

對外合作組織與機構 動態報導

2018/3/30

PAINTING A CLEAR PICTURE OF HOW NITROGEN OXIDES ARE FORMED

解開氮氧化物如何形成的細節

By [Jared Sagoff](#) • March 9, 2018



Nitrogen oxides (NO_x) are
some of the most

significant pollutants in our atmosphere — they
contribute to the formation of smog, acid rain

報告摘要 (KEY INFORMATION)

1. 氮氧化物是我們現今大氣中影響最大的污染物之一，導致光煙霧、酸雨，和地表臭氧的產生。研究燃燒的學者與引擎相關公司已經深耕此領域三十餘年，試圖瞭解氮氧化物產生的過程，以便有效減少其產生。
2. 砷化銦鎵奈米線，可廣泛作為光電子學之應用。美國阿岡實驗室的新研究，以 Bragg Ptychography 方法，觀測奈米線的兩種缺陷，並將觀察結果與理論相比較，提出這些奈米線上的缺陷，也會影響使用奈米線結構的器件。
3. 近來國際石油市場受金融市場因子的影響愈來愈大，如股價、匯率、利率等。而液化天然氣市場，因全球市場規模擴大，也面對益加增大的季節性需求波動，尤以中國格外明顯。因此，開發具有彈性與高流動性的液化天然氣市場以吸收這樣的震盪，可謂十分迫切。
4. 今年初日本外務省成立了氣候變遷諮詢小組，由 NGO、研究人員與企業積極參與討論，遞交三點能源建議：佈署可再生能源外交；確定日本能源轉型路徑；主導邁向脫碳社會的過程，創建新的經濟體。同時，國際的動向仍難以預測：在去年 COP23 會議上，白宮國際能源與環境特別助理曾非正式透露有關乾淨煤炭聯盟與高效化石燃料的概念，然而該特別助理於上個月辭職，乾淨煤炭聯盟究竟是否建立仍未可知。
5. 「愈巨大的愈難被摧毀」，這樣的觀念在治療抗藥性細菌感染上可能並不成立。史丹佛研究團隊發現了一個基因的調控紐，可以放大病原菌如大腸桿菌的體積，使其對抗生素療程更加敏感。

and ground-level ozone. Because of this, combustion researchers and engine companies have been working since the 1980s to understand how these gases are produced during combustion so that they can find ways to reduce them.



In a new review paper published in *Progress in Energy and Combustion Science*, researchers from the U.S. Department of Energy's Argonne National Laboratory and the Technical University of Denmark explain how they synthesized more than a decade's worth of combustion studies to create a new overarching model of how nitrogen oxides are produced.

"Our understanding of how these pollutants are produced in different engine environments has deepened dramatically." — Stephen Klippenstein, Argonne chemist

"NO_x production is one of the main concerns for engine companies," said Argonne chemist Stephen Klippenstein, an author of the paper. "Our understanding of how these pollutants are produced in different engine environments has deepened dramatically."

A wide array of different chemical interactions occur within the mixture of fuel and air in an engine, and the new model identifies several different routes to NO_x formation.

In one pathway, called prompt NO (nitrogen monoxide), atmospheric nitrogen combines with carbon to form an intermediary of one carbon and two nitrogen atoms, which eventually combine with oxygen to form nitrogen monoxide. In another pathway, called thermal NO, nitrogen monoxide is produced directly from nitrogen and oxygen. In a third, called fuel NO, a compound of nitrogen, carbon and oxygen forms the intermediary step on the way to nitrogen monoxide.

"Trying to put together these pathways to create a model that accurately reproduces experimental observations has always been a bit of a guessing game," said Argonne chemist Branko Ruscic, another author of the study. "However, because so many scientists from around the world are contributing information about different segments of the larger picture, we're closer than ever before to a model that truly represents reality."

According to Klippenstein, one of the main characteristics of the combustion process — temperature — makes a big difference in the quantity of NO_x produced. "The temperature affects the lifetimes of the molecules in the mix," he said. "Being able to accurately model and predict the behavior of some extremely short-lived molecules is crucially important to determining the pathways of the reaction."

"If you can run your engine at a lower temperature, you can avoid the formation of much of the NO_x," he added.

Another factor in the combustion process that dramatically affects NO_x production involves what researchers call the richness of the fuel mixture — that is, the proportion of fuel to air as combustion takes place in the engine. Engines that run richer will have molecules with more methyl groups, Ruscic said, which tend to promote the formation of NO_x.



“We’re getting to a place where we understand NO_x production pretty well,” said Ruscic. “It’s really a good example of the triumph of community science.”

“It’s like putting together a jigsaw puzzle where some of the pieces might seem to fit but haven’t yet been painted,” said Klippenstein. “It’s our role to figure out how to paint a few more pieces so that our collaborators can put together the picture better.”

The study, “[Modeling nitrogen chemistry in combustion](#),” appeared on February 22 in *Progress in Energy and Combustion Science*.

SCIENTISTS HAVE A NEW WAY TO GAUGE THE GROWTH OF NANOWIRES

量測奈米線增長的新方法

By [Jared Sagoff](#) • March 19, 2018



In a new study, researchers from the U.S. Department of Energy’s (DOE) Argonne and Brookhaven National Laboratories observed the formation of two kinds of defects in individual nanowires, which are smaller in diameter than a human hair.

These nanowires, made of indium gallium arsenide, could be useful for a wide range of applications in a field scientists have termed optoelectronics, which encompasses devices that work by converting light energy into

electrical impulses. Fiber optic relays are a good example.

The effectiveness of these devices, however, can be affected by tiny defects in their components. These defects, which can change both the optical and electronic properties of these materials, interest scientists who seek to tailor them to boost the functionality of future optoelectronics, including materials that will be able to manipulate quantum information.

In the study, the team, which also involved collaborators from Northwestern University and two European universities, observed two kinds

of defects in a single nanowire. The first kind of defect, caused by strain, affects the entire nanowire, preventing it from growing perfectly straight. The second kind of defect, called a stacking fault, occurs close to the atomic level, as individual planes of atoms are laid down to lengthen the nanowire.



“To visualize the difference between stacking faults and strain, you can think of shuffling a deck of cards,” said Argonne materials scientist Stephan Hruszkewycz, a study author. “A stacking fault occurs when a card from the deck is shuffled imperfectly — as if two cards come from the right hand before one can come from the left.”

Strain, Hruszkewycz explained, “looks as if a tower of decks of cards were tilted in a certain direction instead of standing perfectly straight.”

Because stacking faults and strain occur at such different scales, understanding how they interact to change a nanowire’s characteristics requires scientists to use sophisticated imaging technology and complex mathematical algorithms.

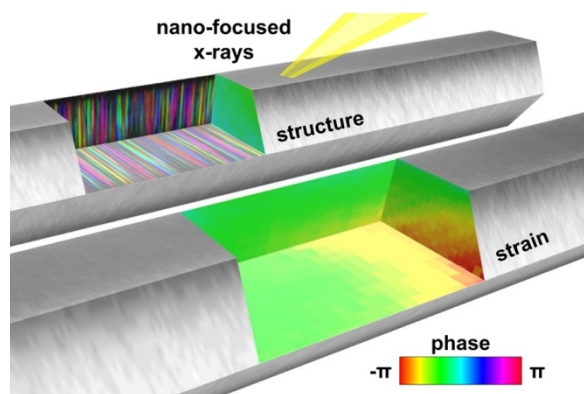
By using a technique called Bragg ptychography to observe the defects, the Argonne researchers created a method they could use to see the nanowire within its operating environment.

“We’ve developed a technique that allows us to investigate the actual local structure in the material,” Hruszkewycz said. “This will allow us to make valuable comparisons to theories that people have come up with that describe how these defects could affect not only the nanowire, but the entire device of which it is a part.”

“The method provides a missing link between nanoscale defect structure and variations in strain on longer length scales that will enable us to better control the optoelectronic properties of nanowires,” said Northwestern University materials science professor Lincoln Lauhon.

In Bragg ptychography, researchers shine an X-ray beam at a series of overlapping spots all over the material, like a stagehand slowly moving a spotlight across a stage. The information produced by the atoms’ scattering of the X-rays gives researchers a three-dimensional view of the material at close to atomic resolution. The researchers used the technique at Brookhaven’s Hard X-ray Nanoprobe at the National Synchrotron Light Source II (NSLS-II), a DOE Office of Science User Facility.

