CHROMATIC MECHANICAL RESPONSE IN 2-D LAYERED TMD BASED NANOCOMPOSITES

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IMAPS NEW ENGLAND SYMPOSIUM

https://www.extremetech.com/extreme/211437-extremetech-explains-what-is-graphene

NEW 2D LAYERED MATERIALS



Valance band New 2D Layered TMDs are ideal for energy conversion due to existence of bandgap

Can be chemically/mechanically exfoliated

Large breaking strength E^{2D}/9 for monolayers

Modulate bandgap with strains opening up "Straintronics"

Photovoltaics, Photo-detectors and Solar Cell

Material	Thickness	Efficiency %	Weight g/m²	Power density
GaAs	1 μm	29%	5.3	54 kW/kg
Si	35 µm	20.6%	92.7	2.5kW/kg
Graphene/MoS ₂	0.9 nm	0.1-1%	3.9 x 10 ⁻³	250-2500 kW/kg
WS ₂ /MoS ₂	1.2 nm	0.4-1.4%	7.9 x 10 ⁻³	450-1800 kW/kg

Bernardi et al., Nano Letters, vol. 13, pp. 3664-3670, Aug/2013.

PHOTONS TO MECHANICAL MOTION

- The ability to convert photons to mechanical motion is a classical problem in condensed matter physics.
- AG Bell used the opto-acoustic effect to produce sound in a gas using sunlight*
- However direct transduction of photons into mechanical energy is only possible with few materials.
- Ex: Liquid Crystal Elastomers, PLZT ceramics, carbon nanotubes...



* A.G. