Materials for extreme environments

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Materials for extreme environments can help to protect people, structures and the planet. Extreme temperatures in aeroplane engines, hypervelocity micrometeoroid impacts on satellites, high-speed machining of ceramics and strong radiation doses in nuclear reactors are just some examples of extreme conditions that materials need to withstand. In this Viewpoint, experts working on materials for different types of extreme environments discuss the most exciting advances, opportunities and bottlenecks in their fields.

Materials for extreme shock and strain-rate environments

Suhas Eswarappa Prameela. Metallic alloys and ceramics are attractive for structural applications because of their durability and mechanical strength. Their use is ubiquitous and is heavily preferred in environments where materials are subjected to shock loading or high-strain-rate deformation, such as in car collisions, launch and re-entry of rockets, or hypersonic vehicles, and as protection materials on the battlefield.

When a material is subjected to shock loading, a substantial amount of energy is absorbed in a very short time. Typical quasistatic mechanical loading involves strain rates of 10^{-3} to $10^{-1}\,s^{-1}$ that can be sustained over minutes to hours. However, the high strain rates achieved during dynamic or shock experiments are often on the order of 10^{3} to $10^{7}\,s^{-1}$ over just a few nano- or microseconds. Because the propagation velocities for energy are finite, the material seeks internal pathways to dissipate this energy. Every material has a spectrum of available pathways or mechanisms. For example, metals can dissipate energy through high-velocity twinning, rapid dislocation motion, void nucleation or adiabatic shear banding. Ceramics can undergo local amorphization, formation of cracks or voids, and adiabatic shear banding. The material's microstructure governs which mechanisms are active, thereby offering an approach to control the material's response.

There are two major categories of shock and high-strain-rate experiments. The first consists of experiments to study the constitutive behaviour, which includes plate impact, laser shock, isentropic compression and Kolsky bar experiments. The second set of experiments is focused on studying deformation mechanisms and failure processes, which include plate impact (recovery), blast, shear band, perforation, confined penetration, impact cratering, dynamic fracture and ballistic experiments. Both categories of experiments help to quantify materials' dynamic strength and failure behaviour. Furthermore, the rich data obtained using state-of-the-art diagnostics, like high-speed photography and time-resolved in situ synchrotron studies, can help to identify and track key deformation and failure mechanisms during extreme events.

Over the past decade, there has been a renewed push to develop metallic alloys that can survive in extreme shock and high-strain-rate environments. In the case of face-centred cubic metals (such as Al, Cu, Ag and Ni), solute concentration, dislocation density and grain boundaries mainly control the mechanical strength. During high-strain-rate deformation, the dislocation density increases, often leading to increased shear strength, for example from nearly 60 MPa at $10^{2}\,s^{-1}$ to 140 MPa at $10^{5}\,s^{-1}$ in the 1100 Al alloy[1]. As the purity of Al decreases, the strength increases, with a reduction in the normalized rate sensitivity at high strain rates. In body-centred cubic metals (such as Fe, Ta, Mo, V and W), strength strongly depends on the strain rate and temperature. Body-centred cubic metallic alloys retain strength at high temperatures, owing to their high melting point, and plastic deformation is mainly controlled by the motion of screw dislocations, whose mobility is determined by kink formation. The thermal softening and strain-rate effects are strongly influenced by kinks and screws. A study on Fe–Mn alloys showed that the shock waves are disrupted by a metastable volumetric contraction at the atomic scale during phase transformation[2]. In the case of hexagonal close-packed alloys (such as Mg, Ti, Zr and Y), the hexagonal crystal symmetry complicates the plastic deformation mechanisms, resulting in anisotropic behaviour. Diverse dislocation reactions and twinning are common in these alloys and are strongly influenced by the solute type, concentration and grain characteristics. A study showed that micrometre-sized slag particles often found in commercial Mg alloys accelerate spall failure, a phenomenon where the material rips open from the inside out during shock loading[3]. This occurs because of void nucleation at the interface between matrix and slag particles. Slag particles do not play a significant role at quasistatic strain rates, but they can be detrimental at extreme strain rates. Several efforts are ongoing to produce a high density of nanoscale precipitates with coherent interfaces to improve mechanical properties across a wide range of strain rates; other efforts are focused on altering the microstructure of materials to minimize spallation and penetration during ballistic impacts[4]. For example, a pre-compression process called pre-twinning resulted in stable, ordered twin structures that changed the dominant failure mechanism in Mg alloys from discing to ductile hole growth[5].

Advanced ceramics made of carbides, nitrides, oxides, silicides and borides have also been studied at high strain rates. Dislocations are hard to move in these materials under normal loading conditions, except at high pressures. These materials show great differences between their tensile and compressive strengths, and their behaviour is dominated by crack nucleation, growth, coalescence and propagation. The mechanical strength of ceramics is

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controlled by the stress state, the sample size (because the fracture is fundamentally a size-dependent process) and the strain rate. Some dominant mechanisms under impact include amorphization, fracture and granular flow. One recent study showed how silicon doping in boron carbide ceramics is an effective way to suppress stress-induced amorphization[6]. Rapid advances in high-throughput dynamic experiments and machine-learning models are proving to be time-efficient and cost-effective ways to rapidly screen thousands of microstructures and/or chemistries, helping to realize the inverse design of structural materials subjected to extreme shock and strain-rate conditions.

Materials for extreme temperature environments

Tresa M. Pollock. Materials must withstand extreme temperatures across a wide variety of engineering applications and operating environments. Robust performance at high temperatures is critical, for example, in propulsion (scramjets, rocket motors, aircraft engines), flight with high Mach number, atmospheric re-entry of space vehicles, nuclear reactors (both fission and future fusion designs), energy generation and storage (turbines for power generation, concentrated solar power), chemical and thermomechanical processing operations (furnaces and reactors) and high-temperature electronics. To operate in such extreme thermal environments, materials must be resistant not only to melting, but also to failure due to thermal or mechanical loading, and degradation caused by thermally induced phase transformations or surface recession resulting from corrosion, oxidation, vaporization or ablation.

The many degradation and failure mechanisms that limit the application of materials demonstrate kinetics that tend to scale with the melting temperature, making this a material property of primary importance. The melting temperatures of the major classes of materials available for operation at temperatures above 1,000 °C are shown in the first panel of FIG. 1. At the low end are nickel- and cobalt-based superalloys, which have high levels of mechanical damage tolerance and operate in thermomechanical environments with temperatures up to 90% of their melting point. At the higher melting temperature end of the spectrum are carbides, nitrides and borides (as well as graphite and composites that are mixtures of these materials), which can survive extreme temperatures in inert environments but are often limited to operation at much lower temperatures because of oxidation or vaporization, and have limited capacity for plastic deformation. Refractory metals have very high melting points and the ability to tolerate thermomechanical loading at high temperatures, but are limited by their poor oxidation resistance and by a transition to brittle behaviour below about 20% of their melting temperature. An emerging class of refractory alloys, referred to as multi-principal-element alloys or high-entropy alloys, which consist of approximately equiatomic mixtures of three to six refractory elements, shows some promise for strength and ductility across the entire temperature spectrum. Finally, silicides and oxides that melt at intermediate temperatures are often desirable because of their tendency to form surface protective layers at elevated temperatures. In the absence of intrinsic surface protective layers, single or multilayered coatings that are thermochemically and thermomechanically compatible with the substrate must be designed and applied.

In extreme temperature environments, the demands on materials are multifaceted and as a result require optimization of a suite of properties. This property tuning is typically accomplished by targeted alloying or doping, resulting in materials that may contain 10 or more elements. Thus, the compositional search space for

new materials is very large, and materials discovery is limited by the traditional iterative materials development loop, consisting of hypothesizing promising materials compositions and experimentally synthesizing, testing and analysing them. Over the past few years, the rapid expansion of computational power, improvements in materials theory and simulation, the speedup in the characterization of materials, and the application of machine-learning algorithms to the rapidly expanding materials data have fundamentally changed the materials discovery and development process, enabling substantial acceleration. The remaining bottlenecks promise to be addressed by autonomous synthesis and characterization tools, further development and implementation of artificial intelligence approaches, and expanded availability of high-performance computing resources.

Finally, processing materials for extreme temperature environments into useful components and devices presents extraordinary challenges. Traditional bulk processing methods such as rolling, forging, extrusion and bulk crystal growth are severely challenged by the temperatures required to process the materials in the first panel of FIG. 1, resulting in extremely expensive, energy-intensive processing platforms. One solution is to target near-net-shape approaches, using, for example, 3D-printing methods, in which high-energy-intensity lasers or electron beams locally tailor the material by simultaneously shaping, mixing or depositing. Models for these complex processes remain to be fully developed across the spectrum of materials of interest, owing to the complexity of the physics and the breadth of length scales that must be understood and controlled. Nevertheless, further development of advanced synthesis approaches and better integration into the iterative design loop would enable the fabrication of 'materials on demand', tailored for specific extreme temperature environments.

