these basic materials, has been accomplished [7]. The continued trend in enhancing strength-toughness/ductility combination has been remarkable in high strength sheet steels [8] for automotive applications and high performance bainitic steels [9] for rails.

Corning met the demand made by Steve Jobs for his iPhone and iPads with the Gorilla glass with enhanced strength and damage resistance (M. Panzarino (2012); URL: http://thenextweb.com/apple/2012/03/02/apple- confirms-that-it-still-uses-corning-glass-in-most-iphones/; http://www.corninggorillaglass.com). The structure–process–property paradigm that underlies the extensive development of structural materials has also contributed to advancements in functional materials [10]. Silicon, the bedrock material for semiconductor electronics and solar cells, is appropriately considered by Browne [11] as one of the seven elements that trans-formed the world (other elements being iron, carbon, uranium, gold, titanium and silver). Graphene, the wonder allotrope of carbon, is the strongest material tested [12], and is emerging as an electronic material with promising applications [13**]. By way of extending the magnetic energy product of hard magnets, 60 MGOe NdFeB nanocomposite hard magnets have been made [14]. Significant increase in magnetic recording density to a staggering 103 Gb/in2 has been achieved with the advent of heat-assisted magnetic recording (HAMR) technologies (URL: http://www.seagate.com/about/newsroom/press-releases/terabit-milestone-storage-sea-gate-master-pr/). Prompted by the discovery of high TC ceramic superconductors, several complex oxides have been synthesized chasing room temperature superconductivity. However, they have not seen widespread use because of cost, complexity of their processing and the damping effects of high magnetic fields. Recently Fe-based superconductors, which are partly metallic and therefore more easily fabricated, have been found to carry exceptionally high currents under high magnetic fields [15**].

Multi-component materials

Thanks to the exceptional alloying tolerance of Ni, directionally solidified and single crystal multi-element nickel superalloys have facilitated realization of highly efficient aeroengines to power modern aircraft. The Rolls Royce Trent 1000 aeroengine made with Ni-based super-alloys and inducted into Boeing 787 in 2010 consumes about 20% less fuel and is accompanied by a drop in CO2 emission level of nearly 15%, compared to its predecessor Trent 875 (URL: http://www.rolls-royce.com).

Direct synthesis of compound phases has led to high TC superconductors, discussed in the foregoing subsection. Similarly, the glass forming tendency was proven to increase with the number of components, and a multi- component bulk metallic glass with strength-toughness combination greater than those obtained in structural steels has been made [16]. Among other multi-component alloys that have recently attracted attention are the gum metal from Japan and high entropy alloys from Taiwan. The gum metal is a beta-titanium alloy exhibiting high strength and elastic-plastic behavior with significant strain [17]. The high entropy alloys are materials designed on the basis of near-equal atomic ratio and high entropy of mixing [18].

Benefits of fine-scale microstructure

Solidification, precipitation, precipitation-recrystallization interaction, and thermo-mechanical controlled pro-cessing (TMCP) have been designed to obtain finer micro-structures (19) in bulk materials: for example nano-precipitation hardening (Sandvik-NanoFlex: 2000 MPa) [20], incorporation of amorphous and/or nano-size grains in Fe–B bulk metallic glasses (4000 MPa) [21*] and in nano-super hard steels (6200 MPa) (Technology overview (2009); URL: http://cancade.com/assets/files/). Process innovations such as electromagnetic stirring of castings and equal channel angular processing (ECAP), new generation TMCP, and phase reversion process [22] involving severe cold deformation-annealing sequence have evolved to refine bulk materials to submicron grain size to achieve simultaneous enhancement in strength and toughness. Mechanical alloying, coupled with new rapid powder sintering tech-niques like field-assisted sintering technique (FAST) and flash sintering technique (FST) [23*], rapid solidification, rapid pressurization, sonication, chemical and physical deposition techniques, have enabled production of bulk nano-phase materials. The global pursuit of nanomaterials with unique properties is supported by the advent of characterization tools such as HRTEM, STM, AFM and 3D atom probe [19].

Employing extreme temperature, pressure and strain rate for materials processing

Nature processes materials at high pressures and temperatures to form minerals with multi-component and multi-phase character [19]. Diamond is a result of precipitation of carbon in this structural form from CO_2 saturated magnesium-rich rocks at 50 kbar and 1700 K occurring at depths of 600 km [19]. Ultra-hard aggregated diamond nanorods have been realized in the laboratory by compressing carbon fullerenes to a pressure of 20 GPa at a temperature of 2500 K [24]. Metallization of hydrogen occurs naturally in planets such as Jupiter and has also been experimentally produced in the laboratory at high pressures and low temperatures [25]. At the other extreme, the low temperature-low pressure environment in space has been exploited for new kinds of materials processing. These are selected examples of effort that emulate nature with the aim of obtaining technologically superior materials under extreme processing conditions.

Material deformation at ultra-high strain rates (10^3 and above) is relevant to diverse areas such as dynamic metal forming, for instance electromagnetic forming [26], ballistic penetration of armor materials, asteroid impact on earth, machining and solid particle erosion. At high strain rates in the range of 10^3–10^8, dislocation velocity is largely controlled by viscous damping accompanied by other effects influencing the nature of deformation [27].