“Beamline 3-ID is capable of producing a coherent nanofocused beam, so it is well suited for reconstructing images through techniques like Bragg ptychography,” said Brookhaven lead beamline scientist Yong Chu, an author of the study. “This collaboration has been extremely valuable for advancing Bragg ptychography capabilities at NSLS-II, as well as our understanding of nanowires.”



Scientists have recently improved the algorithms that generate this picture, an improvement that has dramatically changed the X-ray information collection process. Instead of having to use a spot-by-spot grid-based approach as done in earlier ptychographic studies, Hruszkewycz and his collaborators could move their X-ray beam around more freely, collecting useful information from across their sample. “It’s like instead of doing a very simple and repetitive line dance, all we have to do is make sure that we place our feet on each part of the dance floor at one point or another,” he said.

This flexibility has another advantage: it allows researchers to illuminate smaller features using a smaller spot size — enabled in large part by X-

ray zone plates fabricated by Michael Wojcik, a physicist at Argonne’s Advanced Photon Source. These zone plates are a diffractive optic that consists of several radially symmetric rings, called zones, which alternate between opaque and transparent. They are spaced so that light transmitted by the transparent zones constructively interferes at the desired focus.

“When we’re trying to hit our target, we don’t have to be Robin Hood,” Hruszkewycz said. “We just have to get close enough to hit somewhere on the target; we don’t have to split the proverbial arrow.”

An [article based on the study](#), “Measuring three-dimensional strain and structural defects in a single InGaAs nanowire using coherent X-ray multiangle Bragg projection ptychography,” appeared in the January 18 online edition of *Nano Letters*.

The work was performed in part at Argonne’s [Center for Nanoscale Materials](#), a DOE Office of Science User Facility. The U.S.-based part of the research was funded by the U.S. Department of Energy’s Office of Science and the National Science Foundation.

RECENT DEVELOPMENTS IN THE OIL AND LNG MARKETS

石油與液化天然氣之近期發展

By Yoshikazu Kobayashi



The international oil market is becoming susceptible to financial market factors. After rising to \$70/bbl at the end of January, Brent headed downward, reaching the \$62 range in early February and hovering around \$65 since

mid-February. Behind such fluctuation is the strong impact of instability in international financial markets.

Until last year, international financial markets enjoyed “goldilocks” conditions (the moderate temperature), neither too hot nor too cold and

characterized by a combination of a booming global economy and low inflation and interest rates. Since the beginning of January, the combination of rising stock prices and the depreciating dollar prompted buying in the international oil market in anticipation of a supply crunch, pushing Brent into the \$70 range.

However, the "moderate temperature" condition suddenly reversed in February. Oil prices fell sharply in early February as the rise in US long-term interest rates caused stock prices to plummet, raising concerns for the global economy and inducing a selloff of oil futures. Price fluctuations are now calming down and the oil market is adopting a wait-and-see attitude as of mid-February. However, oil prices could remain susceptible to financial market factors including US interest rate policy under the new FRB Chair Jerome Powell who took office on February 5, the possible end of quantitative easing by the European Central Bank, and resulting exchange rate fluctuations.

Of course, finance is not the only factor causing swings in oil prices. On the supply side, American shale oil production is expected to surge due to the rise in oil prices. In its latest oil market report, the International Energy Agency

predicts that US oil output will grow by more than 1.5 mb/d in 2018. On the other hand, output is plunging in Venezuela where there is a looming debt crisis, due to the impact of US economic sanctions and a cash crunch of the state-run oil company PDVSA. Production has fallen from more than 2 mb/d in July 2017 to 1.6 mb/d in January 2018, with some experts predicting a further drop to as low as 1 mb/d. These supply and risk factors will certainly cause price fluctuations in the international oil market going forward.

In the international LNG market, the spot LNG price of Northeast Asia has dropped to as low as \$8/mmbtu (April delivery). The demand period is ending, and the price is likely to continue to fall. One of the reasons for the jump in spot prices this winter was the increase in seasonal demand volatility as the overall global LNG market expanded. China, where volatility is particularly high, needs to build up storage capacity, although this will take time. In the meantime, the international LNG market will have to live with powerful seasonal volatility, and there is a great need to develop a flexible, high liquidity LNG market that can absorb such volatility.