Materials for extreme corrosion and hydrogen environments

Dierk Raabe. Corrosion is the degradation of materials (primarily metals) due to interactions with their environment. It limits the longevity, safety and function of products, sometimes resulting in abrupt and catastrophic failure. Corrosion is a system phenomenon in which such diverse factors as material, coating, environment, microbiology, stresses and/or electromagnetism act together. Every year

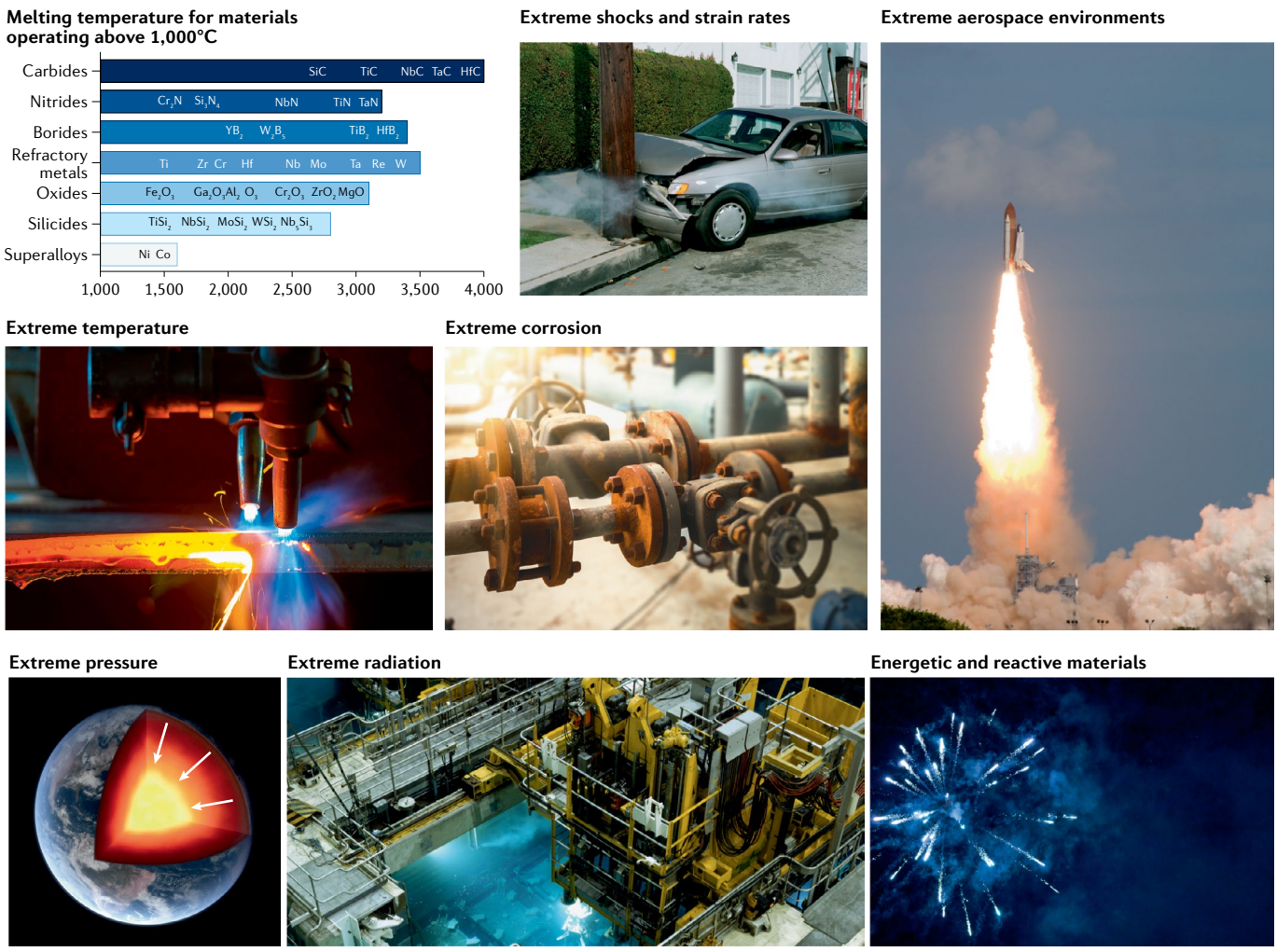

Fig. 1 | **Examples of extreme environments.** Materials for applications in extreme environments need to withstand very harsh and challenging conditions, as in the examples illustrated. Credit: extreme shock and strain rates: Erik Von Weber/Getty; extreme temperature: AROON PHUKEED/Getty; extreme corrosion: jia yu/Getty; extreme pressure: fpm/Getty; extreme radiation: Steve Allen/Getty Images; energetic and reactive materials: Junao Li/Getty; extreme aerospace environments: Mooneydriver/Getty.

it irreparably destroys about 4–5% of the world's gross domestic product, with annual costs above 2 trillion US dollars. A third of that could be saved through the use of better materials and corrosion protection.

This makes corrosion science (which includes the study of hydrogen-related material decay) the discipline with the highest leverage in the transition from the age of the fossil industry to the age of sustainability. It enables higher longevity of materials and thus helps to reduce global warming, because products and infrastructures that do not need to be replaced help to cut synthesis and manufacturing-related greenhouse gas emissions and energy consumption. Examples of infrastructure in which sustainability hinges critically on materials' resistance against corrosion are wind farms; direct solar thermic power plants that use liquid salt; fusion and fissile reactors, which suffer from hydrogen embrittlement and corrosion; power plant turbines and aero-engines that use green hydrogen as (additional) fuel; pipeline infrastructures carrying hydrogen; and desalination plants that provide water for drying-out regions in times of global warming.

