Diamond Semiconductor: “deep elastic strain engineering”

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Department of Materials Science and Engineering

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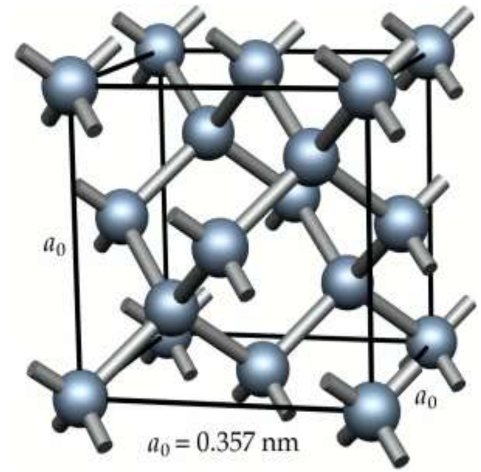
2021

Diamond as the hardest (tooling) material

Covalent bond, sp^3 hybridization



Drilling

（武汉）段隆臣教授团队和李大佛教授团队参加了部分钻探方案设计和钻探模拟试验等工作，为"嫦娥"配上金刚钻，采用表钻镶合、多点采样的方式，设计了钻具钻取和机械臂表取两种"挖土"模式，超硬材料助力圆中国梦！

Cutting

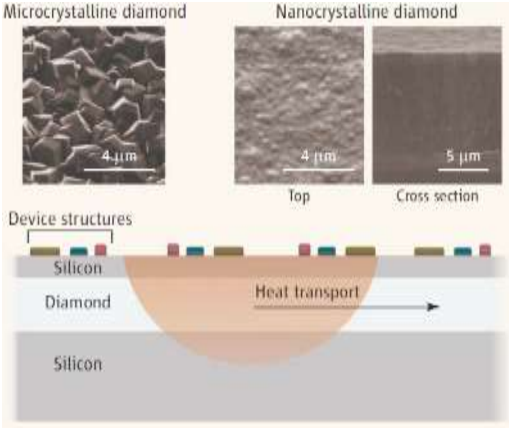
Grinding/polishing

"harder than (natural) diamond…" --- YSU, JLU…

Also, “Mount Everest” of Electronic/Photonic Materials…

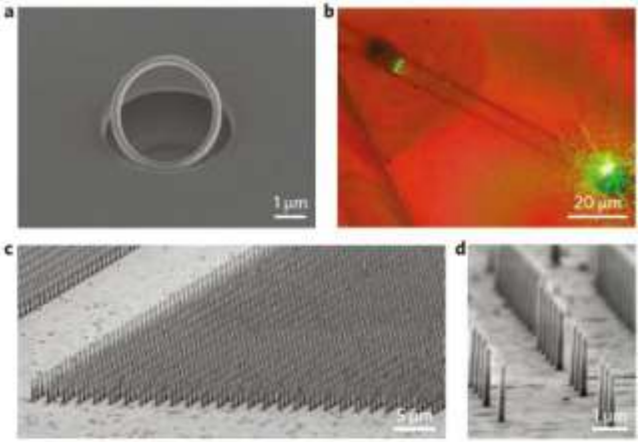
Ultrawide bandgap semiconductor with high thermal conductivity, dielectric breakdown strength, carrier mobility… (& NV center)

Si-diamond-Si integrated circuit



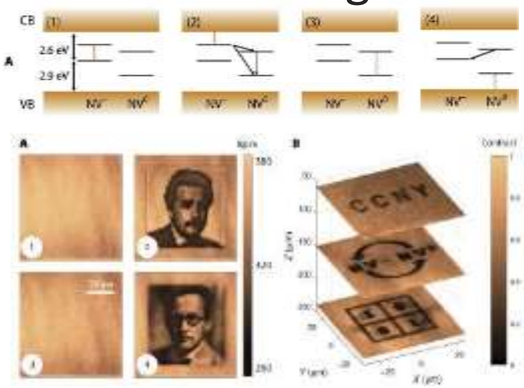
Science **319**, 1491 (2008)

Diamond photonic structures



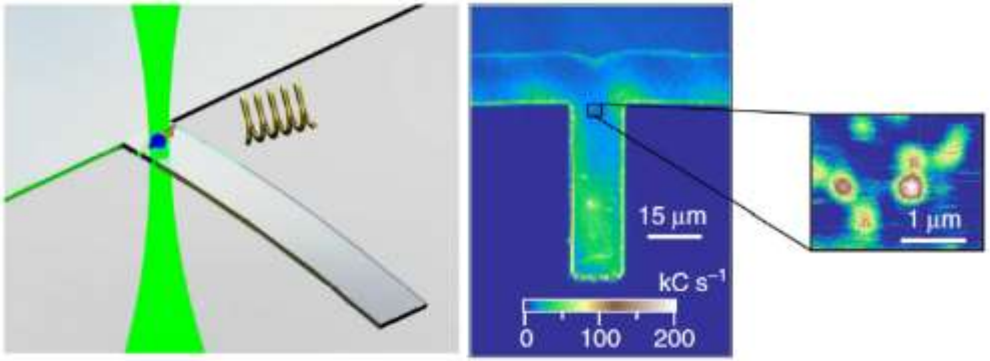
Nat. Photonics. **5**, *397–405 (2011)*

Data storage



Sci. Adv. 2016, 2, e1600911

MEMS; Quantum Nanomechanical Resonator

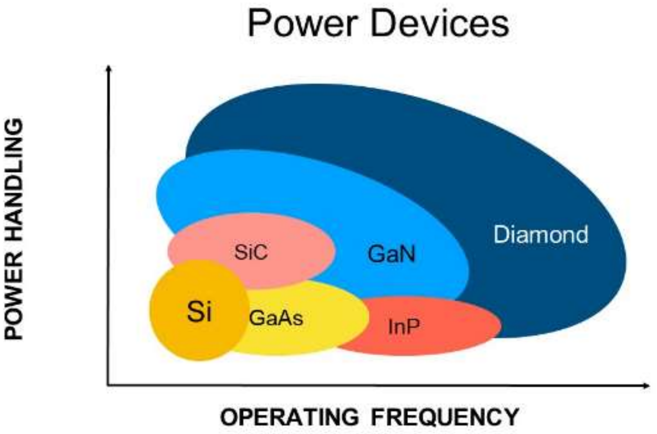


Nat. Commun. 2014, 5, 4429

Ultimate Semiconductor for High Power/Frequency Applications

The properties that make diamond shine..

Parameters	Si	SiC	GaN	Diamond
Bandgap E_g (eV)	1.11	3.26	3.39	**5.47**
Breakdown field E_c (MV/cm)	0.3	3.5	3.4	**10.0**
Electron mobility μ_e (cm^2/Vs)	1,500	800	900	**2,200**
Thermal conductivity (W/cmK)	1.5	4.9	2.2	**21.3**



https://www.wired.com/insights/2015/01/the-rise-of-diamond-technology/

WIRED

Moore's Law and Moving Beyond Silicon: The Rise of Diamond Technology

PARTNER CONTENT ADAM KHAN, AKHAN SEMICONDUCTOR

MOORE'S LAW AND MOVING BEYOND SILICON: THE RISE OF DIAMOND TECHNOLOGY

John Bardeen, William Shockley and Walter Brattain, the inventors of the transistor, 1948 -- the birth of Silicon Valley.

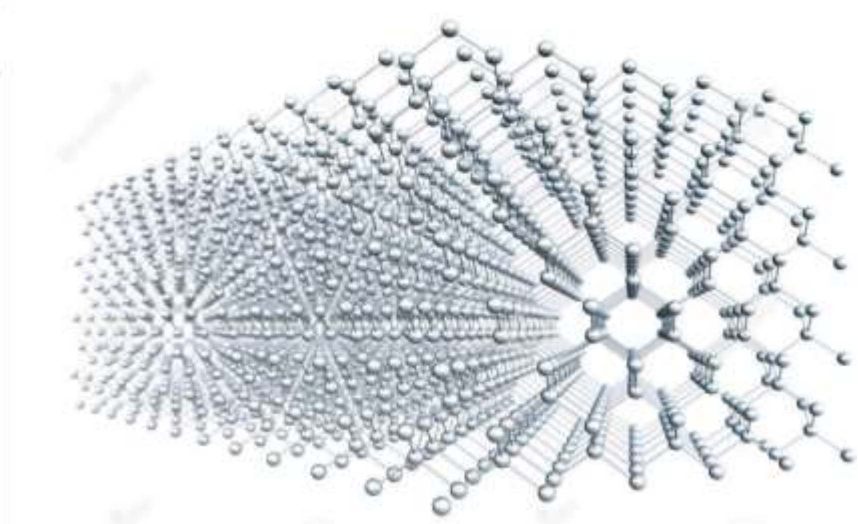
Obstacle in realization diamond electronics

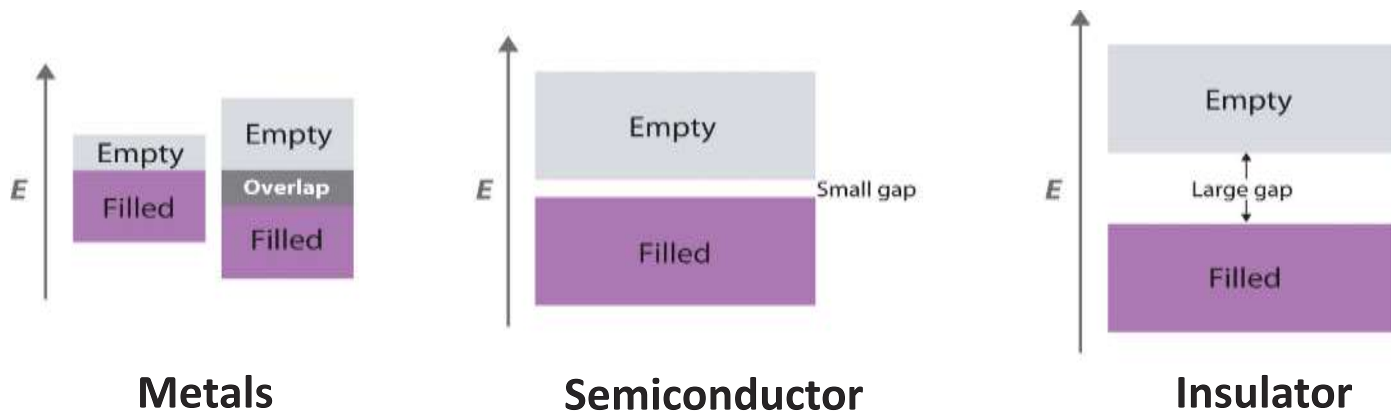
Doping for diamond is difficult, especially N type

Tight crystal lattice;

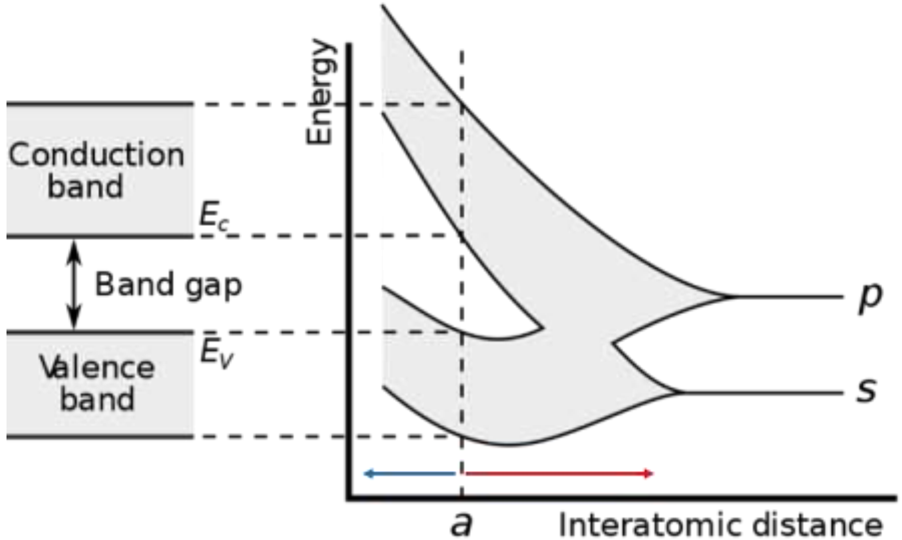
Small atomic number (limited doper);

