Iron and steel warm up

S ANANTHANARAYAN REPORTS ON A STUDY THAT REPRESENTS THE COMING TOGETHER OF QUANTUM MECHANICS, STATISTICAL MECHANICS, THERMODYNAMICS AND THE USE OF SUPERCOMPUTERS THAT ENABLES A DESCRIPTION OF THE 'COMPLEX DYNAMIC PHENOMENA TAKING PLACE INSIDE ONE OF THE MOST USED STRUCTURAL MATERIALS'

Iron, the material we find everywhere — from pots and pans to tools and ships and then to beams and trusses in skyscrapers and bridges — displays peculiar a behaviour when it is heated. Till it reaches the temperature of 912° Celsius, the crystal structure of metallic iron remains the same, *Body Centered Cubic*, but when it crosses that temperature, it changes to *Face Centered Cubic*, which is a closer-packed form that remains so till 1, 394° Celsius, when it changes back to BCC, till it melts at 1,538° Celsius. And there is also a *hexagonal close packed* structure when iron is under very high pressure.

This apart, iron is magnetic. This property — of responding to magnetic fields, or to retain magnetism as a permanent magnet — arises from something known as *spin*, of the particles that make up the iron atom. In the atoms of iron, and other metals that display iron-like *ferromagnetism*, there are odd numbers of electrons and, hence, an *unpaired* electron, the one that results in a net magnetic effect. At lower temperatures, metallic iron forms domains, or regions a few microns across where the magnetic effects of a group of atoms are aligned to act like a small magnet. But with mutual interaction, these domains position themselves so that they cancel each other out and a piece of iron normally shows no magnetism.

But a further peculiarity is that when iron is heated to 770° Celsius it loses its magnetic property. There are reasons to hold that it is the magnetic property that favours the low temperature, loosely packed, BCC structure that iron assumes at lower temperatures. But there is clearly more to be said as iron stays this way till 912° Celsius, even after magnetic behaviour is left behind at 770° Celsius.

"The newly gained insight of how thermodynamic stability is realised in iron will help to make the design of new steels more systematic," says Jörg Neugebauer, Max Planck Institute at Düsseldorf.

Mauger L, Lucas MS, Muñoz JA, Tracy SJ, Kresch M, Xiao Yumin, Chow Paul and Fultz B, of Caltech, Air Force research lab, Ohio, from California and the Carnegie Institute of Washington at Illinois, report in the journal *Physical Review B* that their study of the behaviour of the mechanical vibration and order and disorder in magnetic alignment in metallic iron, as the temperature changes, indicates a correlation between the energy stored in the two reservoirs. The finding has allowed the researchers to conclude, for the first time, that it is this interaction at moderate temperatures that allows the BCC structure of iron to remain even after the alignment of magnetic elements has disappeared.

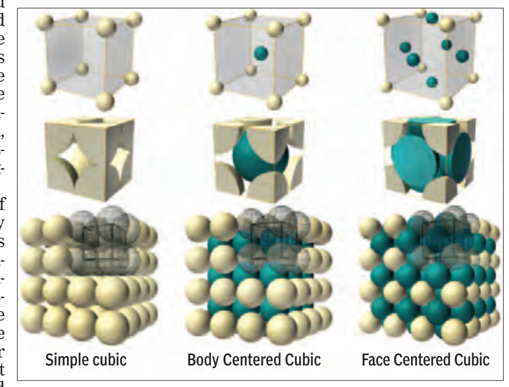
The finding also agrees with the results of a theoretical calculation made by Mauger, Fultz and others, with Jörg Neugebauer at his laboratory in the Max Planck Institute at Düsseldorf, thus validating the computation carried out.

Thermodynamics

The way systems of particles, like solids, liquids or gases, behave depends on the way the total energy of the system is distributed. The simple gas laws, for instance, are explained by statistical models of molecules of gas bouncing off each other and the walls of the container. This is also true of liquids, where molecules, which are the particles, hold on to each other in a lower energy state but are still able to flow and take the shape of a container. And the masses and other properties of the molecules dictate when this stability will break down and change the state into that of a gas. At lower energies still, we have the solid state, where the atoms constituting the material are in fixed positions, held together by electrical forces, and sometimes magnetic forces. The energy of the system shows itself in the motion of the atoms or groups of atoms, generally of vibration, like masses supported by springs that stretch and compress. And different crystal structures, each of which may be the most stable at different levels of energy, may be favoured at different temperatures.