One of the issues in this field is the inverse relationship between the strength of a material and its corrosion resistance. Particularly in the transport sector, and especially for electric vehicles, lightweight construction is essential. For this purpose, ultra-high-strength alloys such as medium manganese and multiphase steels, as well as zinc-, copper- and magnesium-blended aluminium alloys, are increasingly used. Their high strength mainly comes from complex microstructures, chemical compositions and internal stress fields. All three types of features make such materials susceptible to corrosion and particularly to hydrogen embrittlement, acting through mechanisms such as accelerated diffusion along lattice defects, formation of multiple local galvanic elements, and stress-driven trapping and accumulation of hydrogen at internal interfaces. Countermeasures have been suggested, such as the introduction of intentional heterogeneities into the microstructures of high-strength steels that can suppress hydrogen-driven crack growth[7]. In high-strength aluminium alloys, the chemical interaction of magnesium and zirconium with hydrogen can lead to embrittlement, so that passivation of the affected interfaces and control and/or replacement of these elements can increase the material resilience[8]. In titanium and nickel alloys, nanohydrides have been identified as critical for the initiation of corrosion and embrittlement.

Another area where more work is needed is the development of materials for the use of hydrogen as an energy carrier. This requires designing grids for high hydrogen partial pressures, with steels that resist hydrogen embrittlement. The negative Joule–Thomson coefficient must be also taken into account, as the expansion of hydrogen does not lead to cooling but to heating, and thus to higher hydrogen absorption. In this context, embrittlement-resistant bainitic and tempered martensitic steels are being developed for safe hydrogen infrastructures. Feeding hydrogen as fuel into gas turbines can also lead to embrittlement, due to the alternating mechanical loads and heating/cooling cycles, during which hydrogen-related damage can be initiated. Specifically, it can lead to hydrogen-stabilized superabundant vacancies which accumulate into pores, hydrogen-enhanced local plasticity and/or hydrogen-enhanced interfacial decohesion. The materials used in such turbines (flying or stationary) range from high-temperature steels to titanium alloys and nickel-based superalloys, all susceptible to hydrogen embrittlement. Recent findings indicate that some medium- and high-entropy alloy variants, doped with interstitials, have beneficial corrosion and hydrogen-embrittlement resistance that could potentially compete with those of some of the established alloys.

A further challenge is the increase of the recycled content used in alloys (for reducing greenhouse gas emissions in the primary synthesis sector) and the corrosion-related effects arising from it[9]. In some products, the recycled content can exceed 80%, in part containing contaminated post-consumer scrap. Producing high-performance materials with the highest possible recycled scrap content is an essential pillar of a coming circular economy. However, this approach introduces impurities into previously largely corrosion-resistant alloys, influencing corrosion and hydrogen attack, and leading to liquid metal embrittlement. Examples include the formation of galvanic elements by intermetallic phases caused by impurities such as iron, copper, magnesium or zinc, and hydrogen embrittlement in high-strength aluminium alloys. Similar effects result from increasing amounts of manganese in steel scrap, which can lead to higher corrosion susceptibility of advanced steels. A particularly big problem is the accumulation of copper and zinc in steel scrap. The impurities lead to a notorious form of liquid metal embrittlement through low-melting eutectics, which can lead to catastrophic failure. Both elements are very hard to remove from liquid steel scrap melts during recycling.

Other important research topics in this field are advanced corrosion inhibitors; cathodic protection; advanced coatings; ab initio-based computational corrosion science; the use of artificial intelligence in corrosion science; advances in analytical and in-operando methods for high-resolution hydrogen probing and quantification of galvanic features; corrosion in the oil and gas industry; and corrosion in nuclear facilities.

Materials for extreme pressure environments

Marc André Meyers. High pressures can substantially change materials' properties. The interiors of the Earth and exoplanets are striking examples of the importance of pressure: the inner core of the Earth is solid iron, whereas the outer core is liquid. This configuration is directly responsible for the Earth's magnetic field and the retention of the atmosphere. By contrast, Mars, which has a solid iron core, is virtually devoid of atmosphere. There are substantial ongoing research efforts to study materials under high pressures, with or without coupled temperature changes. These experiments can be static or dynamic.