Large bandgap energy…



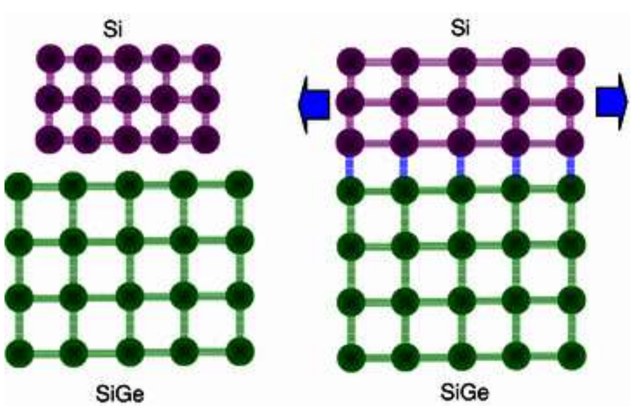


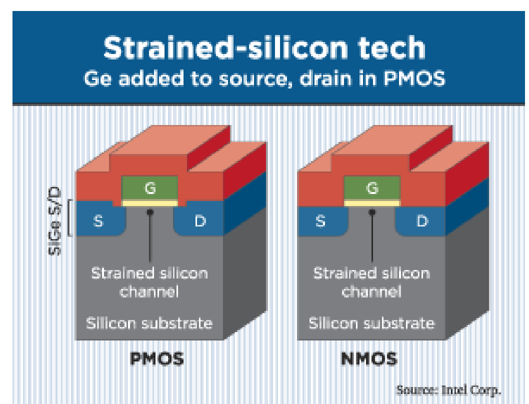
An alternative strategy --- elastic strain engineering



Wikipedia

Applying lattice/elastic strain can considerably change the materials' properties!





http://www.eetimes.com/document.asp?doc_id=1217259

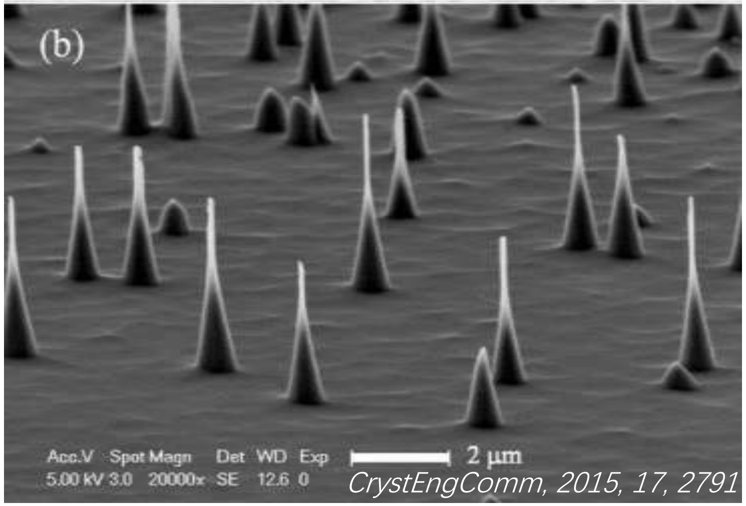
Deform diamond elastically?

If you manage to deform a bulk diamond, it usually means you have broken it

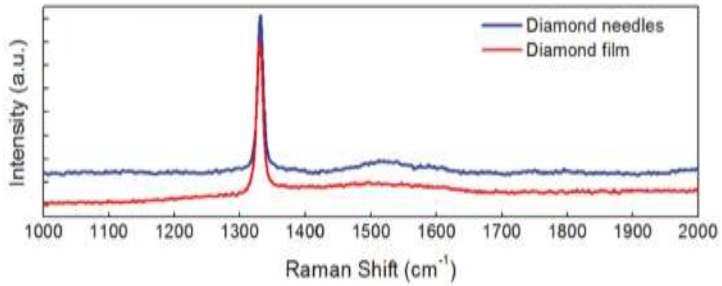
Crazy Hidraulic Press https://youtu.be/YHU0aM9rCFA

What about nanoscale?

Firstly, diamond nanoneedles --- from COSDAF Prof. WJ Zhang

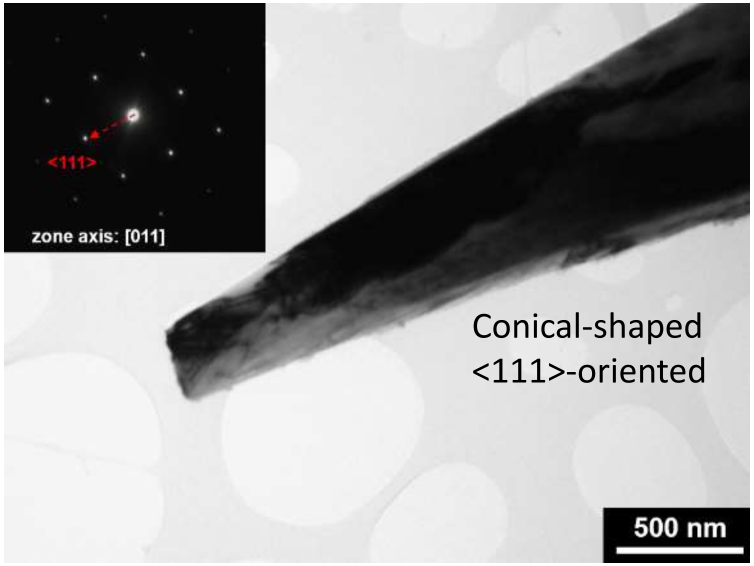


Micro-Raman

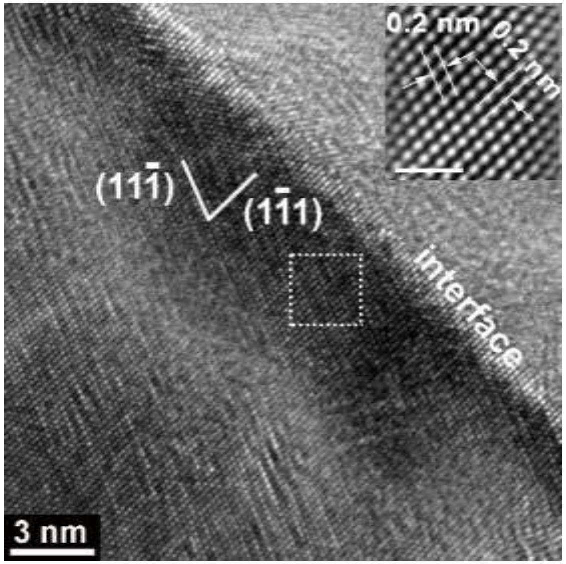


1332 cm^{-1}: sp^3 hybridized C-C bond structure

Plasma-induced etching of diamond thin films etching of diamond thin films



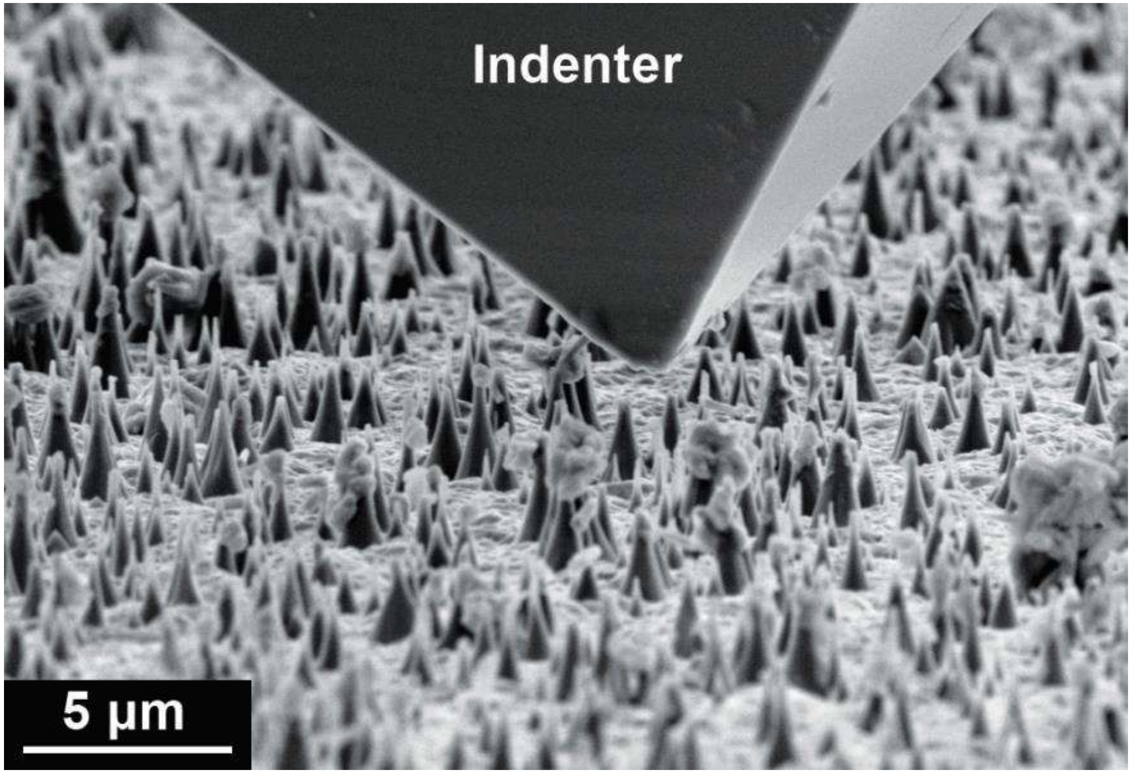
HRTEM
SAED

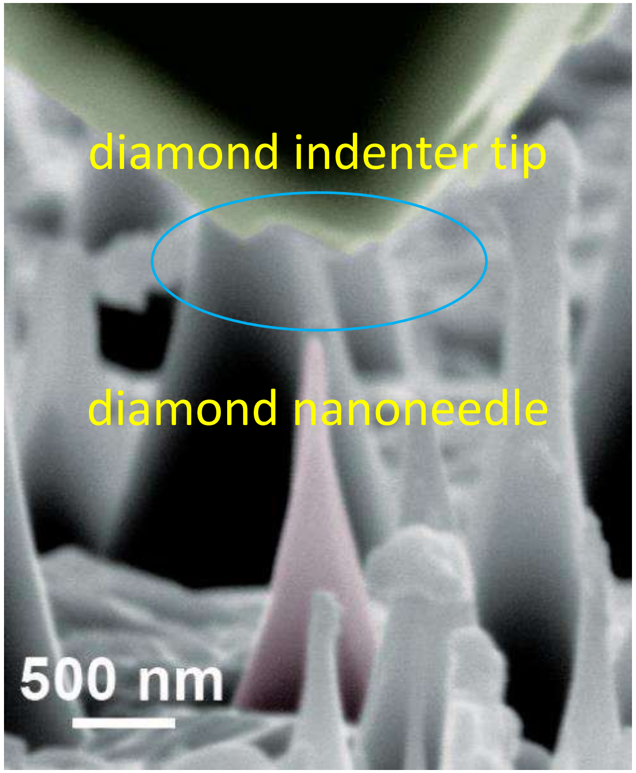


single-crystalline nanoneedles

Atomic-level smooth surface

Experiment challenge: using a nanoindenter, however…





shield VS. spear paradox…

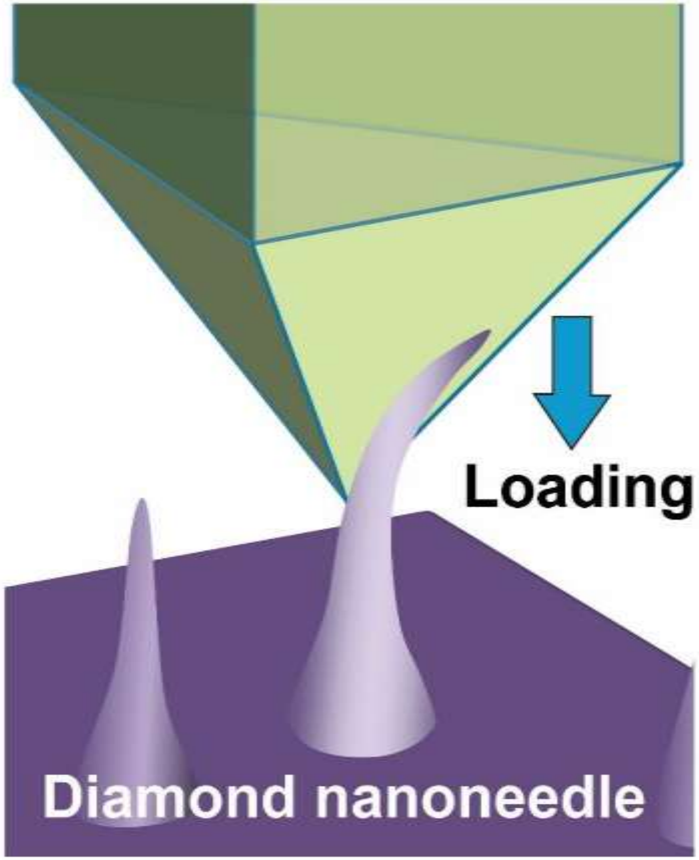
Size effect

“Push-to-Bend” strategy

Quantitative force-displacement (F-D) data recorded;