The water molecule, for instance, forms different forms of ice as it warms to the melting point. A feature of the water molecule is that the two hydrogen atoms are not symmetrically placed on either side of the one oxygen atom. This makes the molecule behave like a pair of charges at moderate distances and this results in complicated changes in crystal structure as temperature varies. This feature even causes structure to dominate the liquid state just after melting, with shrinking rather than expansion, as water warms from freezing, at 0° Celsius to four degrees Celsius.

In iron also, on account of ferromagnetism, the energy of an assemblage of atoms has energy of magnetic linkage in addition to the electrical forces that keep the crystal together, along with the mechanical energy of lattice vibrations. It would appear that this is the reason that iron exhibits diversity and anomaly in its disposition as the temperature changes.



The Caltech group assessed the actual nature of vibration energy in iron, as the temperature is raised from to the point where magnetism is lost and then to the point where the crystal structure changes from BCC to FCC. As the particles that are vibrating are individual atoms and the distances are at the scale of the interatomic, the dynamics follow the rules of quantum mechanics. The vibrations move as very high frequency waves within the crystals and the waves have a particle character and manifest as *phonons*, just like light waves move in packets that are known as *photons*. Energy stored in the alignment of magnetic moments also shows itself as waves to appear as particles known as *magnons*, and there is theoretical computation of their behaviour.

The Caltech group assessed the vibration modes present in iron by the scattering of specific X-Ray frequencies by the phonons. The X-Rays were generated in the particle accelerator at Argonne National Laboratory in Argonne, Illinois. This facility works on the principle that accelerated charges emit light of frequency that depends on the acceleration. Thus, by varying the energy of the particles in the accelerator, it is possible to obtain X-Ray emission at frequencies of choice.

When the vibration measurements that were recorded were considered along with the known magnetic behaviour of iron at the different temperatures, it was found that energy stored in vibration was more than expected, with the excess, arising out of frequencies that were not harmonics of characteristic frequencies, corresponding to the levels of energy stored in magnetic effects. This suggests that magnetic effects and lattice vibrations act together at moderate temperatures. At higher temperatures, the force between atoms in the lattice were seen to grow weaker, which allows the BCC structure to continue after magnetic effects are lost due to higher energies. This would also correspond to the loss of tensile strength of iron and steel at higher temperature.

The work represents the coming together of different disciplines, quantum mechanics, statistical mechanics and thermodynamics and the use of supercomputers to enable us "to describe the complex dynamic phenomena taking place inside one of the technologically most used structural materials," says Neugebauer of Düsseldorf . The development of grades of iron and steel, over the centuries, has been largely "trial and error". Said Neugebauer, "The newly gained insight of how thermodynamic stability is realised in iron will help to make thedesign of new steels more systematic."

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World Trade Centre

The collapse of the steel frame of the Twin Towers in New York came as a surprise to many. Why should a fire in the upper floors cause the buildings to collapse? One reason given was that the fire caused the steel frame to melt. But this was discarded as the temperature of burning gasoline is not so high. But then, the steel really did not need to melt to become incapable of supporting the load. The temperature in some of the higher floors rose high enough to reduce the strength of the steel, though well below its melting point, and those floors collapsed. The impact of falling steel and concrete then communicated to the lower floors, which also collapsed.

CELLS AND ORGANELLES

TAPAN KUMAR MAITRA
EXPLAINS A COMPLEX NETWORK

A fundamental distinction in biology is the one between the prokaryotes (eubacteria and archaea) and the eukaryotes (animals, plants, fungi and protists). Equally fundamental is the distinction between the eubacteria and the archaea. In fact, analyses of ribosomal RNA sequences and other molecular data suggest a tripartite view of organisms, with eukaryotes, eubacteria and archaea as the three main groups.

A plasma membrane and ribosomes are the only two structural features common to all three groups. All other organelles are found only in eukaryotic cells, where they play indispensable roles in the compartmentalisation of function. Prokaryotic cells are relatively small and structurally less complex, lacking most of the internal membrane systems and organelles of eukaryotic cells, which have at least four major structural features: a plasma membrane that defines the boundaries of the cell and retains its contents; a nucleus that houses most of the cell's DNA; a variety of organelles; and the cytosol with its cytoskeleton of tubules and filaments. In addition, plant cells almost always have a rigid cell wall and animal cells are usually surrounded by an extracellular matrix of collagen and proteoglycans.

The nucleus is surrounded by a double membrane called a nuclear envelope and the chromosomes within the nucleus contain most of the DNA of the cell, complexed with proteins.

Mitochondria play an important role in the oxidation of food molecules to release energy, which is used to make ATP. Chloroplasts trap solar energy and use it to "fix" carbon from carbon dioxide into organic form and convert it to sugar. Mitochondria and chloroplasts are surrounded by a double membrane and have an extensive system of internal membranes in which most of the components involved in ATP generation are embedded.