Static experiments were pioneered in the early twentieth century by Percy Williams Bridgman, who received the Nobel Prize for this work. Bridgman used two anvils to apply pressures of up to 10 GPa to materials[10]. Later developments at the National Institute of Standards and Technology (NIST) in the 1950s, using diamond anvils, increased the maximum pressures to 50 GPa. In 1961, Sergei Stishov synthesized the high-pressure phase of silica, found deep in the Earth's mantle and around meteor impact craters[11]. This required a pressure of 16 GPa and represents an important discovery in geochemistry. This phase was rightfully named 'stishovite'. Nowadays, pressures as high as 350 GPa can be reached. Diagnostic tools can be used to monitor phase transitions, reactions and changes in physical properties in real time.

High pressures can also be obtained dynamically, through explosive detonation, the impact of a projectile on a material (using one- and two-stage gas guns and powder guns), the collapse of a hollow cylinder (in the 'Z pinch' configuration), and the pulsed deposition of energy in the form of lasers or X-rays. Explosive detonation

has the downside of offering limited control of experimental conditions. Nevertheless, Paul S. De Carli and John C. Jamieson used this method to synthesize diamonds from graphite[12]. This was later accomplished also by static high pressures. Guns have been the workhorse of high-pressure shock research, enabling the determination of the equations of state of numerous materials and the identification of new structures. A particularly important result was achieved in 1996, when William Nellis and co-workers used a two-stage gas gun to accelerate a projectile to a velocity of 6 km s^{-1} and generate a pressure of 140 GPa, which allowed them to synthesize metallic hydrogen, the holy grail of high-pressure physics[13]. Metallic hydrogen, thought to comprise the interior of Jupiter, was later also formed statically using a diamond-anvil cell. A limitation of dynamic experiments using shock compression is that the resulting sharp front leads to high associated temperatures. However, the sharp temperature rise can be attenuated by creating a ramped, rather than abrupt, pressure rise, using conditions commonly known as quasi-isentropic. Using this stratagem, one can reach pressures characteristic of the core of the Earth (~350 GPa) at temperatures below the melting point of iron.

Developments in pulsed laser compression and advances in diagnostics are enabling the exploration of material behaviour in the extreme strain-rate regime of 10^6 to 10^9 s^{-1}. These strain rates are nine orders of magnitude higher than the conventional values to which we are accustomed. Associated pressures are in the hundreds of gigapascals, and even terapascals, much higher than the stresses that materials can sustain. In these experiments, powerful laser beams are applied to specimens with dimensions in the millimetre range. This can be done either by directly applying lasers and using face plates to create a more uniform pulse or by using an intermediate hohlraum capsule, a cavity in radiative equilibrium, into which the lasers are directed to generate powerful X-rays.

In metals, three carriers of plastic (permanent) deformation are operative: dislocations, twins and phase transformations. In the extreme regime of high stresses and strain rates, a fourth mechanism gains importance: amorphization. The structural changes in the materials are mainly recorded through two classes of diagnostics: VISAR (velocity interferometry system for any reflector), which tracks the shock and particle velocities, and X-rays (either monochromatic or white radiation), which measure the changes in lattice parameter and distortions, or monitor the changes in preset fluctuations. These measurements are then compared with predictions: hydrocode or finite-difference methods, which provide macroscopic values of pressure, temperature and equation-of-state parameters, and nanoscale simulations, mostly based on molecular dynamics. Potentials for metals, alloys, intermetallics and ceramics are under constant development and are effectively used to predict deformation mechanisms. On a more fundamental level, the empirical potentials are replaced by calculations based on density functional theory, which are more precise but more computationally intensive.

In conclusion, novel shock and isentropic pulse launching technologies, combined with newly developed diagnostic tools, are driving the exploration of materials response in a heretofore prohibited regime. We are gradually approaching the theoretical limit for the strain rate and discovering new deformation mechanisms.

Materials for extreme radiation environments

Assel Aitkaliyeva. In most industries, materials must satisfy standard design criteria based on tensile properties, thermal creep, cyclic fatigue and creep fatigue. In the nuclear industry, structural materials must meet two additional criteria: resistance to radiation damage, and chemical compatibility (resistance against corrosion, stress corrosion cracking and so on). These additional requirements stem from the fact that materials used in nuclear reactors need to withstand intense radiation fluxes, high temperatures, pressure, corrosive conditions, stress and strain for as long as 80 years[14]. These extreme conditions can lead to dynamic and highly synergistic processes that result in premature material failure. Take void swelling, for example, which is an issue for stainless steel components in nuclear reactors operating at temperatures higher than 400 °C. Swelling is the volume expansion associated with the formation of voids; it tends to be an order of magnitude smaller in ferritic steels (such as HT-9) than in austenitic steels (such as 316SS). As a result of the delicate balance between net defect fluxes and their interaction with various microstructural features, swelling and irradiation creep tend to go hand in hand.