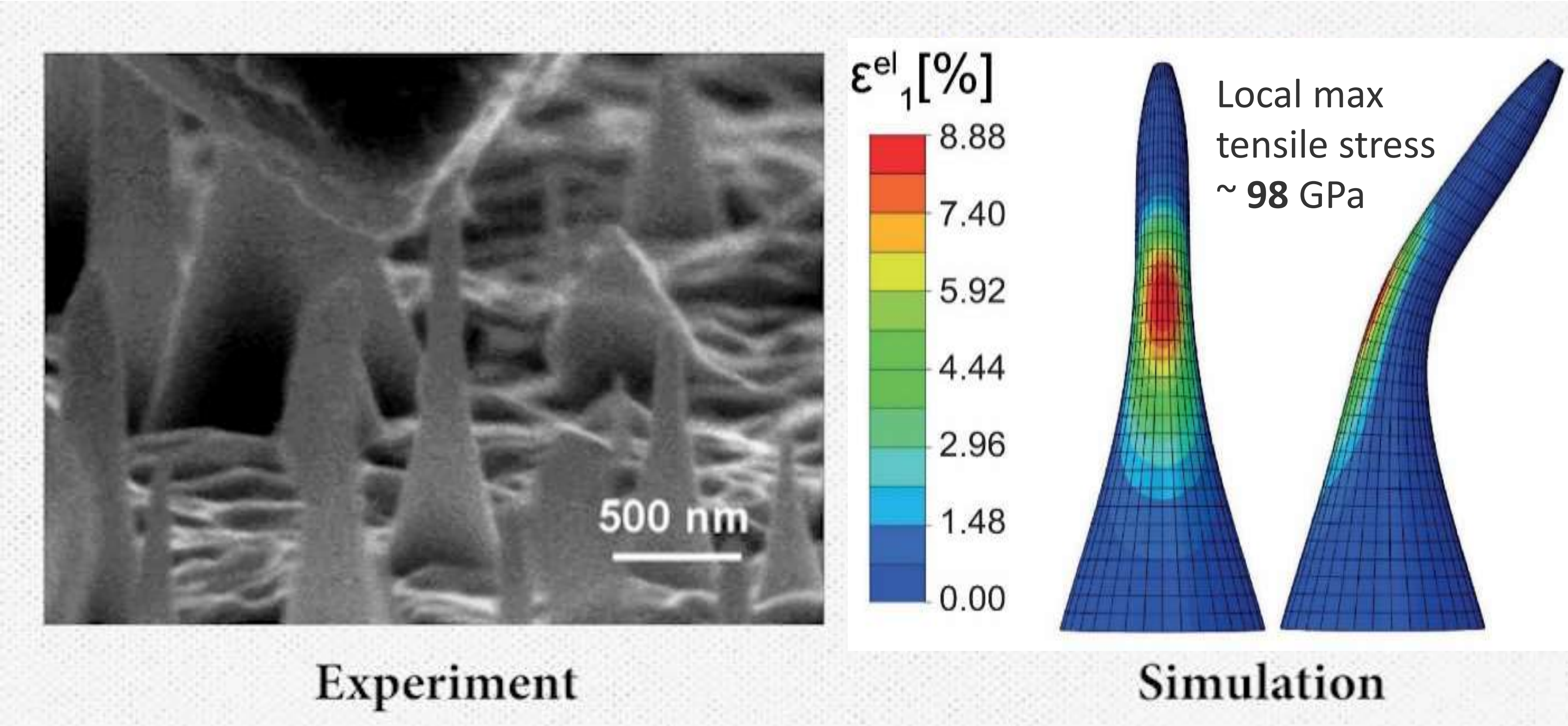
in situ SEM imaging of real-time deformation geometry

(From left: Dr. Hongti Zhang, Dr. Yang Lu and Mr. Amit Banerjee)



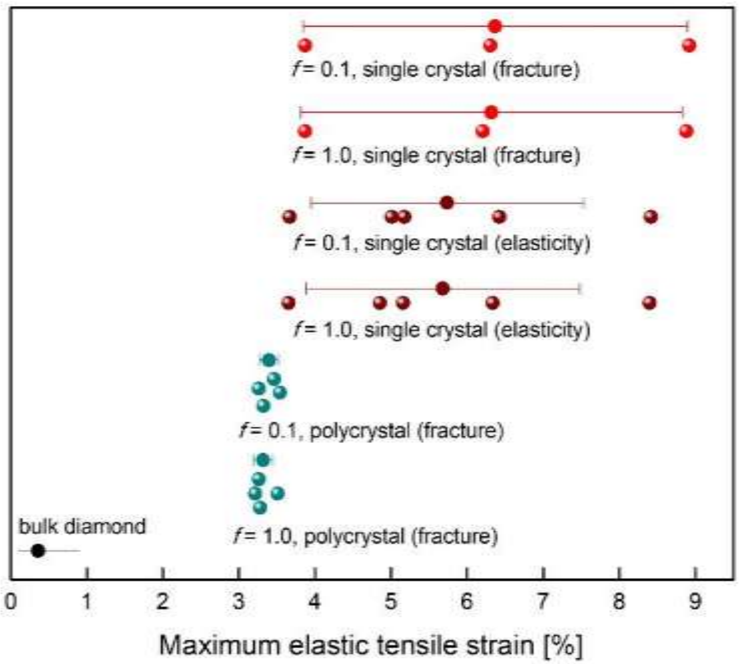
Push-to-Bend

Single-crystalline diamond nanoneedle: deep elastic bending



Bending of a single-crystalline diamond nanoneedle inside SEM, with
fully recoverable flexural deformation

Reducing size for enhanced elasticity



Science

Science **360** (6386), 300-302.
DOI: 10.1126/science.aar4165

Ultralarge elastic deformation of nanoscale diamond

Amit Banerjee,[1,2*] Daniel Bernoulli,[3*] Hongti Zhang,[1,4*] Muk-Fung Yuen,[2,5] Jiabin Liu,[1] Jichen Dong,[6] Feng Ding,[6,7] Jian Lu,[1,4] Ming Dao,[3]† Wenjun Zhang,[2,5]† Yang Lu,[1,2,4]† Subra Suresh[8]†

MATERIALS

On the quest for the strongest materials

Diamond nanoneedles have strength approaching the theoretical maximum

By Javier LLorca[1,2]*

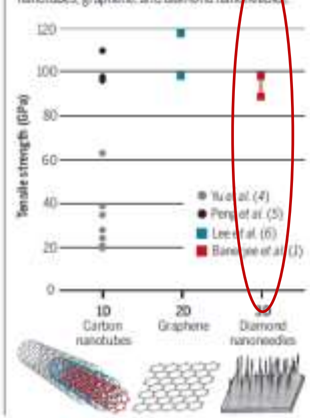
The strength of a material is a measure of its ability to withstand a load without breaking. Scientists in search of the strongest materials have recently turned their attention to nanomaterials, which have few of the defects that typically reduce a material's strength. On page 300 of this issue, Banerjee *et al.* (*1*) show that when nanoscale single-crystal diamond needles are elastically deformed, they fail at a maximum local tensile stress of ~89 to 98 GPa, which is very close to the theoretical limit for this material.

The maximum possible strength that a material can have in either tension or shear is controlled by the fracture of the interatomic bonds and is on the order of 10% of the elastic or shear moduli, respectively. However, it is difficult to achieve these strengths in practice because defects in the solid will lead to inelastic relaxation or brittle fracture well before the atomic bond can be stretched to the theoretical limit. Maximum elastic tensile strains supported by bulk solids are between 0.2 and 0.4%, whereas tensile strains of up to 4% have been measured in micrometer-size whiskers (*2*). Recent progress in nanomaterial synthesis and nanomechanical testing has opened the possibility of probing the strength of material systems that are practically free of defects (*3*). In parallel, atomistic simulations based on density-functional theory and molecular dynamics can predict accurately the fracture strength of perfect crystals and allow the influence of defects and free surfaces on this property to be explored.

Because the carbon-carbon bond is the strongest in nature, the search for the strongest material has focused on one-dimensional carbon nanotubes and two-dimensional graphene nanoscale objects (see the figure). Experimental results and ab initio calculations indicate that the elastic modulus of carbon nanotubes and graphene is ≈1 TPa (*4*–*6*). The strengths measured in both types of nano-objects are thus very close to the theoretical limit (see the figure). By contrast, the reported tensile strength of bulk cubic diamond is much smaller (<10 GPa) (*7*). These differences in strength have been partially attributed to brittle fracture from defects during tensile deformation of bulk samples. Higher tensile strengths (up to 20 GPa) for diamond have been reported from Hertzian indentation tests (*8*), but these values must be treated with caution because of the uncertainties associated with the spherical indentation to determine the tensile strength. Regardless of the experimental technique, diamond fractures by cleavage along the (111) plane, which has the lowest fracture energy. The strengths reported by Banerjee *et al.* (which correspond to a tensile strain of ≈9%) are very close to the theoretical limit for diamond and to the maximum strength values reported for carbon nanotubes and gra-

Strong, stronger...

Experimental measurements have shown similarly high tensile strengths for multiwall carbon nanotubes, graphene, and diamond nanoneedles.



[1]IMDEA Materials Institute, C/Eric Kandel 2, 28906 Getafe, Madrid, Spain. [2]Department of Materials Science, Polytechnic University of Madrid, E. T. S. de Ingenieros de Caminos, 28040 Madrid, Spain. Email: javier.llorca@imdea.org

Allowing electronic property modulation through **deep** straining

PNAS

Deep elastic strain engineering of bandgap through machine learning

Zhe Shi[a,b,1], Evgenii Tsymbalov[c,1], Ming Dao[a], Subra Suresh[d,2], Alexander Shapeev[c,2], and Ju Li[a,b,2]

[a]Department of Materials Science and Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139; [b]Department of Nuclear Science Engineering, Massachusetts Institute of Technology, Cambridge, MA 02139; [c]Skolkovo Institute of Science and Technology, 121205 Moscow, Russia; and [d]Nanyang Technological University, 639798 Singapore, Republic of Singapore

Contributed by Subra Suresh, December 18, 2018 (sent for review November 1, 2018; reviewed by Yonggang Huang and Devendra K. Sadana)

PHYSICAL REVIEW LETTERS 123, 195504 (2019)

Smooth Flow in Diamond: Atomistic Ductility and Electronic Conductivity

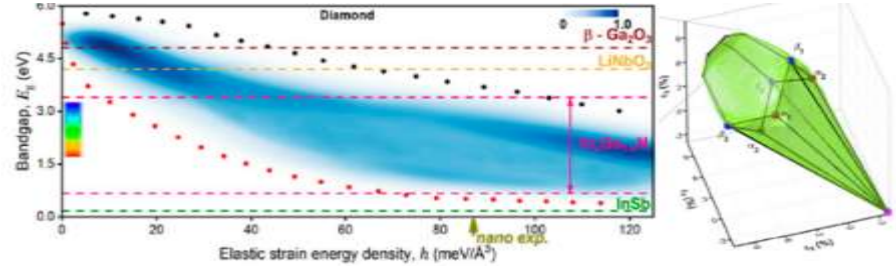
Chang Liu,[1] Xianqi Song,[1] Quan Li,[1,2,3] Yanming Ma,[1,2] and Changfeng Chen[3,1]

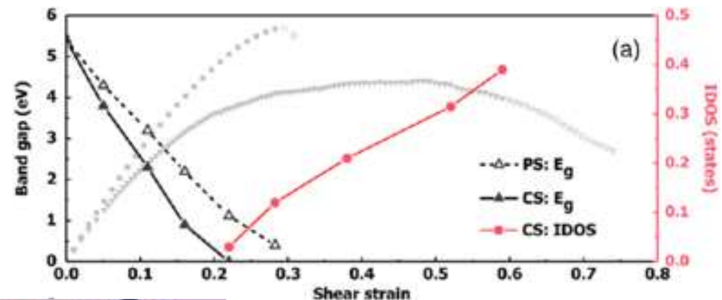
[1]*State Key Laboratory of Superhard Materials, Key Laboratory of Automobile Materials of MOE, Department of Materials Science, and Innovation Center for Computational Physics Method and Software, Jilin University, Changchun 130012, China*

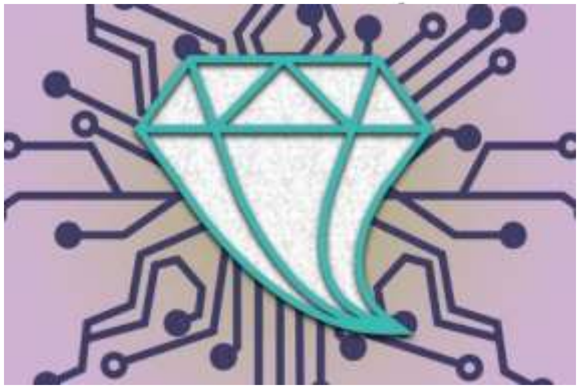
[2]*International Center of Future Science, Jilin University, Changchun 130012, China*

[3]*Department of Physics and Astronomy, University of Nevada, Las Vegas, Nevada 89154, USA*

(Received 1 July 2019; published 6 November 2019)





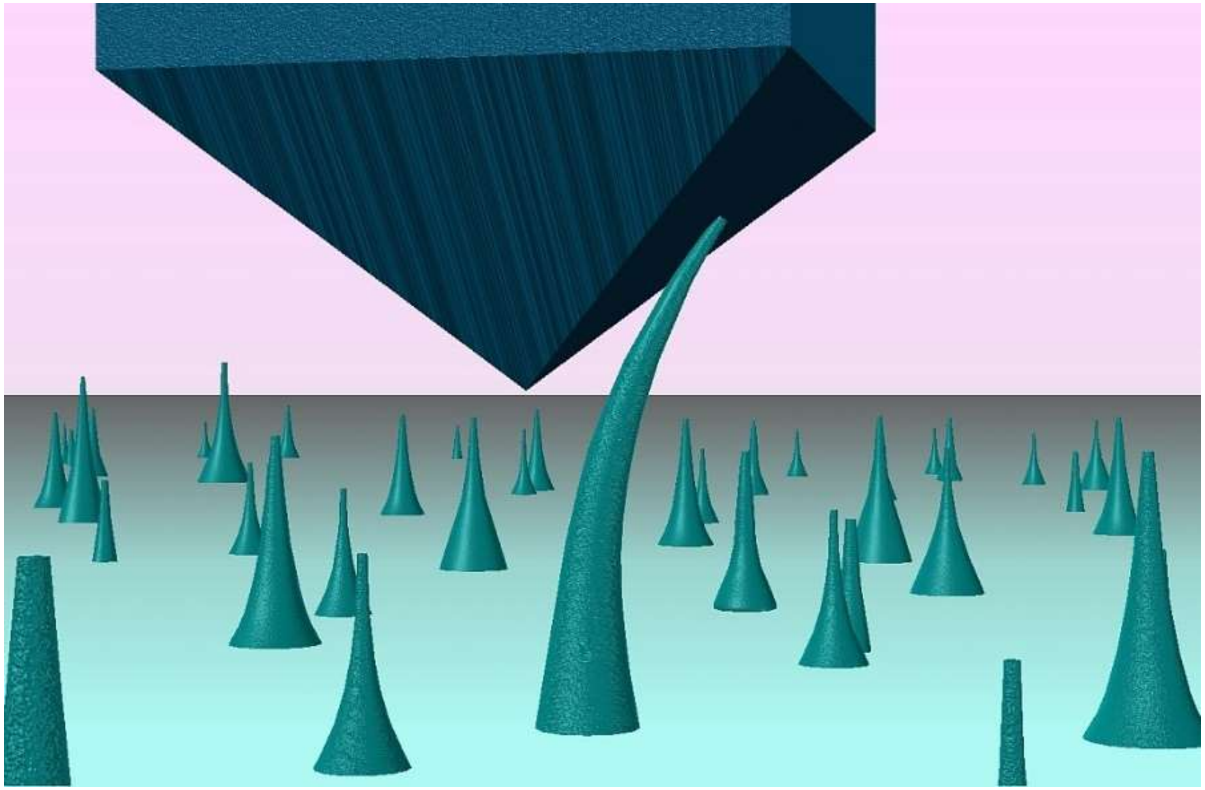


“These discoveries have opened up new avenues to explore how devices can be fabricated with even **more dramatic changes** in the materials’ properties.”

https://news.mit.edu/2019/artificial-intelligence-engineer-microchips-0211

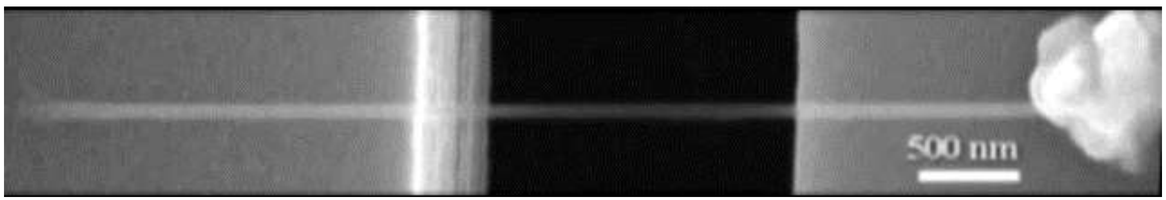
Secondly, for real device application…

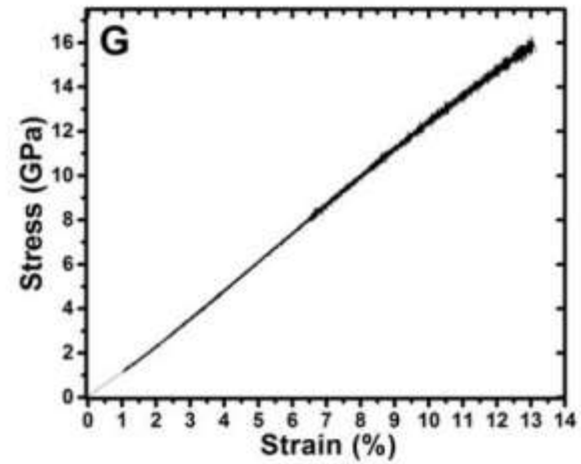
- Device geometry; Straining method; Strain distribution…



Tensile Elastic Straining of Silicon Nanowire

13% global deformation

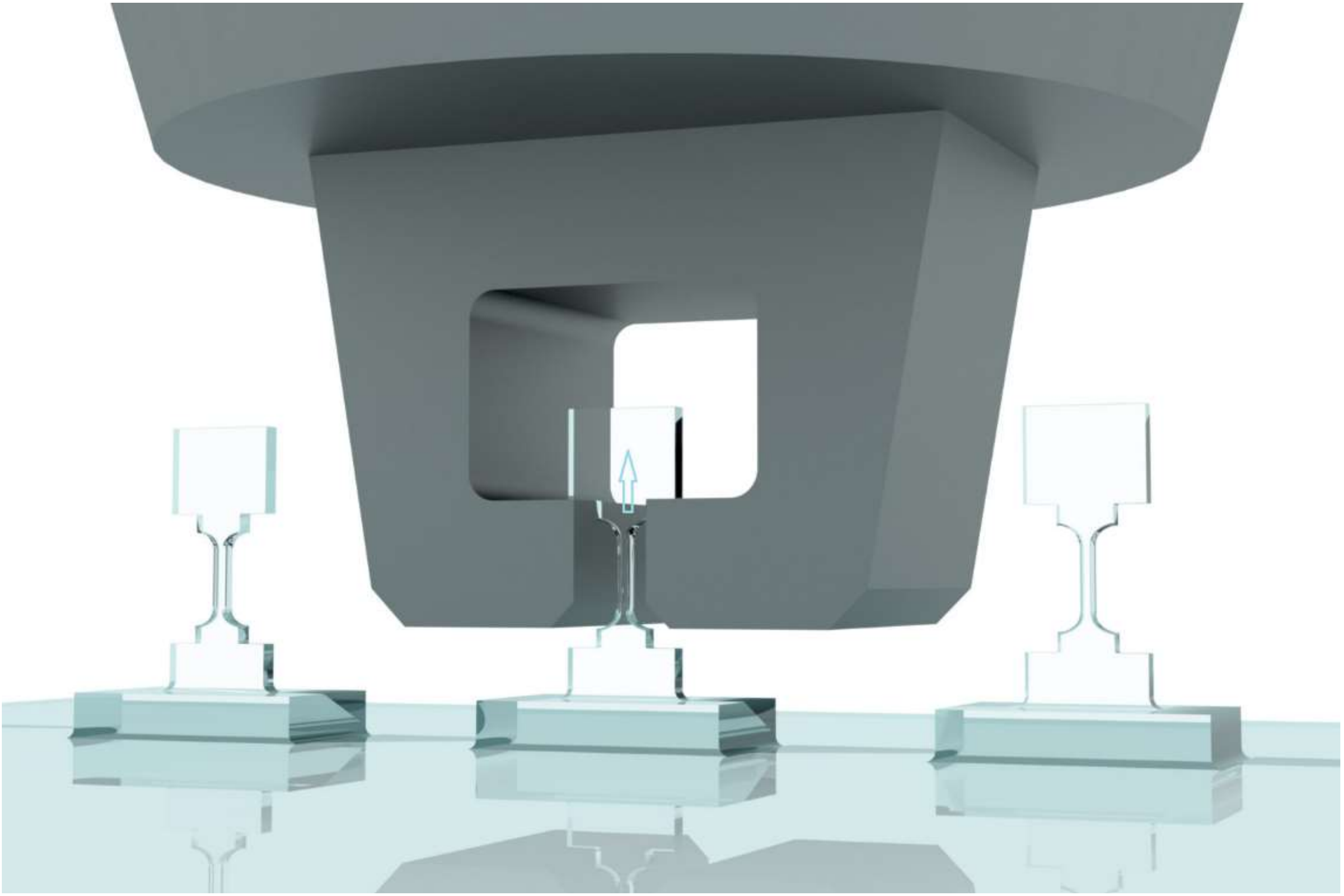




ScienceAdvances
AAAS

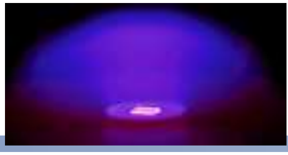
Approaching the ideal elastic strain limit in silicon nanowires
Hongti Zhang, Jerry Tersoff, Shang Xu, Huixin Chen, Qiaobao Zhang, Kaili Zhang, Yong Yang, Chun-Sing Lee, King-Ning Tu, Ju Li and Yang Lu (August 17, 2016)
Sci Adv 2016, 2:.
doi: 10.1126/sciadv.1501382

So, new configuration...

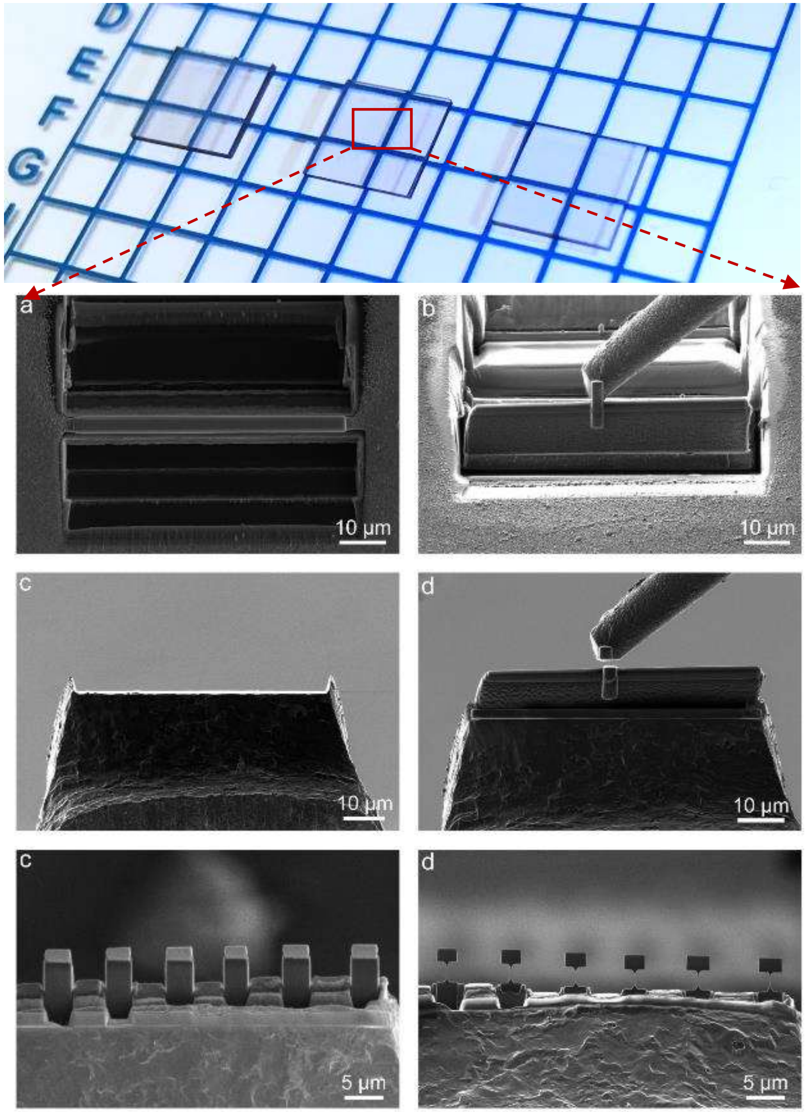


Uniaxial tensile straining of microfabricated diamond structures

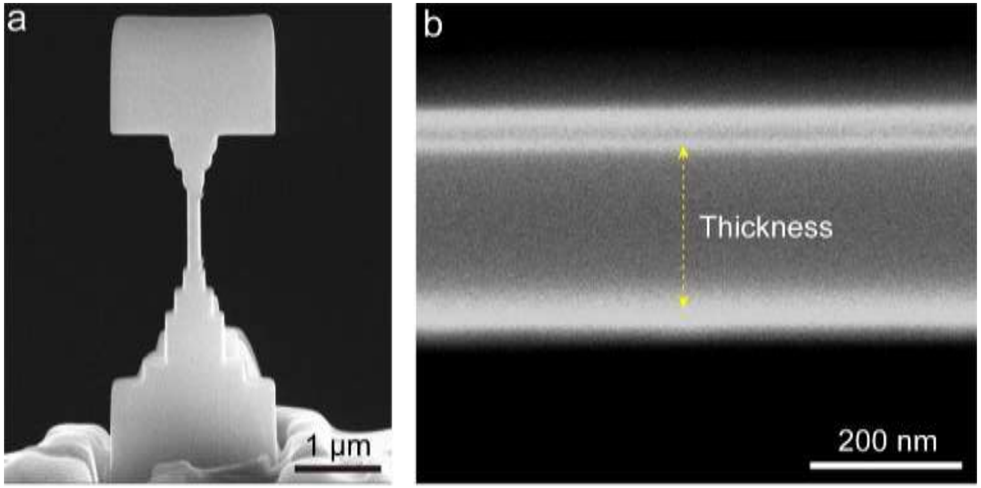
Microfabricated tensile specimen---by Bing Dai, Jiaqi Zhu @HIT