The endoplasmic reticulum is an extensive network of membranes that are either rough (studded with ribosomes) or smooth. Rough ER is responsible for the synthesis of secretory and membrane proteins, whereas smooth ER is involved in lipid synthesis and drug detoxification. Proteins synthesised on the rough ER are further processed and packaged in the Golgi complex and are then transported to the surface of file cell by secretory vesicles.

Lysosomes contain hydrolytic enzymes and are involved in cellular digestion. These were the first organelles to be discovered on the basis of their function rather man their morphology. Peroxisomes are often about the same size as lysosomes but function in the generation and degradation of hydrogen peroxide. Animal peroxisomes play an important role in the catabolism of long-chain fatty acids. In plants, specialised peroxisomes are involved in the conversion of stored fat into carbohydrate during seed germination and in the process of photorespiration.

Ribosomes serve as sites of protein synthesis in both prokaryotic and eukaryotic cells and also in mitochondria and chloroplasts. The striking similarities between mitochondrial and chloroplast ribosomes and those of bacteria and cyanobacteria, respectively, lend strong support to the endosymbiont theory that these organelles are of prokaryotic origin.

The cytoskeleton is an extensive network of microtubules, microfilaments and intermediate filaments that gives eukaryotic cells their distinctive shapes. The cytoskeleton is also important in cellular motility and contractility.

Viruses satisfy some, though not all, of the basic criteria of living things. They are important both as infectious agents that cause diseases in humans, animals and plants and as laboratory tools, particularly for geneticists. Viroids and prions are infectious agents that are even smaller (and less well understood) than viruses. Viroids are small RNA molecules, whereas prions are thought to be abnormal products of normal cellular genes.

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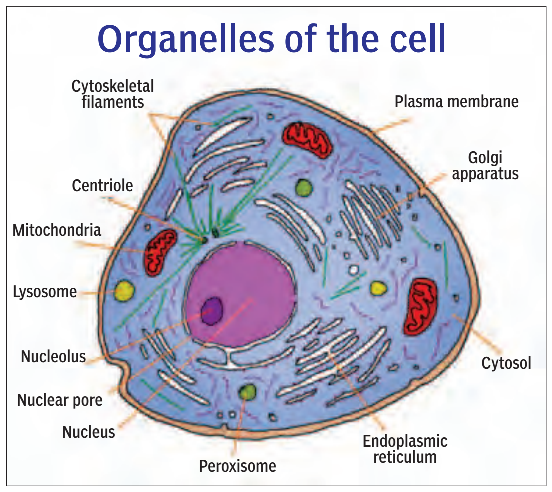
Organelles of the cell



Wind-up to end of days

RESEARCHERS HAVE LISTED TERRIFYING WAYS IN WHICH THEY BELIEVE HUMAN CIVILISATION IS MOST LIKELY TO END, WRITES **JON STONE**

Scientists from the Global Challenges Foundation and the Future of Humanity Institute, Oxford University, have compiled a "scientific assessment about the possibility of oblivion" that involves 12 most likely ways human civilisation could end on planet earth. "(This research) is about how a better understanding of the magnitude of the challenges can help the world to address the risks it faces, and can help to create a path towards more sustainable development," the study's authors said.

The likelihood of global coordination to stop climate change is seen by them as the biggest controllable factor in whether the environmental catastrophe can be prevented. They also warn that the impact of climate change could be strongest in the poorest countries and that mass deaths from famines and huge migration trends could cause major global instability.

A mushroom cloud rises from the waters of Bikini Lagoon during the USA's first series of underwater atomic tests on 7 August 1946. Ships of a "Guinea Pig" fleet can be seen against the huge bank of water at the base of the explosion. While the researchers concede that a nuclear war is less likely than in the previous century, they say evidence suggests "the potential for deliberate or accidental nuclear conflict has not been removed".

The biggest fact that they say would influence whether one happens would be how relations between future and current nuclear powers develop.The again, "there are grounds for suspecting that such a high impact epidemic is more probable than usually assumed," the researchers believe.

The ability of the world's medical systems to respond to a pandemic was important in preventing a catastrophe, they said, but the biggest threat was simply whether there was an uncontrollable infectious disease out there or not.

They warned that an asteroid impact larger than five kilometres in size would destroy an area the size of the Netherlands. These events happened every 20 million years. "Should an impact occur, the main destruction will not be from the initial impact but from the clouds of dust projected into the upper atmosphere… The damage from such an 'impact winter' could affect the climate, damage the biosphere, affect food supplies and create political instability."