The complex relationships between individual phenomena pose a challenge for identifying the mechanisms underlying materials degradation in extreme radiation environments. Understanding and mitigating these mechanisms requires unravelling the origins and evolution of damages over a broad range of spatial and temporal length scales. One must start with the formation of individual defects, which typically occur in femtoseconds, and evaluate material performance on the macroscale over a period of years. As a result of this wide range of length scales and timescales, many fundamental questions on the mechanisms of defect production and damage evolution remain unanswered.

Fortunately, continuous advances in experimental and computational methods are bringing us closer to overcoming this limitation. Advances in in situ characterization methodologies now allow capturing the production and migration of defects as they are created and observing the microstructural evolution during loading. With progress in machine learning, we can develop empirical interatomic potentials to improve the accuracy of atomistic simulations and the size of systems that can be simulated, establish correlations between individual phenomena (such as swelling) and processing conditions (such as the material composition and the irradiation parameters), and interpolate between data points to values that have not been measured to understand the contribution of different microstructural features or properties. Machine learning can also be integrated with automated experiments to achieve high-throughput testing and characterization in extreme environments; for example, systems that autonomously quantify defects as they form in situ during irradiation with high-resolution microscopy or conduct nanoindentation studies of irradiated materials may soon become mainstream. This combined use of experiments, machine learning, and modelling and simulations will help to capture multiscale damage evolution processes.

Another advantage of the combined experiments/modelling/data analytics approach is that it can help with an integral part of materials development: qualification. For some industries, the timescale for new materials design is now as short as 3 years, but this is not the case for materials used in extreme radiation environments. The combination of physics-based multiscale modelling and simulations, experimental testing and characterization, and machine learning methods can allow rapid assessment of new materials proposed for use in reactor

environments. For example, SiC–SiC composites, nanostructured nickel-based superalloys, high-entropy alloys and additively manufactured materials could come to the market first, once their radiation performance has been evaluated. Finally, understanding material behaviours under irradiation can help design improved materials systems for use in other industries, as irradiation can be used as a tool or a design parameter that can be used to tailor material properties and potentially improve materials performance.

Materials for extreme energetic and reactive environments

Kerri-Lee Chintersingh. Energetic and reactive materials generate extreme environments (temperatures above 2,000 K, high pressures in the range of 10 to 100 atmospheres, turbulent flows and shock waves) by rapidly releasing energy as they burn. In energetic materials, the oxidizer and fuel are usually combined into molecules, which decompose readily. The decomposition can occur on a submicrosecond timescale and yields predominantly gas-phase products, such as CO, CO_2 and NO_x. These materials are commonly metastable crystals based on carbon, hydrogen, oxygen and nitrogen (such as trinitrotoluene, TNT). Reactive materials, on the other hand, combine distinct reactants, like thermites, Al/Fe_2O_3. Their exothermic reaction is rate-limited by the transport of components towards each other and typically occurs on the millisecond timescale. The products can include both gas and condensed phases. Both energetic and reactive materials are used in pyrotechnics (fireworks, flares), propellants (air-breathing ramjets, space rocket boosters) and explosives (used in construction and mining, emergency escape devices and automobile airbags). Reactive materials are also used in cutting and welding (railroads, electronics) and in-situ heat sources (ready-to-eat meals).

Traditionally, material design relied on combinations of chemical and structural characteristics leading to the fast release of large amounts of energy. Thermodynamic equilibrium calculations and phase diagrams served as reliable tools for material design. Recent advances in diagnostic capabilities (such as high-throughput experiments like laser-driven flyer plate or high-velocity microprojectile impact testing; nano- or femtosecond pulsed lasers; quantum cascade lasers; piston-free shock tubes; temperature-jump/time of flight mass spectrometry) led to a much broader range of characteristics that can be quantified at faster timescales and finer spatial resolution. For example, the rates of thermally and shock-initiated ignition can be separated and reactions occurring across multiple timescales can now be identified using state-of-the-art optical tools. Progress in material synthesis has enabled combinations of multiple species into one structure with complex phases and widely tunable structures with different crystal orientations, sizes and shapes, all affecting their performance[15]. Studies have demonstrated that combining common fuels such as aluminium with nitrides/nitrates, oxides or multiple transition metals (such as Zr, Ti, Hf) by ball-milling or magnetron sputtering results in a nanosized scale of mixing as bilayers or inclusions, leading to reactive materials with lower ignition thresholds and higher combustion efficiencies. Advances in nanomaterials produced materials with distinct and unusual morphologies, including nanopowders, flakes and spherical powders with tunable porosity. Furthermore, when designing new materials, it is important to combine attractive energetic characteristics with other properties, such as structural strength, hardness, density, the safety of handling and storage, or the capability of generating specific products. For example, generating halogenated products in explosive blasts is desired to destroy harmful biological agents like anthrax.