Sample fabrication process

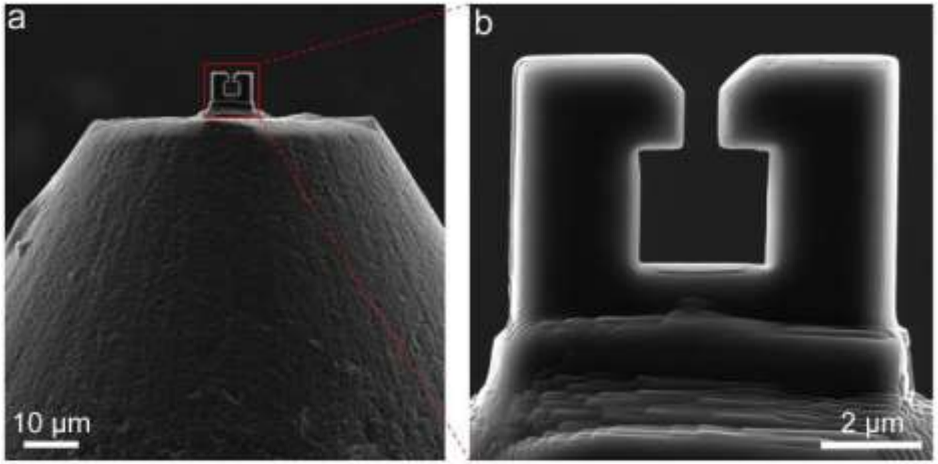


Single crystalline diamond microbridge



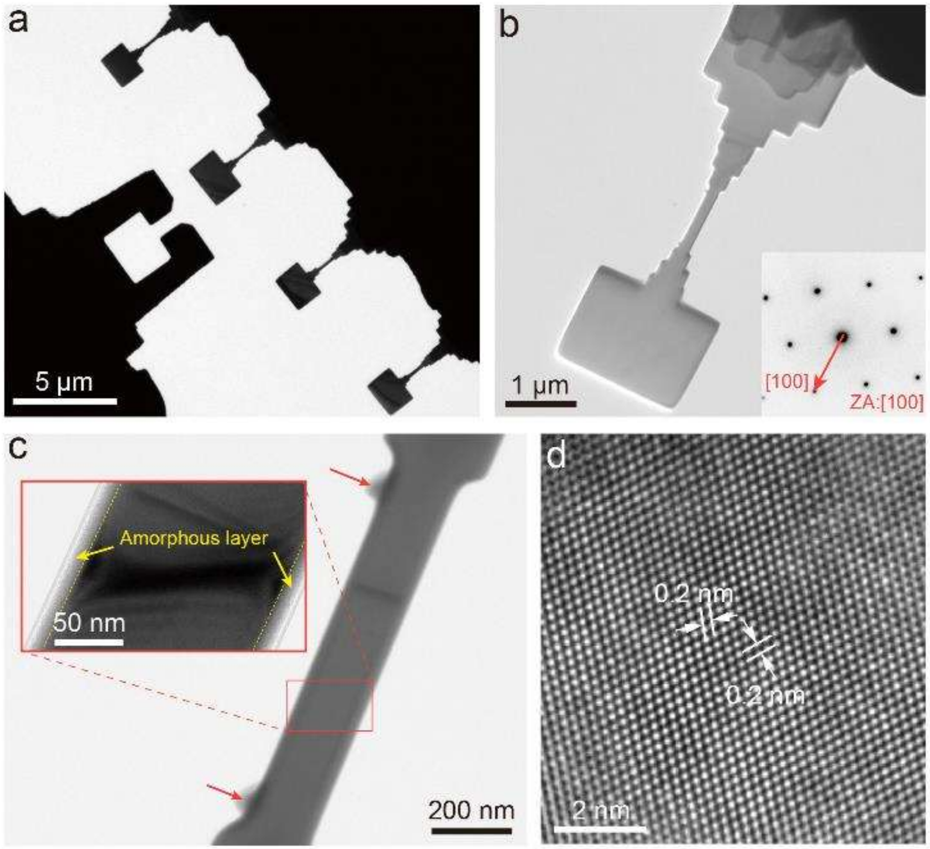
Side view **Top view**

FIB-sculpted diamond tensile gripper



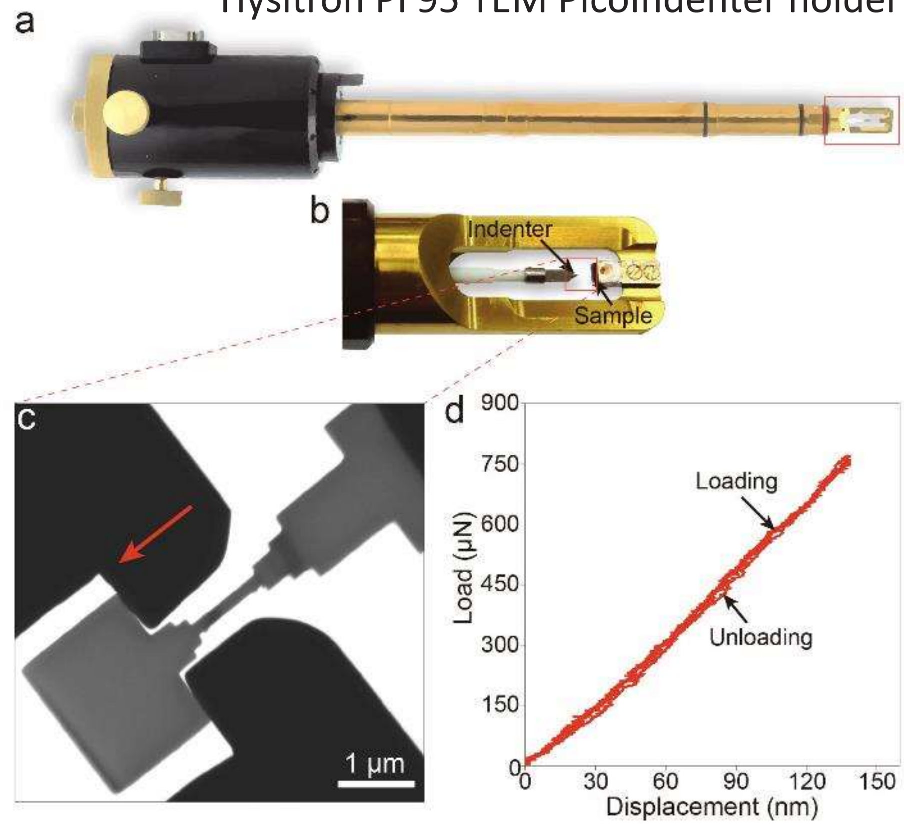
in situ TEM tensile straining

Sample characterization

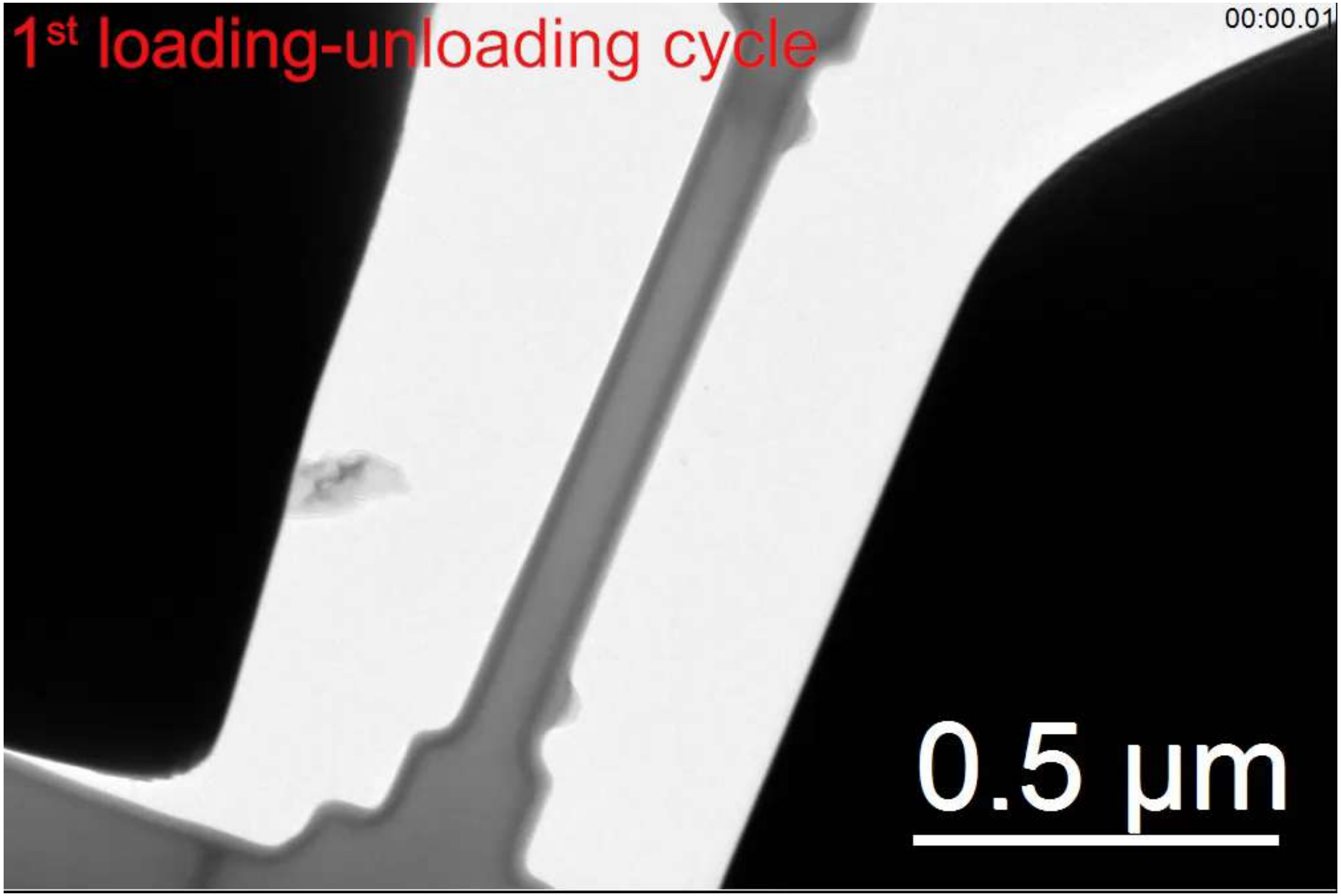


in situ TEM tensile testing setup

Hysitron PI 95 TEM PicoIndenter holder

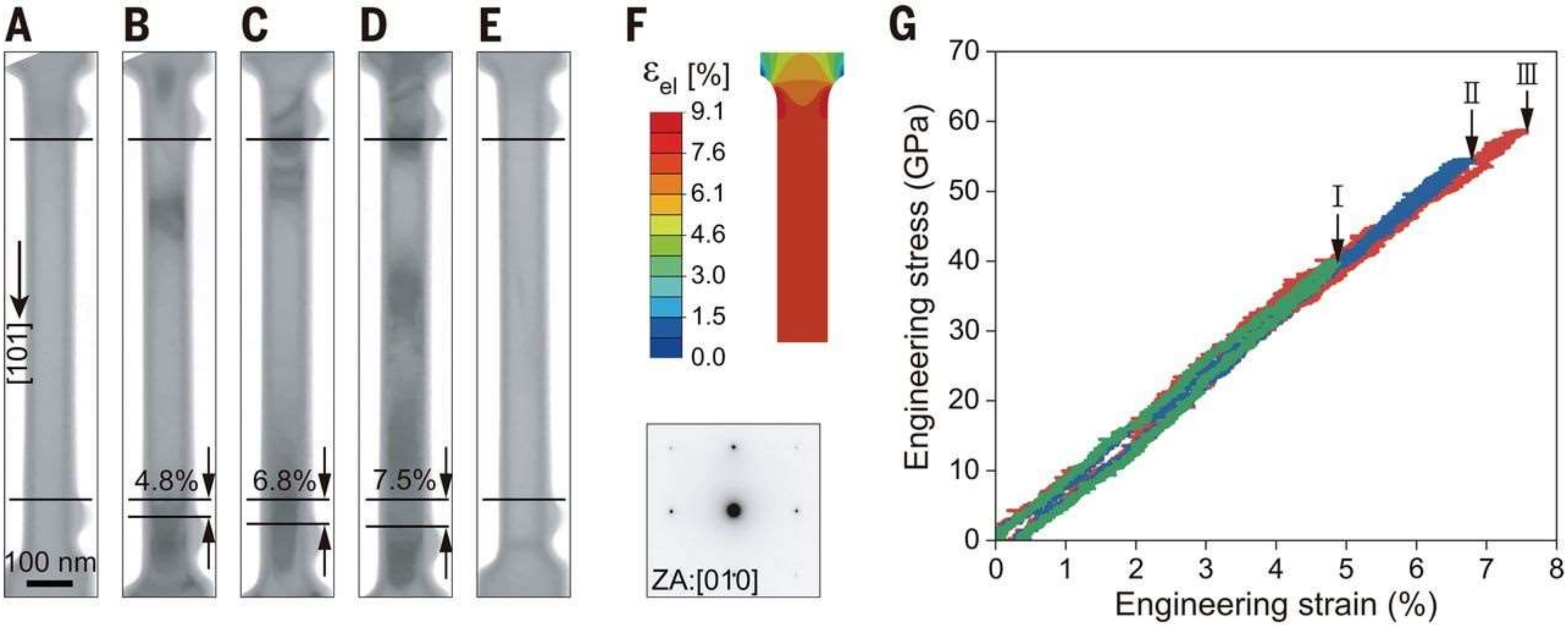


in situ Loading-unloading tensile straining



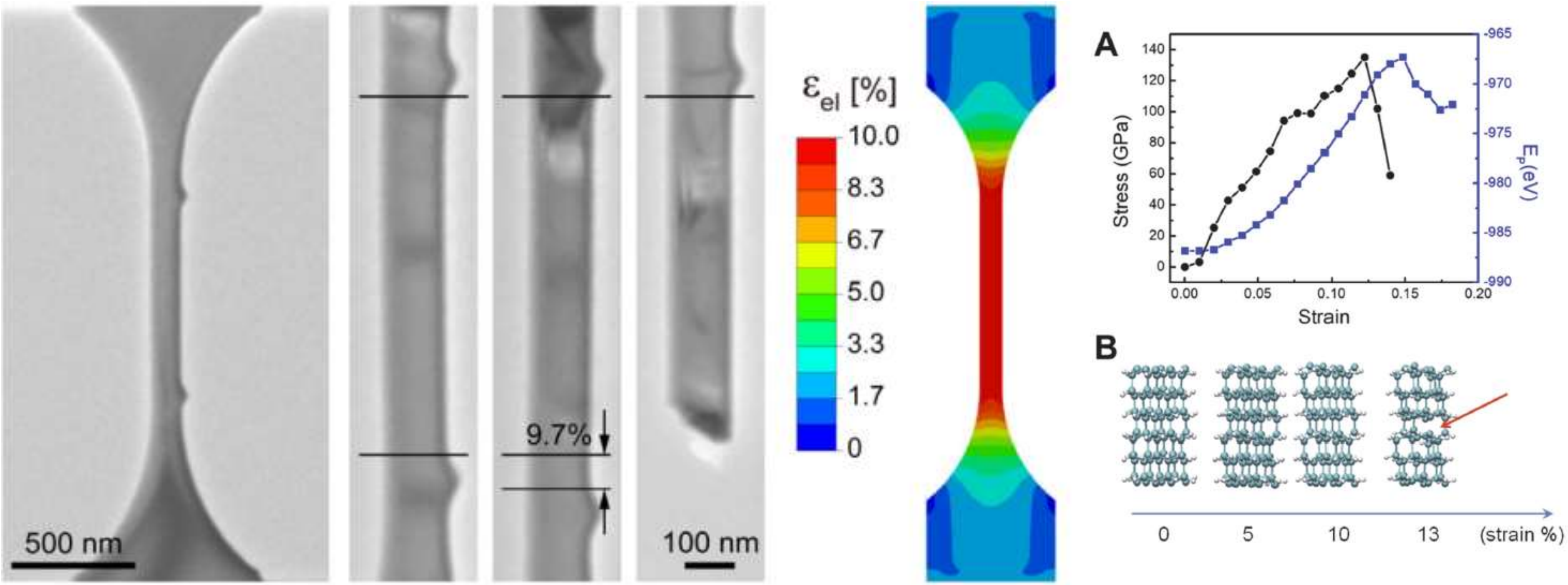
