Electrostatic shape control of a charged molecular membrane from ribbon to scroll

Scientific Achievement

Through experimental and theoretical studies, molecular reordering driven by variations in electrostatic screening length is shown to induce micrometer scale structural changes in crystalline membranes of charged, chiral molecules.

Significance and Impact

Our study suggests that these structural changes should be general to charged bilayers possessing a spontaneous curvature, and applicable to many applications, including drug delivery and photocatalytic production of hydrogen.

Research Details

- With the addition of NaCl, high aspect ratio $C_{16}K_1$ ribbons formed in zero salt conditions transform to isotropic sheets, prior to rolling up to form cochleates.
- A simplified model demonstrates that the ribbon to sheet transformation is a first-order transition induced by the reduction in the range of electrostatic interactions.
- Theoretical models show that rolling of membranes into cochleates is the combined effect of molecular chirality and tilt.

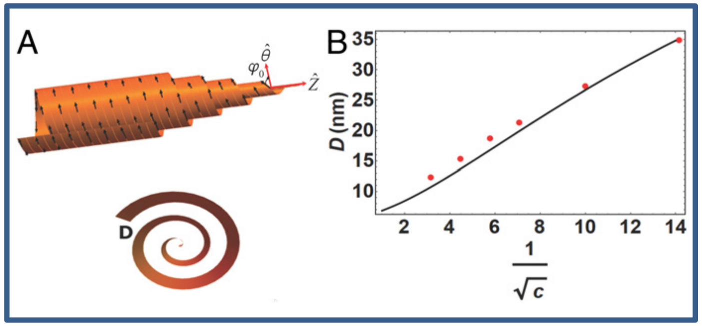


Figure. (A) The geometry of the cochleates. D is the interbilayer separation. Arrows represent the projection of the tilt vector in the local tangent plane. (B) Theoretical prediction showing a roughly linear relationship between interbilayer spacing D and c−1/2, where c is NaCl molar concentration.

Changrui Gao, et al., *PNAS* 116, 22030-22036 (2019); DOI: 10.1073/pnas.1913632116

Work was performed at Northwestern University

How to Build a DOE Office of Science Highlight Slide

Title

Attention grabbing and accessible but not exaggerated

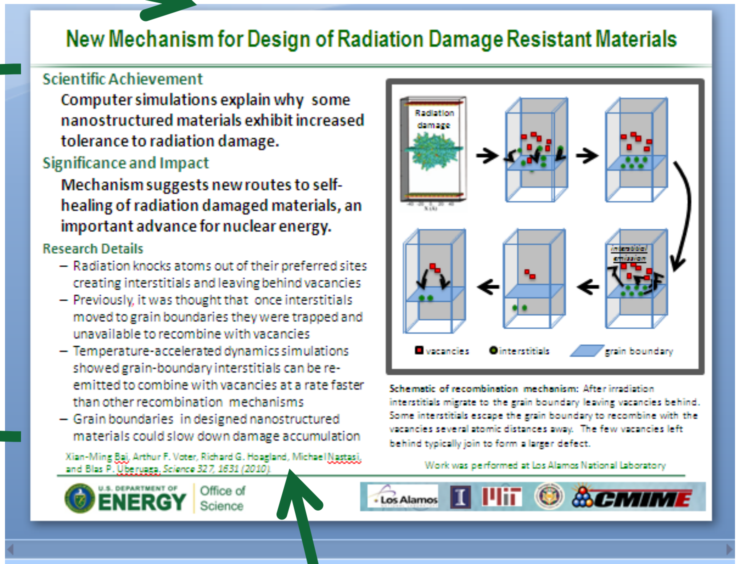
Text

All text should be short and to the point – minimize words and stress significance to society

- **Scientific Achievement** – 50 words or less
- **Significance and Impact** – 50 words or less
  Importance, relevance, or intriguing component of the finding to the field
- **Research Involved** – Address the research approach in 2-4 bullet points
  Give a ~175 word detailed explanation plus additional description of figure if needed in the PowerPoint Notes section

Citation

Full citation with all authors' names is preferable



A new mechanism has been discovered that holds promise for reducing the damage experienced by materials in fission or fusion reactors by enhancing the "healing" of the point defects (interstitials and vacancies) created by the exposure to energetic neutrons in these environments. Using a combination of modeling tools, researchers at the Center for Materials under Irradiation and Mechanical Extremes (an Energy Frontier Research Center at Los Alamos National Laboratory) examined the role of grain boundaries on damage production and defect evolution. Molecular dynamics calculations showed that the boundaries have a complex effect on damage production reducing the number of defects remaining after the cascade and leaving the boundary loaded with interstitials. By evolving the damage structure to longer time scales with temperature-accelerated dynamics calculations, it was found that these interstitials can emit from the boundary and annihilate nearby vacancies. This can take place over many atomic distances and occurs much faster than alternative recombination mechanisms. This result, published in *Science*, may explain the decreased radiation damage resistance found in nanostructured materials, which have a large number of grain boundaries, and could be used to design improved materials for reactor applications