The broadened ranges of material compositions and structures, and the data describing their properties and performance, make it difficult to rely on conventional data analysis tools to design, optimize and modify new reactive and energetic materials. The composition–structure–property–performance correlations have become increasingly multidimensional, and more data are available from a wide range of sources. This makes it critical to implement machine-learning tools to accelerate data analysis and processing, identify and predict relationships from simplified complicated functional dependencies, and bridge gaps in our understanding of physical and chemical phenomena across multiple timescales and length scales. The task is challenging because diverse datasets, including high-speed optical and X-ray phase-contrast imaging, X-ray diffraction patterns, scanning electron microscopy images, thermogravimetric analysis, ignition delays, burn times, reaction propagation rates and detonation velocities, need to be combined into meaningful models. The models are important to theoretically describe behaviours and phenomena on practical scales, which may be difficult to probe experimentally. Work on such models has begun, and more are expected soon. Recent work showed that machine learning helps to bridge the gap between the phenomena occurring on the molecular scale in explosives, described by molecular dynamics models, with meso- and macroscale phenomena described by hydrodynamic codes. It has also been used to simulate the role of void shape and size on the initiation mechanism of energetic crystals, to derive kinetic parameters for reactions leading to ignition and combustion, and to quantify uncertainties in experiments and models to guide material design in extreme environments. Separately, computer vision enables a new level of understanding of rapid reactions occurring in metal-based reactive materials.

Materials for extreme aerospace and space environments

Zachary Cordero. From micrometeoroid impacts on the James Webb and other telescopes to harsh radiation conditions in space, extreme aerothermal heating during flight/re-entry of hypersonic vehicles to strongly oxidizing conditions in propulsion devices, materials in aerospace and space applications often face complex extreme environments, where many stimuli such as temperature, strain rate, shock and oxidation act in concert to push materials to their physical limits. Such multidisciplinary challenges are exemplified by the high-performance reusable rocket engines recently developed by SpaceX and Blue Origin, and newer ones in development for low-cost heavy-lift launch vehicles that will enable next-generation space economics. Unlike expendable rocket engines, which are optimized for reliability, weight and fuel efficiency, reusable rocket engines must also consider the competing criteria of re-entry and launch cycle life (reusability). Challenges include temperature swings from cryogenic temperatures to over 2,000 °C, high pressures and heat fluxes, and ultra-high-pressure oxygen environments. These give rise to potentially catastrophic failure modes, from metal fires and oxidation-assisted fatigue to strain-ratcheting-driven rupture. Legacy materials were used to design and fabricate current reusable rocket engines. Companies are now racing to update technology and develop new platforms, but the challenges are formidable and require collaborative teams. There are exciting

opportunities to apply modern design and development tools and to exploit huge advances in materials over the past 20 years to specifically tailor materials to meet the extreme environments of reusable propulsion systems.

The three components that dictate the life of a reusable boost-stage staged-combustion rocket engine are the thrust chamber, turbopump and nozzle. Each operates in disparate conditions that drive distinct failure modes, motivate different material choices and present unique research opportunities. Regeneratively cooled thrust chambers, for example, are essentially high-pressure, complex heat exchangers with thin cooling channels running along their length. Fuel or oxidizer cools the walls to maintain structural integrity under very high heat flux (5 to 50 MW m^{-2}) from the combustion products, which have gas temperatures in the range of 1,000 to 2,500 K at pressures over 300 bar. Limiting the peak temperature and thermal stresses in the hot wall motivates the use of copper-based alloys with high thermal conductivity and thin-walled cooling channels. Failures typically initiate in the hot wall and arise from a combination of high-temperature creep, plastic yielding from transient thermoelastic stresses during engine startup and shutdown, and erosion due to rapid cycling between oxidizing and reducing conditions. Current thrust chambers begin to crack after tens of firing cycles, a major challenge for reusable boost-stage engines that must restart multiple times during a single flight cycle and that should fly tens of flights before an overhaul. Substantial improvements to thrust chamber lifetimes require a greater understanding of how the composition and microstructure of a material can be tailored with cooling channel geometry to mitigate cyclic plasticity and creep at high temperatures. Low-cost high-throughput maintenance procedures to periodically rejuvenate the structural integrity of the hot wall are also needed to extend its lifetime.

A second life-limiting component is the turbopump that pressurizes the propellants. In oxidizer-rich turbopumps, the turbine entry temperature and O_2 partial pressure are typically 350 to 750 K and 300 to 600 bar, respectively; these O_2 partial pressures are so high that they can cause conventional engineering alloys to ignite and burn uncontrollably. There are two main ignition mechanisms in the oxygen-rich turbine: frictional ignition due to rubbing of rotating components, and particle impact ignition when small foreign objects entrained in the flow strike a solid surface. Both mechanisms have caused launch failures in expendable engines and delayed the development of next-generation reusable rocket engines. Currently, high-strength superalloys are used to withstand high centrifugal stresses and temperatures, despite being highly flammable. The physics underlying ignition phenomena are poorly understood, in part because of the experimental challenges with reproducing these processes in the laboratory. However, this understanding is critical for developing new ignition-resistant ox-compatible materials and coatings, which will in turn unlock new approaches for extending the life of the turbine.