Loading-unloading cycles of a single-crystalline diamond bridge sample along **[101]** direction, with fully recoverable deformation (played at 30× speed)

Ultralarge, uniform tensile elastic straining



Large, uniform tensile elasticity in the microfabricated diamond bridge

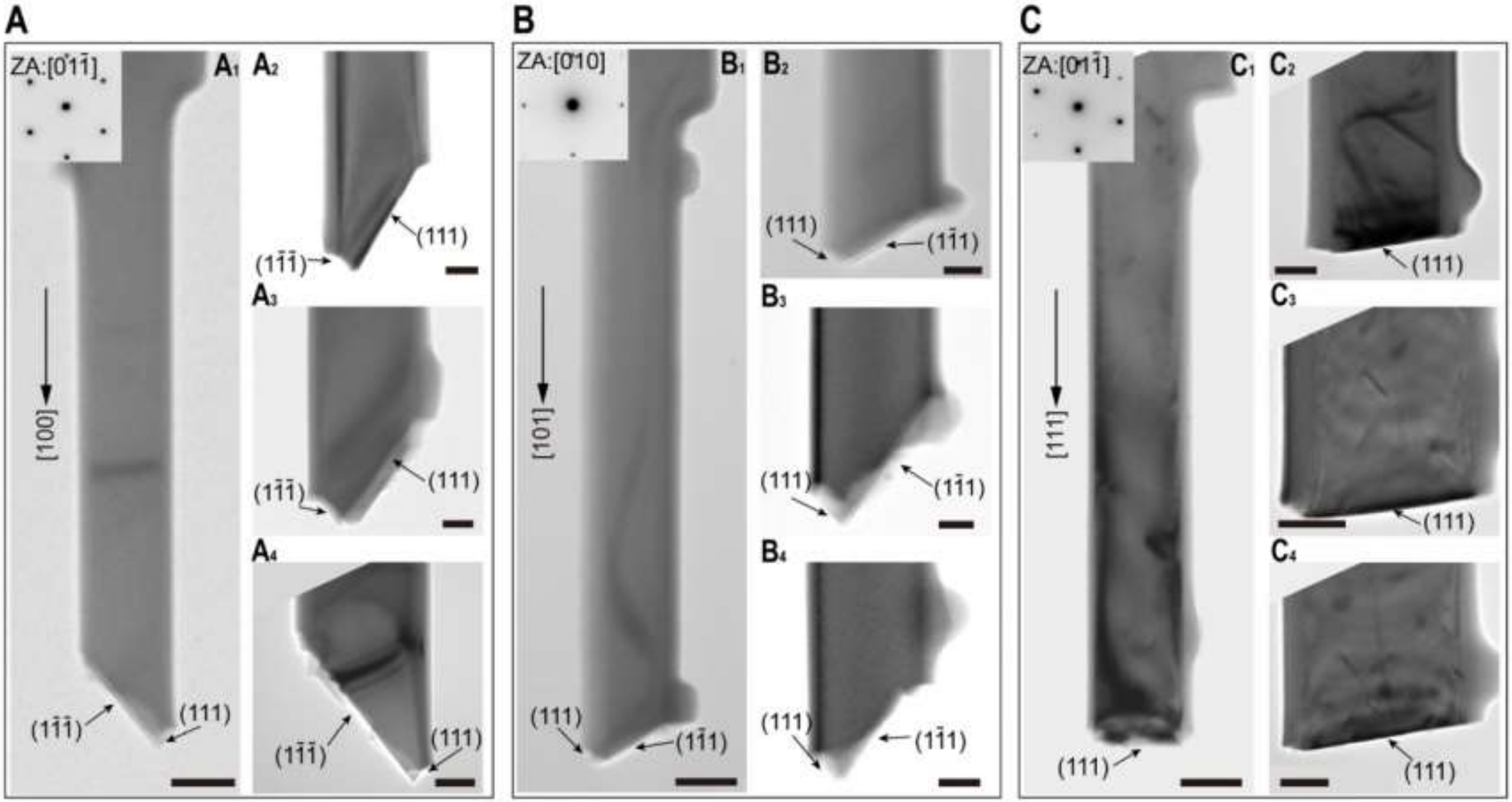
Optimization of sample geometry for extreme



Science 2018

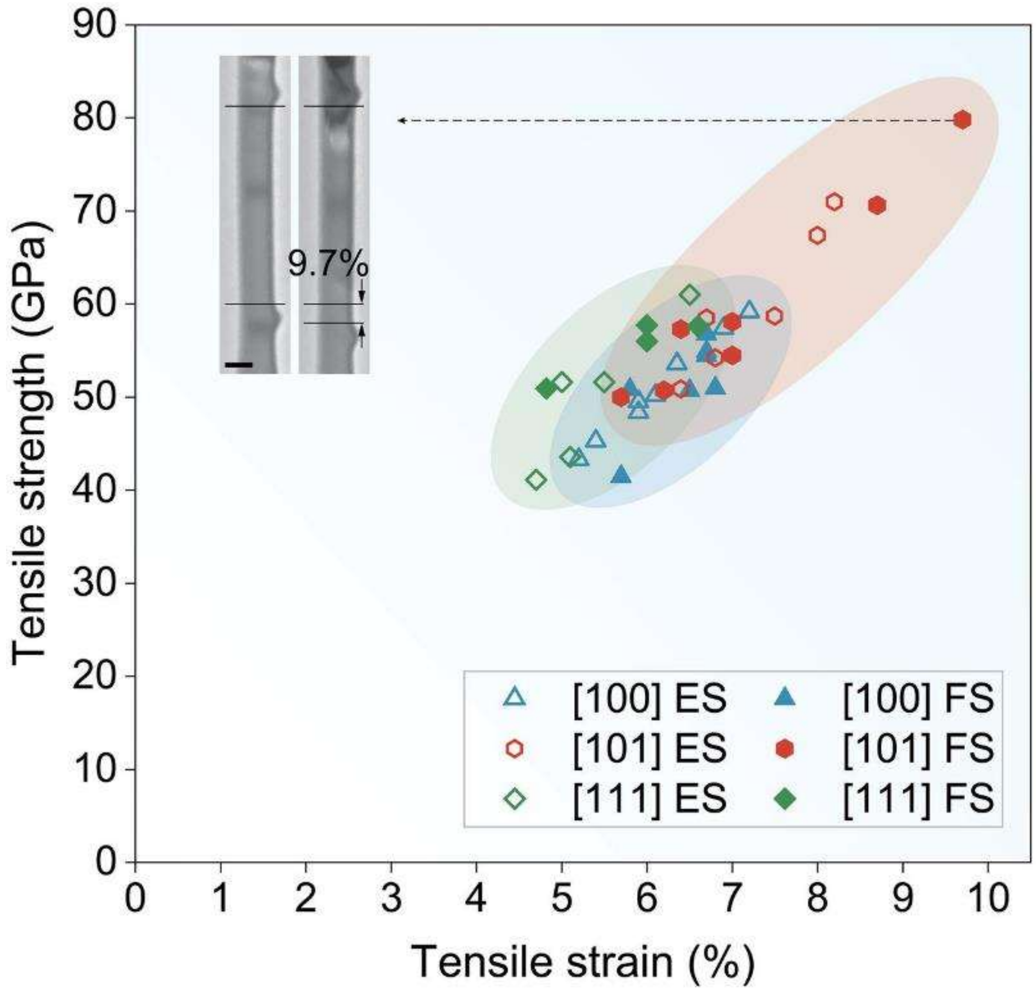
- Optimized by American Society for Testing and Materials (**ASTM**) standard
- Up to 10% sample-wide uniform elastic strain --- **near ideal limit**!