Like an asteroid impact, the greatest threat from a super-volcano was a global dust-cloud that would block the sun's rays and cause a global winter. "The effect of (historic eruptions) could be best compared with that of a nuclear war," they said.

Humanity either had to conserve the ecosystem or hope that civilisation was not dependent on it. "Species extinction is now far faster than the historic rate," the study warned. Humanity had to develop sustainable economies in order to survive this one. "The world economic and political system is made up of many actors with many objectives and many links between them," the study warned. "Such intricate, interconnected systems are subject to unexpected system-wide failures caused by the structure of the network." Economic collapse could lead to social chaos, civil unrest and a breakdown in law and order.

With plans on to artificially replicate the polio virus, the scientists were worried that someone would intentionally build an "engineered pathogen" to wipe out the human race. "Attempts at regulation or self-regulation are currently in their infancy, and may not develop as fast as research does," they warned.

Nanotechnology's proponents may tout it as a way to solve problems, but the researchers believe it could present serious problems. "(Nanotechnology) could lead to the easy construction of large arsenals of conventional or more novel weapons made possible by atomically precise manufacturing," they warned. "Of particular relevance is whether nanotechnology allows the construction of nuclear bombs."

They also believe that "extreme" artificial intelligence "could not be easily controlled" and would "probably act to boost their own intelligence and acquire maximal resources". Rather spookily, they said that one of the key factors in our survival was whether "there will be a single dominant AI or a plethora of entities".

Finally, the researchers warned of "unknown unknowns" and called for "extensive research" into "unknown risks and their probabilities".

THE INDEPENDENT

PLUS POINTS

Attendees examine bacterial samples at the "Art and Science of Bacteria" workshop at MIT.

Beauty of bacteria

On a cold January afternoon, a group of science students and artists pored over Petri dishes in the Massachusetts Institute of Technology Museum Studio examining the bacteria growing within them. These were not just any bacteria but components of the participants' own microbiomes that had formed visible colonies in an incubator overnight, thanks to systems biology postdoc Tal Danino.

He and artist-in-residence Anicka Yi led a two-day workshop on "The Art and Science of Bacteria" as part of their scientific and artistic collaboration set up by Meg Rotzel at MIT's Centre for Art, Science, and Technology. "I wanted to work with bacteria on multiple levels," Yi told the workshop attendees, describing the inspiration for her work with Danino. In addition to the traditional visual view of colourful colonies growing on agar, "there's a smell or scent component to the bacteria", said Yi. "I wanted to work with real live bacteria in the way you all have done in the experiment."

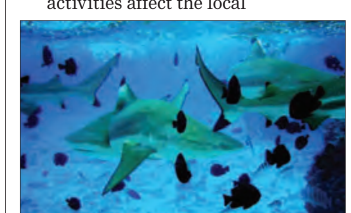
Danino, who has been manipulating microbes since his graduate school days, recalled his early discussions with Yi on personal microbiome and scents. Yi is using these scents in an upcoming gallery show, "You can call me F"," opening at The Kitchen in New York City on 5 March. There, visitors will be immersed in her interpretation of bacterial samples collected from 100 female art professionals acquainted with her. Not only will they see a seven-foot-tall "bacterial billboard", a giant Petri dish displaying the 100 live samples, but they will also smell synthesised perfume designed by Yi based on the scents of the microbes blended with air sampled from traditionally male-dominated spaces.

"We're really developing an entirely new art form that revolves around using biological elements," Danino said. "That's something that I really loved talking about and sharing at the workshop."
"I'm just living in bacteria these days," said Yi with glee.

JENNY ROOD/THE SCIENTIST

Ecosystem

The entire ecosystem of Mo'orea, a volcanic island in French Polynesia, will be captured in a computer model that seeks to understand how climate change and human activities affect the local



environment. Last month, an international group of researchers announced they wanted to feed decades of Mo'orea research from various fields into a computer-based model of the 132-square km island.

The Moorea Island Digital Ecosystem Avatar (MooreaIDEA) will model the island from its peak to the surrounding sea, including fish, corals, plants and its population of around 17,000 people. It is designed to enable researchers and local people to visualise and predict how different factors relating to climate change and human development influence each other and the island.

Mo'orea is already well studied. France has operated a field station there — the Centre for Island Research and Environment Observatory (Criobe) — there since 1971, while the University of California, Berkeley's research station will celebrate its 30th anniversary next month. "We have a lot of data," says Joachim Claudet, one of the ecologists behind the project.

He works at the National Centre for Scientific Research in France. His own project aims to model the complex relationships between human activities, such as fishing and tourism, and natural ecosystems in Mo'orea's coastal areas.

Local decision-makers will be encouraged to use the model to test and visualise different policy scenarios.

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