UPDATE ON POLICIES RELATED TO CLIMATE CHANGE

氣候變遷相關政策近況

By Takahiko Tagami



In his speech on January 14 at the Ministerial Roundtable of

IRENA's 8th Assembly held in Abu Dhabi, Japanese Foreign Minister Taro Kono said that

"Japan significantly lags behind the world in the deployment of renewable energy" and "I am seriously concerned with our current situation." Ahead of this speech, on January 9, the Ministry of Foreign Affairs of Japan established an Advisory Panel to the Foreign Minister on Climate Change, with a view to discussing global trends in renewable energies and climate issues. The Panel is comprised of NGOs, researchers, and enterprises actively engaged in climate actions. The Panel met eight times before submitting "Recommendations on Energy" to Foreign Minister Kono on February 19.

Subtitled "Promote new diplomacy on energy through leading global efforts against climate change," the recommendations propose (1) Deploy renewable energy diplomacy, (2) Define Japan's pathway towards the energy transition, and (3) Take a leading role in realizing decarbonized society and create a new economic system. For Item (2), the recommendations include presenting a roadmap for phasing out coal-fired thermal power in Japan, promptly stopping public assistance for coal-fired thermal power exports, and minimizing dependence on nuclear power.

Some consider that this move is intended to influence the review of the Strategic Energy Plan which is being undertaken by the Ministry of Economy, Trade and Industry. The Advisory Panel is scheduled to meet several times in March and submit comprehensive recommendations around April.

Meanwhile, at COP23 held last November, David Banks, the then White House special assistant for international energy and environment (a National Economic Council member) had informally revealed the idea of a Clean Coal Alliance for promoting clean and highly efficient fossil fuels. This initiative reportedly was formulated by "internationalists" in the State Department and National Economic Council to demonstrate that climate change remains of interest to the US despite its withdrawal from the Paris Agreement. This Alliance is also expected to counterbalance the Powering Past Coal Alliance led by Canada and Britain also announced at COP23.

The countries rumored to be joining the Clean Coal Alliance include Australia, India, African countries, Ukraine, Japan, Indonesia, China, and Poland. There have been media reports that the US is considering establishing Major Economies Ministerial, reminiscent of the Bush Administration's Major Economies Meeting on Energy and Climate Change, and taking leadership again. However, it is not yet clear whether the Clean Coal Alliance will indeed be established, and particularly with the resignation of Mr. Banks on February 13 as White House special assistant, the future has become harder to foresee.

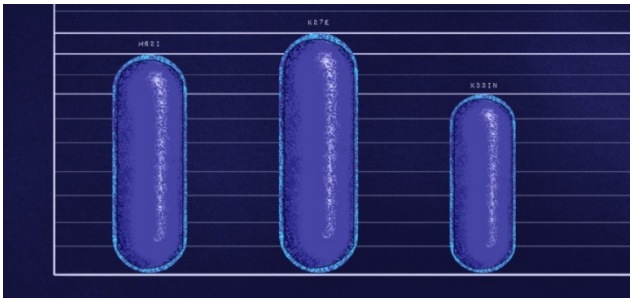
ARE BIGGER BACTERIA EASIER TO KILL?

放大細菌，更易殺菌？

By Tom Abate • March 12, 2018



It's been said that the bigger they come the harder they fall, an adage that turns out to be uncannily accurate when it comes to finding new ways to treat antibiotic-resistant bacterial infections.



Researchers in the lab of [K.C. Huang](#), associate professor of bioengineering, have found that a single mutation to an important protein in *E. coli*—the bacteria you hope never to find in your vegetables—can cause these cells to bloat up by more than 500 percent. If the same were true of humans, a typical 150-pound adult might find that their nearly identical twin—the one with the single mutation that affected the size of every cell in its body—would weigh as much as a grizzly bear.

And the best part, says Huang, is that the bigger bacteria come, the harder they fall. For *E. coli* cells, which look like microscopic hot dogs, as they become longer and plumper they also become more susceptible to certain antibiotics.

“Most strategies to killing bacteria are linear: You find a very specific target and block it with a drug.”