The third life-limiting component in next-generation reusable rocket engines is the rocket nozzle. When a booster is returning to the landing site, it re-enters the atmosphere travelling engine-first at hypersonic velocities, subjecting the nozzle to brief but extreme aerothermal heating. This heating is especially problematic because the engines are not running, meaning there is no regenerative cooling. Although it is possible to limit the extent of heating by using fuel to slow down during re-entry, this approach sacrifices payload to orbit and therefore launch economics. Outstanding questions related to the design and lifing of reusable nozzles include uncertainties in the aerothermal loads during re-entry. Optimal combinations of thermal protection materials, nozzle design and trajectories are needed to mitigate excessive heating to extend the number of flight cycles before retirement. Given the intrinsically multiphysics nature of this problem, there is a need to couple reduced-order models with multidisciplinary optimization frameworks to substantially improve performance.

These examples highlight instances where a new understanding of materials performance in extreme environments can unlock advances in reusable rocket engine technology. In charting a path forward, it is helpful to consider the history of bespoke materials in aero-engines. The development of modern gas turbine engines benefited greatly from sustained collaborations between subject-matter experts in the industry, who understood the critical technical challenges, and academics, who focused on fundamental science underlying materials development and workforce training. The advance of reusable rocket engines will undoubtedly benefit from similar collaborations on materials performance under extreme operating conditions.

Integrative approach for materials design in complex extreme environments

Lori Graham-Brady. As highlighted in the previous sections, extreme environments present a considerable challenge in materials design, due to the activation of multiple competing and cooperating mechanisms during extreme events. However, the targeted development of new materials for these extremes, through integrated, automated and autonomous materials design, is now within reach. This process not only promises to accelerate materials design and discovery, but it also democratizes science and engineering advances through data access and remote operation capabilities[16]. Advances in robotics, high-throughput testing, data sciences and artificial intelligence (AI) are starting to enable such a materials design process, even for challenging and complex extreme environments.

AI-driven automated frameworks for materials design rely on several elements: the availability of extensive materials data; efficient data- and physics-driven models; effective data-informed decision-making; the ability to act rapidly on decisions; and a well-integrated data system. Each of these elements presents unique challenges when attempting to address materials in extreme environments, given the complexity and the range of material length scales and timescales relevant during extreme events. However, recent advances in all five areas show a promising path forward for the field. High-throughput testing promises to provide statistically significant data, but full-scale high-throughput testing at the application scale is not currently feasible. However, new high-throughput approaches that characterize fundamental mechanisms in extreme events, even if they are not at the full application scale, have started to emerge. These tools promise to provide materials data for extreme environments in unprecedented quantity and quality, through novel high-throughput materials fabrication (such as additive manufacturing and sputter deposition), characterization (such as X-ray diffraction, X-ray fluorescence, electron backscatter diffraction and optical microscopy) and testing (such as nanoindentation and laser shock). Moreover, natural language processing has progressed to the point where it can mine rich materials datasets in the scientific literature. Putting these sources together, a critical mass of materials data is emerging that can support data-driven materials design.

Traditionally, guidance regarding future exploration in the materials design space has relied on ad hoc expert advice, which leads to a slow and potentially biased decision-making process. The advent of machine learning and other efficient data-driven surrogate models for complex materials behaviour enables rapid data-driven and/or physics-based predictions of material performance. Such efficient predictions support AI-driven approaches that make reliable, optimal design decisions based on large quantities of heterogeneous materials data. These decisions inform both human users and robotic controls regarding future actions.

Many handling and testing processes for evaluating material behaviour under extreme conditions rely on intensive human-in-the-loop intervention. Often these processes are rote, time-consuming activities that take researchers' time and energy away from higher-level strategy and design. Robotic automation in materials science has advanced in its ability to remove the human-in-the-loop from rote material manipulations, for example through automated polishing, staging and transfer of specimens. Human–robot collaborations that make use of expert judgement to help guide important elements of the automated process while maintaining the operation of routine automation are the coming wave of innovation in this domain. Finally, it is important to recognize that any autonomous materials design process must be fuelled by properly managed and leveraged data. This requires the development of new ways of conceptualizing and organizing data, which must connect scientific evaluations, automation, AI models and decision processes. There are several groups, such as the Materials Research Data Alliance, working towards open, accessible and interoperable materials practices across the entire community working on accelerated materials discovery.

Clearly, there are numerous obstacles that remain before fully integrative approaches to materials design for extreme environments are available, but many of the necessary ingredients are emerging rapidly. Research advances towards autonomous design provide an exciting opportunity for collaborative research that will transform materials design for extreme environments.

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