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Figures

Visually compelling figure(s) to explain the research

Include legends and descriptive caption

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Institutional logo(s)

Include affiliations or institutional logos

Indicate institution where research was performed (if possible); EFRC and Hub research should include those logos as well

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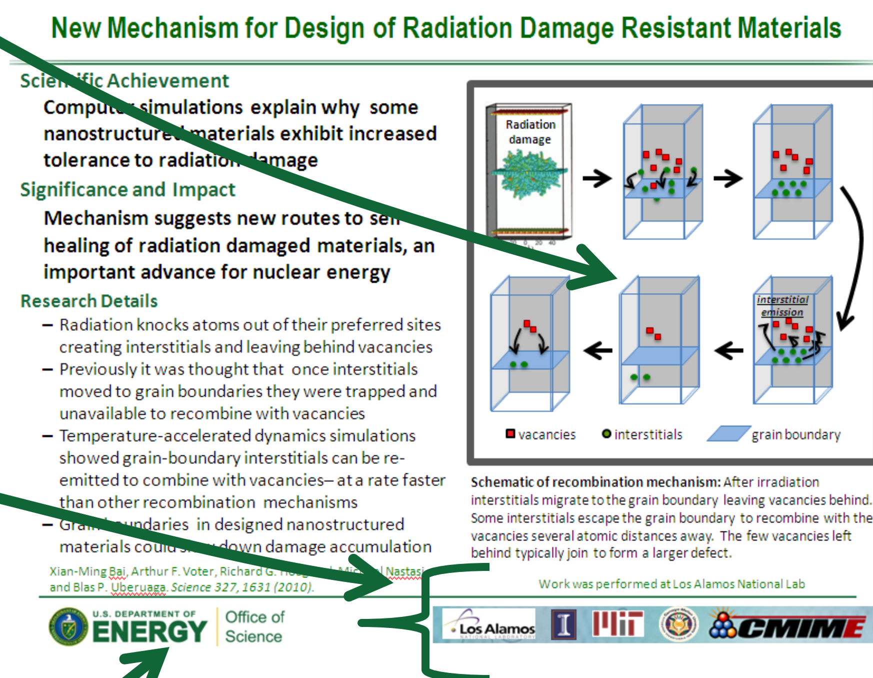


New Mechanism for Design of Radiation Damage Resistant Materials

Scientific Achievement

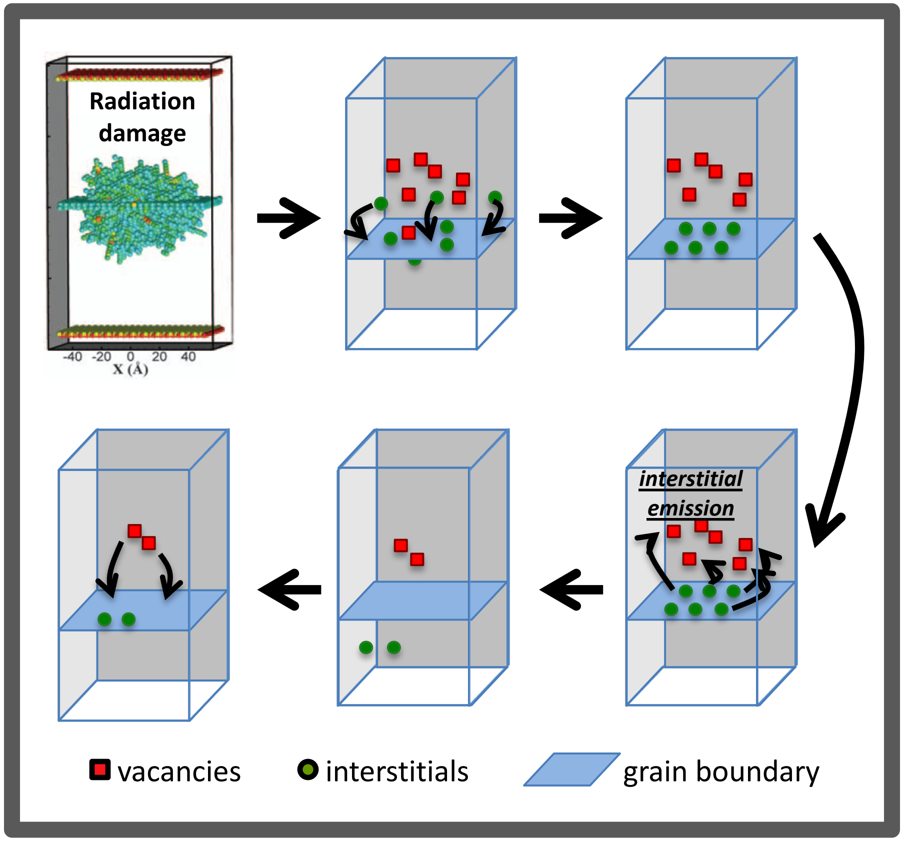
Computer simulations explain why some nanostructured materials exhibit increased tolerance to radiation damage