“These findings point in the direction of totally orthogonal therapies, in which you predispose cells to death by tweaking a global property like their size,” Huang said.

Remarkably, researchers in the Huang lab found a genetic “tuning knob” that allowed them to make both subtle and extreme modifications to the shape and size of bacterial mutants. By twisting this dial the team could study how the dimensions of the bacteria impacted their lifestyle. The immediate application was to find that fattening up bacteria prepared for the kill. But as a basic research tool this “dial the size” technique allowed the team to ask questions about the evolution of life.

The power of a protein

The findings in the paper are motivated by questions from the science of cellular biophysics. Much as astrophysics examines the forces that push and pull the stars and planets and galaxies, and thereby give shape to the universe, biophysics explores how forces and physical principles affect the basic building blocks of life, and thereby give shape to cells and organisms.

Inside cells, the fundamental units of life, lies a menagerie of DNA, RNA and proteins that collectively encode the programming instructions necessary for all cellular processes. To many of us, proteins are simply material to be consumed as part of our diet, but proteins are the heroes of all life as we know it. They make up the magnificent machines that perform complex tasks such as making ATP (the fuel that powers cells), dividing cells in two and building the home (the cell itself) in which they live. In fact, the surface of the cell is far more than just a boundary between inside and outside, it defines the geometry in which all proteins organize and the concentrations of all cellular components.

The number of proteins inside a typical cell is in the millions, with many thousands of different varieties. Given this complexity, understanding how cells are constructed would appear to be a daunting task. One of the surprises that emerges from this paper is that a single protein called MreB serves as a master regulator of cell size. MreB acts as a platform that spatially coordinates the machinery that builds the cell wall, which ultimately dictates the size and shape of every cell. Huang's team, led by graduate student Handuo Shi, discovered that changing just one out of the 347 letters in MreB's genetic code was a prescription to bring about dramatic increases in size and,

consequently, antibiotic susceptibility that has the researchers so excited.

Mutation, mutation, mutation

Like all proteins, MreB is a macromolecule: A long chain of smaller molecules, known as amino acids. To make any protein, the cellular machinery reads off its instructions, three letters at a time, from the four letters—A, T, G and C—of the genetic code. This simple set of instructions explains all of life on our planet. Remarkably, the long, gangly chain of amino acids produced by genetic coding somehow folds up into a perfectly shaped protein machine. All of the atoms and molecules in the protein machine engage in minute pushing and pulling that enable this macromolecule to precisely arrange itself and move with a purpose. From a biophysics perspective, life is composed of the interactions of gazillions of protein machines, with all their composite atoms interacting with each other according to mathematical rules that researchers aim to make as predictable as the movements of the stars and planets (perhaps the big breakthrough will require an apple to fall on the head of a modern-day Newton).

Rather than waiting for anything to hit them in the head, the Huang lab wondered just how much a key protein like MreB could tolerate change. You might think that a protein that is absolutely required for survival would be evolutionarily frozen, like the great white sharks prowling the ocean for hundreds

of millions of years. Russell Monds, a former postdoctoral scholar in Huang's lab, identified a strain of *E. coli* that had a mutation in MreB that made cells bigger and also better at dealing with starvation. He then devised an experiment to see what would happen if just one amino acid at a time across all of the 347 amino acids in MreB was subtly changed: Which mutants would survive? To do so, the team manufactured many copies of *E. coli*'s DNA, each one with a change to a randomly selected amino acid in the gene that codes for MreB, using a process called error-prone PCR.

Shi and fellow teammates Alexandre Colavin, Marty Bigos and Carolina Tropini then developed a method that used a cell sorter to pick out individual cells with different sizes, identifying the bigger and smaller needles in the haystack of cells. Armed with this library, they were able to ask fundamental questions about whether and how cells care about their size.

[K.C. Huang](#), associate professor of bioengineering and of microbiology and immunology.

Huang said this was conceived as a basic research study into the ways cell grow and how bacterial populations evolve, but he also highlighted the medicinal benefits.

"We've discovered a single tuning knob that can enlarge or shrink bacteria across a large range," he said. "While we don't yet know how to twist this bacterial size dial in patients, it's good to have such an

exciting new therapeutic approach as antibiotic resistance becomes increasingly prevalent."