Energy efficient materials processing

The projected rise in world population to over 9 billion by 2050 will lead to increased consumption of materials and enhanced usage of energy, leading to rapid depletion of vital energy resources. Development of eco-friendly materials by minimizing the use of energy delineates the way to meet these challenges [28]. Reducing the number of processing steps as well as product weight, minimizing heat and electrical losses during usage and recycling are all being explored. For example, primary Al involves production energy of 149 MJ/kg and 10 kg CO_2 emission per kg: these values are considerably reduced, 13 MJ of energy and 0.9 kg of CO_2 per kg, for recycled Al and similar benefits from recycling are reported in case of steel [29]. With the world annual crude steel production at over 1.5 billion tones, iron and steel industry accounts for 5% of world's energy consumption and over 3% of the world's CO2 emission. Advanced processing technologies such as top gas recycled blast furnace (TGR-BF) with CO2 capture and storage (CCS) are being evolved to reduce CO2 emission [30]. The use of renewable energy will also lower energy consumption [30]. In regard to the low cost alternative and high-power conversion efficiency, dye sensitized solar cells have attracted significant atten- tion since the Gratzel's group developed a solar cell based on nanocrystal mesoporous titania [31]. Advanced energy efficient materials processing technologies like additive topology optimized manufacturing have become avail-able for manufacturing hierarchical structures involving part design for multifunctional properties employing ICME approach (J.M. McQuade, 'Energy efficiency: Materials and manufacturing processes' (2013); URL: http://iee.ucsb.edu/). Additive manufacturing methods are promising for the manufacture of patient-specific biomedical implants [32]. A new energy-efficient process has been recently reported for making functional coatings (Fraunhofer develops an energy-efficient process for making functional coatings (2013); URL: http://www.industrial-lasers.com/articles/2013/03). Improved metal joining techniques, such as the environment friendly and highly energy efficient friction-stir welding process, have been introduced in space shuttle manufacturing by NASA in 2009 (proven friction stir welding technology brings together reliability and affordability for NASA space launch system; URL: http://www.nasa.gov/exploration/systems/sls/12-056.html). The automobile is the quintessential symbol of modern-day life-style across nations and it is anticipated that the world could have more than a billion vehicles by 2020. Batteries are critical for energy efficient, less-polluting vehicles. From the early rechargeable lead-acid batteries that provided a specific energy of 40 Wh/kg to the current values of 150 Wh/kg provided by lithium-ion chemistries, energy storage systems have made unprecedented advancements. Key to this was the development of an intercalating compound LiCoO2 as the cathode that could reversibly accept and release lithium ions. At the other end, the anode was replaced from lithium metal to intercalation of lithium into graphite, a layered structure, to assure safety and provide the cycle life demanded in consumer applications. High capacity positive electrodes paired with Si-based negative electrodes can provide energy densities above 400 Wh/kg. Future developments based on lithium–sulfur (Li–S) and the lithium–air (Li– O2) systems promise energy densities of 2600 Wh/kg and 11,400 Wh/kg [33], respectively. These latter high energy systems are needed to satisfy vehicle range demanded of pure electric propulsion systems if zero-emission vehicles are to become the choice for personal mobility.

Above developments are illustrative of trends underway globally to address concerns consequent to perceived climate change. While energy efficiency in materials processing is receiving increasing attention, there are serious concerns arising due to uneven distribution in the world of resources of energy materials such as rare earths and those needed for photovoltaics. The modern communication and computing devices are built around numerous elements, albeit in small quantities. Several of these materials are being regarded as critical [34] requiring augmented exploration and new internationally accepted policies.

Integrated computational materials engineering (ICME)

Alloy phase diagrams are central to the understanding of materials. While 80–90% of possible binary metallic alloy diagrams have been determined, only 5–10% of possible ternary diagrams are available. The number of quaternary diagrams is even less and minimal for multicomponent crystalline ceramics as well as the emerging polymeric systems. Significant progress was achieved through experimental work guided by Gibbs free energies and phase rule but the experimental approach has proved impractical in the case of higher order phase diagrams. Kaufman's pioneering CALculation of PHAse Diagrams (CALPHAD) method provided the momentum to go forward, but critical to its success are databases of thermochemical and thermophysical properties, as well as quantitative data on diffusivities. When combined with other predictive models CALPHAD approach can help accelerate alloy design and development: for example, the superalloy GTD 262 successfully developed by GE, USA [35,36]. Considerable progress has been registered in designing alloys to possess a given set of properties using the computational materials design approach [37*], involving multi-level designing spanning length scales from several microns down to the electronic level [38]. Following success of the first computationally designed material Ferrium S53 as landing gear steel in 2010, there has been a growing emphasis on computational methods for realiz- ing improved material properties and performance [37*].

The US President announced the 'Materials Genome Initiative for Global competitiveness' in 2011 requiring experimental as well as computational tools besides digital data on properties discussed above [36]. Kaufman and Agren outlined recently [39] how the materials gen-ome can be regarded as DNA 'encoded in the language of CALPHAD thermodynamics and kinetics'. The coming years are bound to witness a wave of interest in the use the materials genome platform for accelerated design of new materials not envisaged hitherto.

Concluding remarks

The science and engineering of materials remains a hall-mark of where the society has reached. Materials defined the Ages. The advent of the optical microscope and the mapping of the iron-carbon phase diagram changed for-ever the course of materials development and the society has benefitted from an explosion in materials develop- ments related to telematics, energy generation, automo- tive, aerospace and other high technology systems. While materials, including those produced on tonnage scale at relatively low cost, have created a memorable past largely based on experimental work, the future of materials developments will be fueled by fresh insights into mech-anisms that will be driven by a combination of theory, experiments and computations to enable design of new materials, several ab initio or customized to the user. Clearly, it is impossible for any single group of individuals or institutions, or for any one country, to cope with this opportunity. We can expect that since materials contrib-uted to interconnecting societies, the collective capability created will now drive materials developments at a far more accelerated pace.

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