Significance and Impact

Mechanism suggests new routes to self-healing of radiation damaged materials, an important advance for nuclear energy

Research Details

- Radiation knocks atoms out of their preferred sites creating interstitials and leaving behind vacancies
- Previously, it was thought that once interstitials moved to grain boundaries they were trapped and unavailable to recombine with vacancies
- Temperature-accelerated dynamics simulations showed grain-boundary interstitials can be re-emitted to combine with vacancies at a rate faster than other recombination mechanisms
- Grain boundaries in designed nanostructured materials could slow down damage accumulation

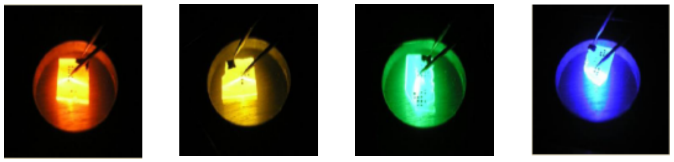


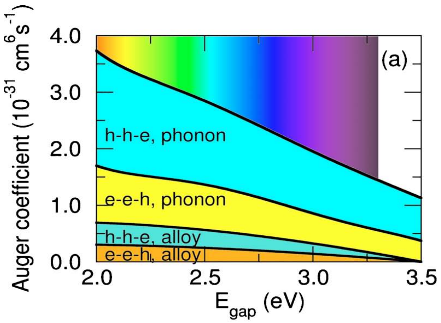
Schematic of recombination mechanism: After irradiation interstitials migrate to the grain boundary leaving vacancies behind. Some interstitials escape the grain boundary to recombine with the vacancies several atomic distances away. The few vacancies left behind typically join to form a larger defect.

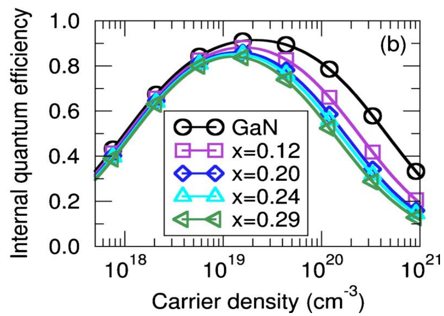
Xian-Ming Bai, et al., *Science* 327, 1631 (2010).

Work was performed at Los Alamos National Laboratory

Understanding Drooping in Light Emitting Diodes (LEDs)







Upper : Images of LEDs.
Middle: Phonon mediated processes substantially affect the Auger coefficient in InGaN.
Lower : Droop in efficiency occurs at high carrier densities in InGaN alloys. Increases in the Indium content (x = fraction of Indium) make the droop worse.

Scientific Achievement

New calculations demonstrate that LED "droop" is dominated by multi-particle interactions. Droop occurs when increasing energy input does not produce proportionally more light.

Significance and Impact

Understanding "droop" may result in cheaper, more efficient LEDs; LEDs are more energy efficient, smaller, and longer-lived than incandescent lamps or fluorescent lighting

Research Details

– Atomistic first-principles calculations indicated that increasing amounts of indium in Indium Gallium Nitride (InGaN) green LEDs caused a decrease in light intensity

– Computational data was confirmed by experimental spectroscopic evidence which showed electron-phonon coupling and alloy scattering (breaking of symmetry due to the insertion of Indium) to be important processes

E. Kioupakis et al., Applied Physics Letters **2011**, *98*,161107

Work was performed at University of California – Santa Barbara

New Catalyst Speeds Conversion of Electricity to Hydrogen Fuel

Scientific Achievement

A newly synthesized nickel complex speeds the production of hydrogen ten times faster than a natural hydrogenase enzyme at room temperature

Significance and Impact

Opens a new research path to develop long-lived catalysts using inexpensive, earth-abundant metals to convert electrical energy to chemical energy