Fracture morphologies



- Without visible sign of plasticity during tensile deformation
- Retain the overall pristine single-crystalline structures
- Typical distinct {111} cleavage surfaces

Experiment summary

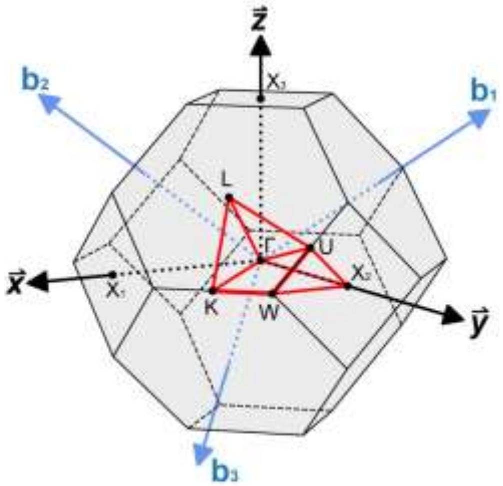


- ES: elastic strains from fully reversible runs; FS: failure-run strains
- **6-9%** sample-wide elastic strains with full recovery

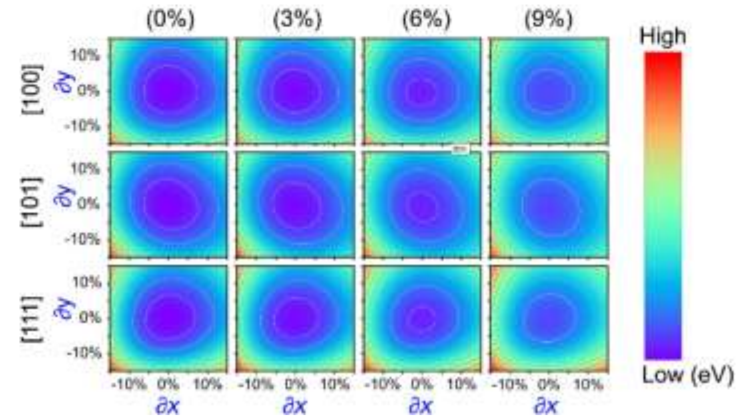
Lastly, electronic properties under deep elastic straining

-- DFT calculation by Andy Chou, JP Chou, Alice Hu

Brillouin zone of diamond primitive cell



Calculated energy

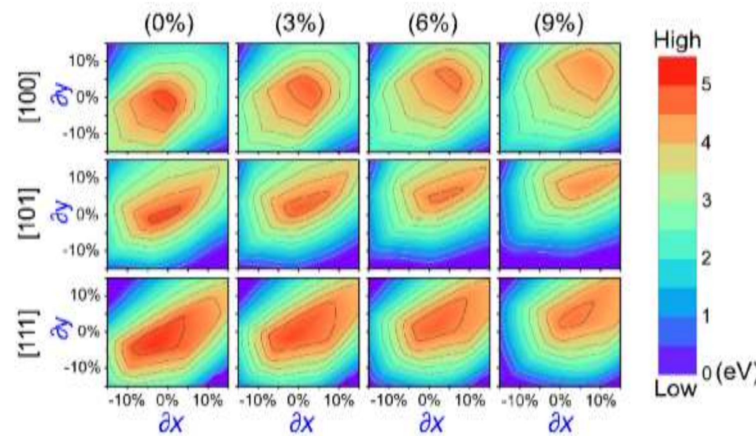


k-point coordinates of primitive cell

k-path: Γ−X_2−U−W−K−Γ−L−W−X_2

symbol	k_1	k_2	k_3
Γ	0.000	0.000	0.000
X_2	0.500	0.000	0.500
U	0.625	0.250	0.625
W	0.500	0.250	0.750
K	0.375	0.375	0.750
L	0.500	0.500	0.500

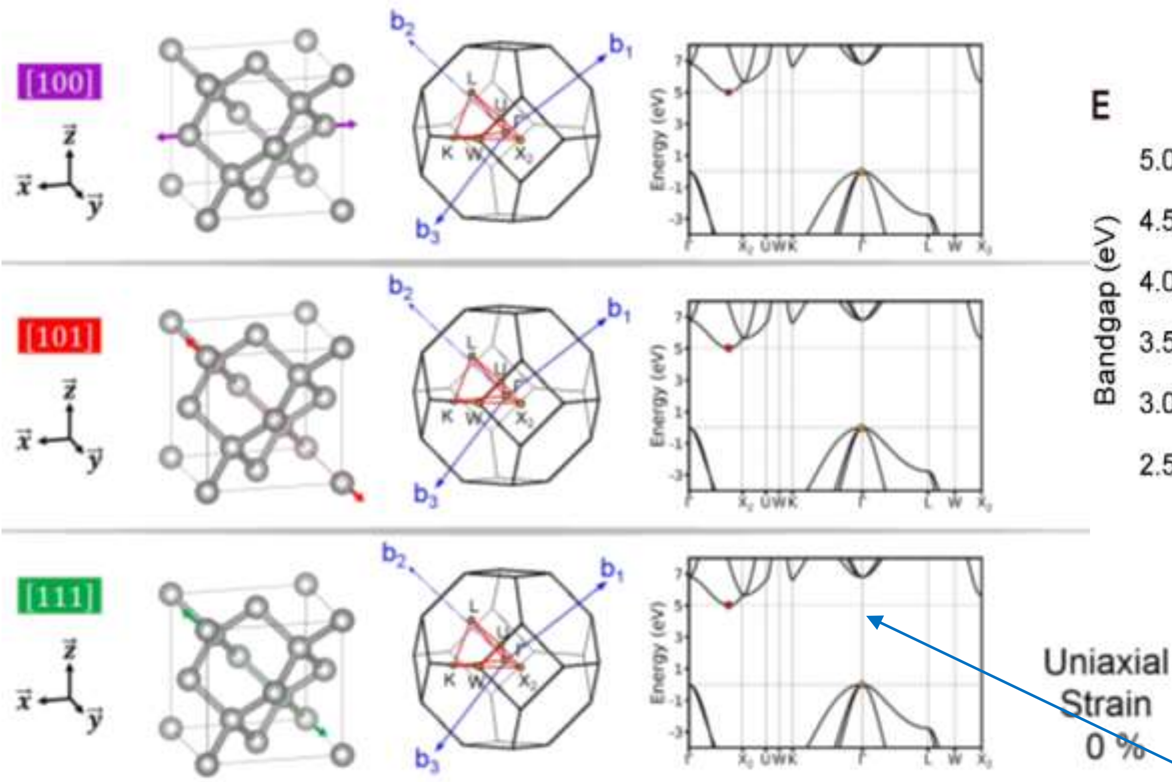
Calculated bandgap

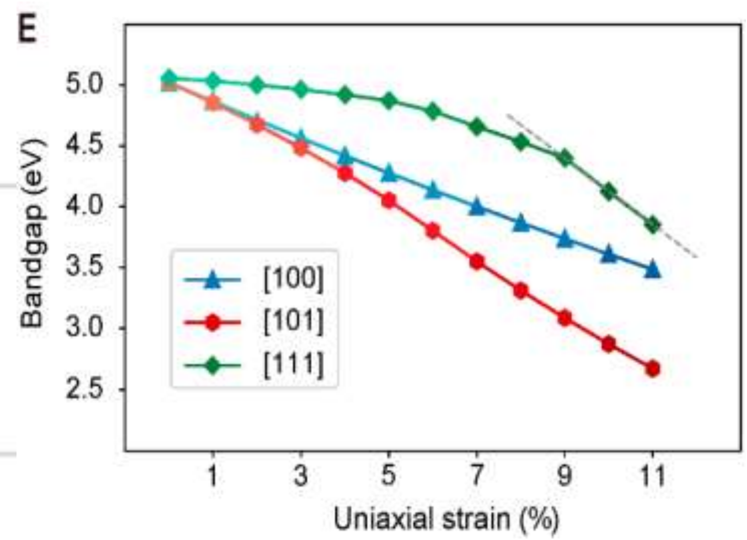


Diamond has small Poisson contraction and barely has transverse change on non-loaded axis

Band structure evolution upon tensile straining

Bandgap changes for each loading direction

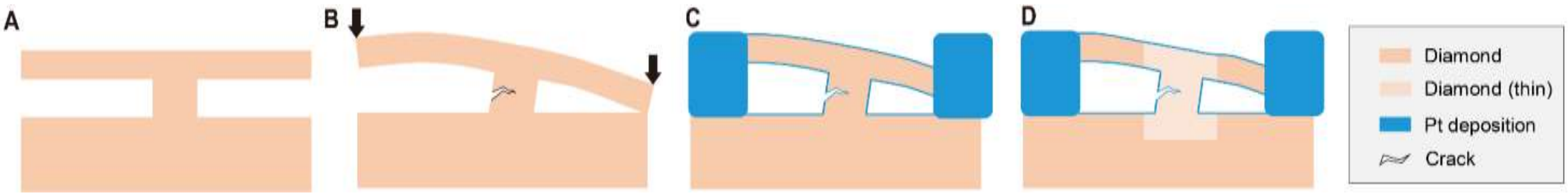


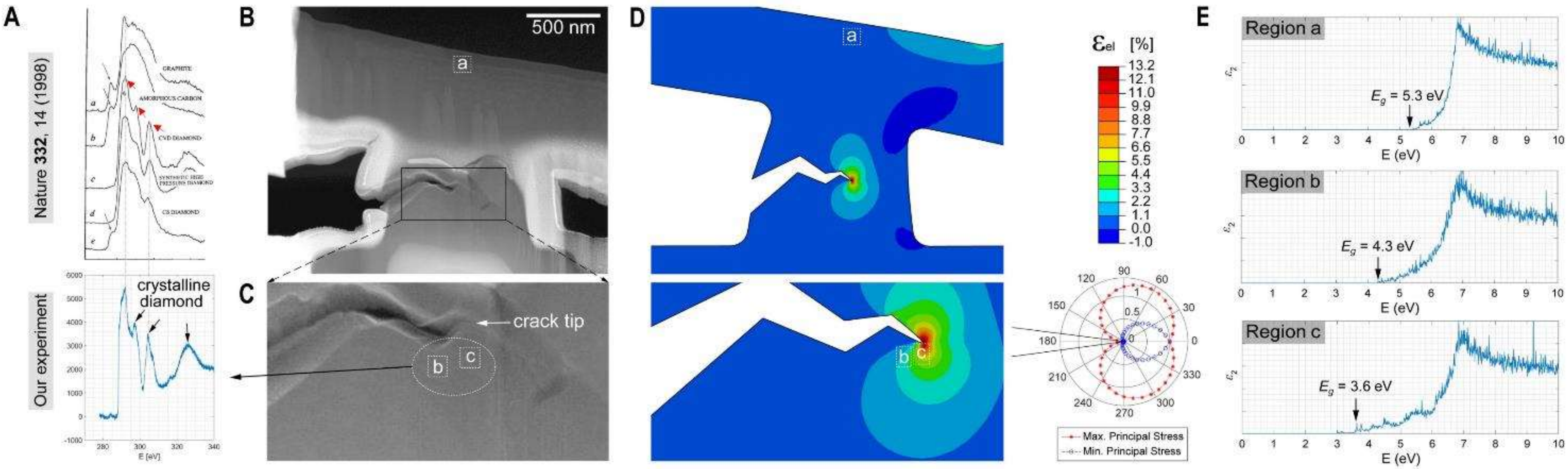


conduction band minimum (CBM)

- [101] direction with the **largest reduction** rate, down to ~3 eV at 9% strain → conventional wide-bandgap semiconductor
- **Indirect-direct** bandgap transition with tensile strains >9% along the [111] direction → optoelectronics