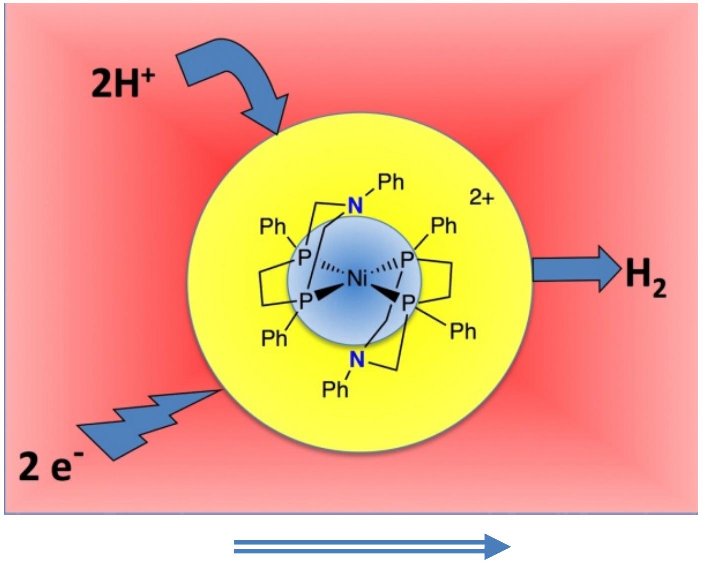
Research Details

– In this process, water molecules are split to produce hydrogen and oxygen. Hydrogen can be used as a fuel

– Using the natural hydrogenase enzyme as a model, a synthetic catalyst using nickel was developed. The metal atom gets its reactive properties from the groups of atoms containing phosphorous and nitrogen that surround it.

– By splitting water, hydrogen gas is formed by combining the H^+ on the nitrogen with the H^- on the nickel center

– Adding an acid or water increased the rate of hydrogen produced from the newly-designed synthetic catalyst

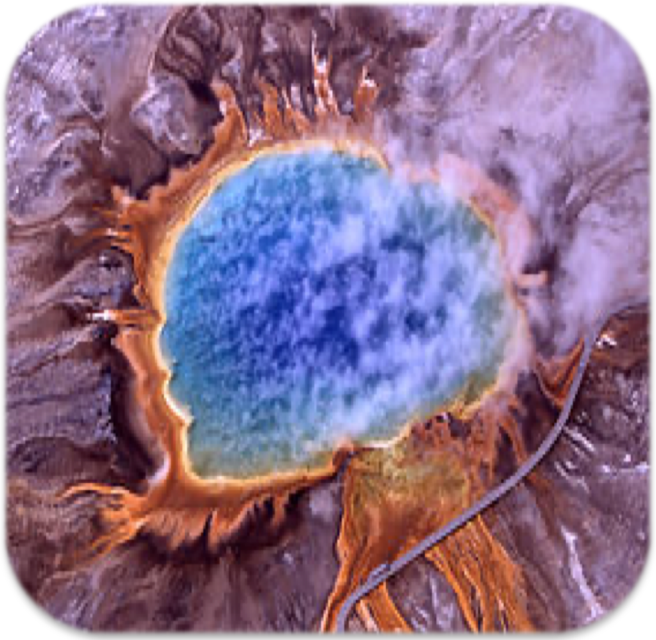


$2 e^- + 2 H^+ \rightarrow H_2$

Schematic showing catalyst operation

ML Helm, MP Stewart, RM Bullock, MR DuBois, DL DuBois Science 12 August 2011: 863

Purple Bacteria Develops Its Own Form of "Sunscreen"



The orange ring surrounding Grand Prismatic Spring, Yellowstone National Park, is due to carotenoid molecules, produced by huge mats of algae and bacteria (Photo from http://en.wikipedia.org/wiki/Carotenoid)

E D. M. Niedzwiedzhi et al. Photosynthesis Research **2011**, 107, 177-186

Work was performed at Washington University in St. Louis

Scientific Achievement

Determined that specific pigments in the light harvesting complex found in photosynthetic bacteria act primarily to protect the cell from damage by excess sunlight

Significance and Impact

Provides insights on how to minimize deleterious effects from over exposure to sunlight in the design of man-made systems to gather and use the sun's energy

Research Details

- In photosynthetic organisms, supplementary pigments called carotenoids capture wavelengths of light that the major pigments can not efficiently harvest
- However, steady-state absorption and fluorescence spectra showed that carotenoids in the photosynthetic bacterium *Thermochomatium tepidum* play a negligible role in energy capture and transfer
- Instead, the composition and structure of the carotenoids have been optimized to protect the light harvesting complex from sun damage