EELS characterization of strained diamond specimen



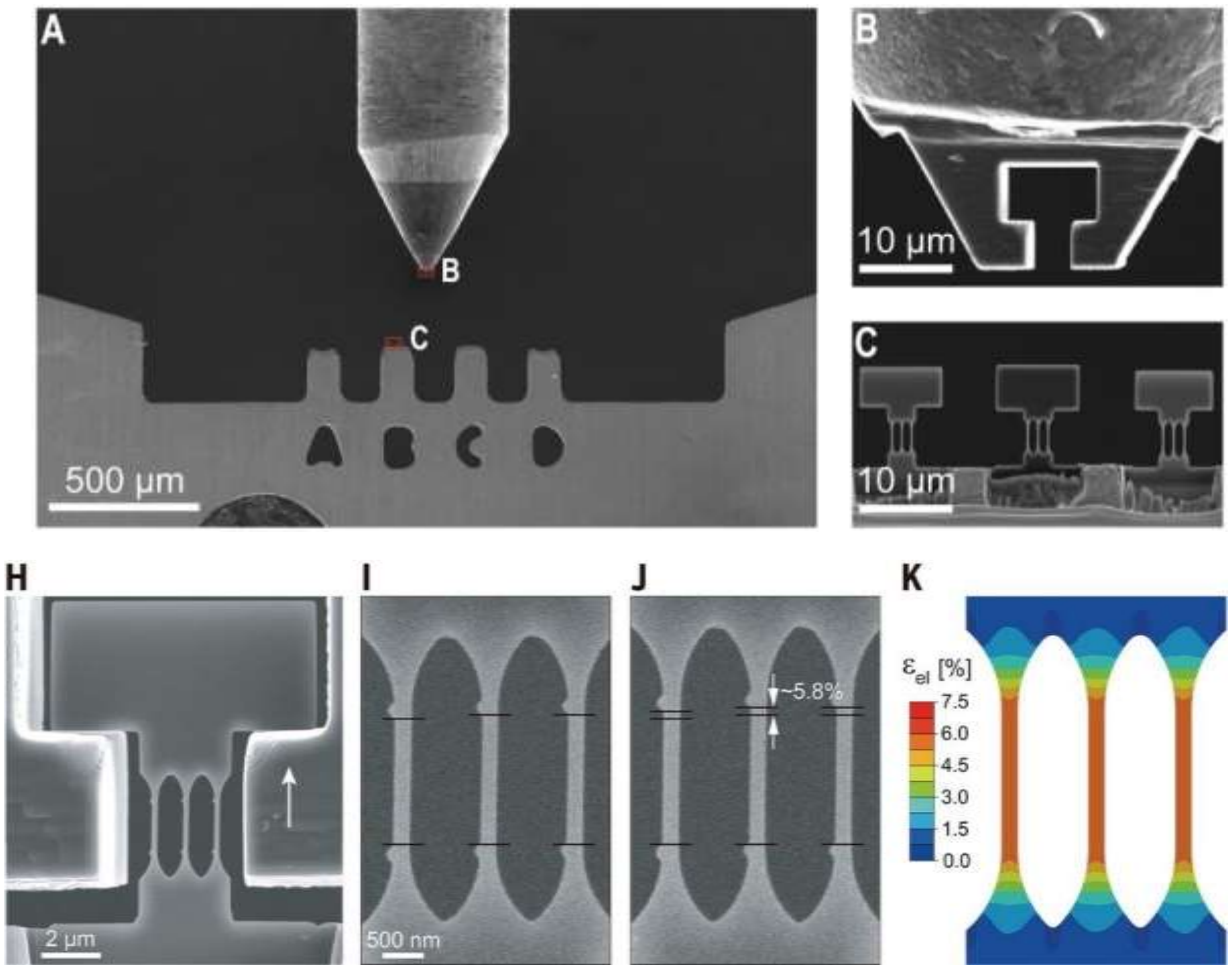


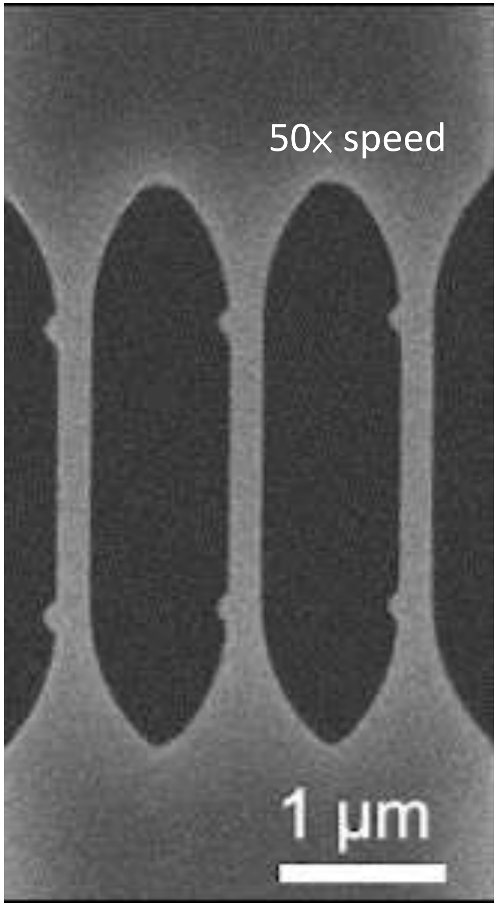
--- EELS by Yang Yang, Andy Minor @LBNL

Measured bandgap energy agrees well with the calculated **bandgap decrease** trend

“strained diamond” device

“Strained diamond” device array





Complete recover after being uniformly strained to ~5.8%, fractured at ~6%

Diamond array samples with multiple bridges (can be scalable)

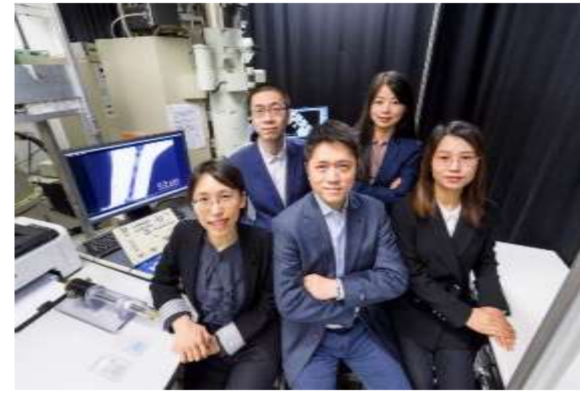
“Strained diamond” for future microelectronics/optoelectronics

Science

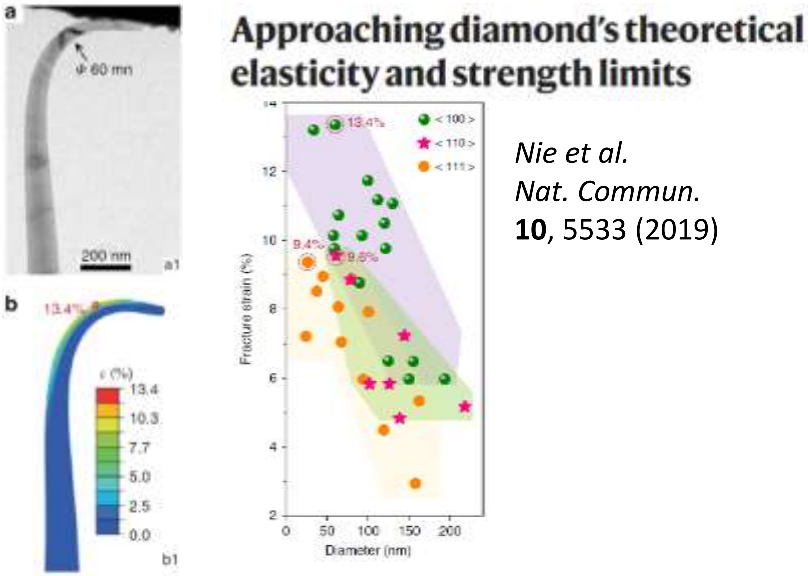
Science 01 Jan 2021:
Vol. 371, Issue 6524, pp. 76-78
DOI: 10.1126/science.abc4174

Achieving large uniform tensile elasticity in microfabricated diamond

Chaoqun Dang[1*], Jyh-Pin Chou[1,2*], Bing Dai[3*], Chang-Ti Chou[4*], Yang Yang[5], Rong Fan[1], Weitong Lin[1], Fanling Meng[6], Alice Hu[1,7]†, Jiaqi Zhu[3]†, Jiecai Han[3], Andrew M. Minor[5], Ju Li[8]†, Yang Lu[1,7,9]†



Pushing to the limit…



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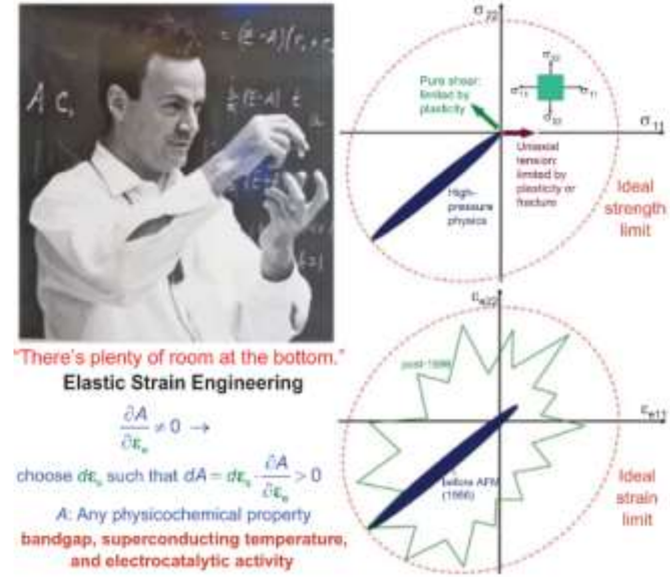

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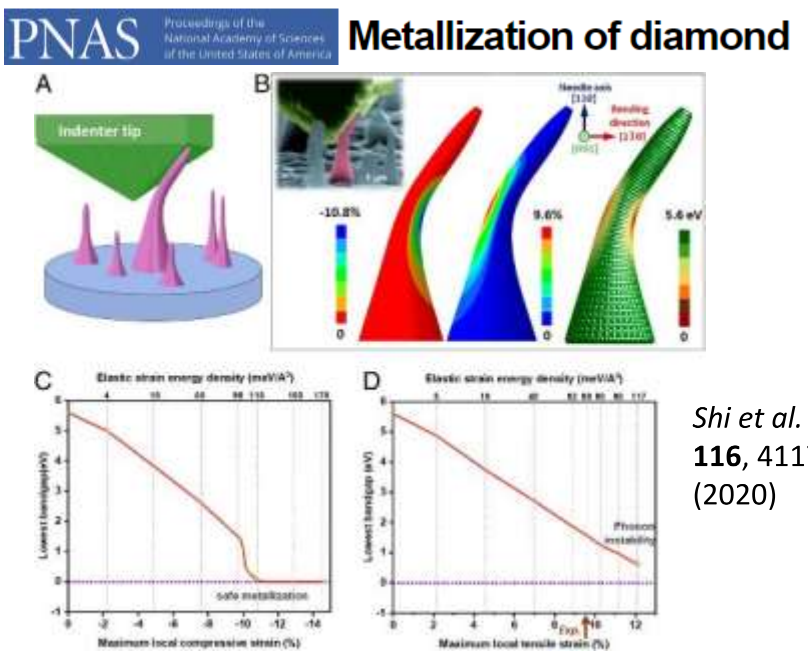

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Editors' Suggestion

Superconductivity in Compression-Shear Deformed Diamond

Chang Liu,[1] Xianqi Song,[1] Quan Li,[1,2,*] Yanming Ma,[1,2,†] and Changfeng Chen[3,‡]

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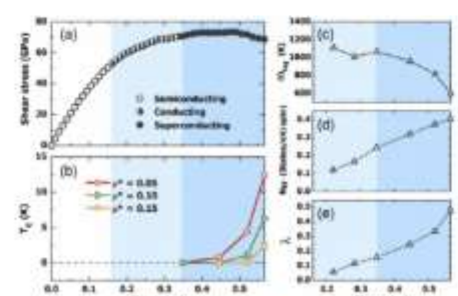


A new diamond age…

VICE

IMAGE: OXYGEN VIA GETTY IMAGES

MOTHERBOARD
TECH BY VICE

Scientists Are Stretching Diamonds to Revolutionize Electronics

Researchers are breaking down diamonds to nano-size and physically stretching them. The eventual results could change everything we know about electronics.

TC By Thobey Campion

January 29, 2021, 10:00pm Share Tweet Snap

> Long story short, if these findings remain consistent, we're sitting pretty for the next ten years of optoelectronics.

While that's a few years out, "The Dawn of a Diamond Age of Electronics," as one industry pioneer puts it, is upon us.

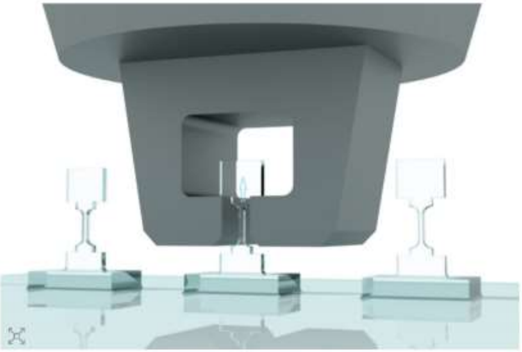
physicsworld Magazine | Latest

semiconductors and electronics

SEMICONDUCTORS AND ELECTRONICS RESEARCH UPDATE

Elastic diamond could be used to make LEDs and lasers

09 Jan 2021



nature reviews physics

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Nature Reviews Physics | https://doi.org/10.1038/s42254-021-00279-5 | Published online: 13 January 2021

MATERIALS PHYSICS

Stretching diamonds

Diamond has a very high carrier mobility and thermal conductivity which would make it ideal for electronic devices, were it not for the very large electronic band gap of 5.5 eV, which effectively makes diamond an insulator. As diamond is an incredibly hard material, modifying its mechanical properties is a challenge. Now, writing in *Science*, Chaoqun Dang and colleagues, demonstrate the ability to stretch diamond by up to 9%. Supporting density functional theory calculations show that such elastic strain engineering can make diamond semiconducting.

Although diamond has been strained before, this has been done by flexural bending (like jumping on a rope bridge) which has led to non-uniform strain. In this experiment, Dang et al. stretched the diamond instead. They created micro-scale "bridges" of diamond and then gripped the ends with tiny pincers and pulled to stretch out along the length of the sample. The diamond completely recovered its original length after strain values of up to 9%. The elasticity depended on the crystal orientation of the direction of strain.

These experiments were followed up with density functional theory calculations to model how the electronic band gap changed as a function of strain. At 9% strain, the calculations show the bandgap reducing to 3.09 eV. This would turn diamond into a direct bandgap semiconductor, making it comparable to GaN or ZnO. The demonstration that diamond can be stretched opens up many possibilities. However, challenges remain, including making electronic measurements of the stretched diamond, sustaining the strain for long periods of time and finally integrating the stretched diamond into practical devices.

Ankita Anirban

Credit: MirageC/Getty

ORIGINAL ARTICLE Dang, C. et al. Achieving large uniform tensile elasticity in microfabricated diamond. *Science* **371**, 76–78 (2021)

Thank you

Q&A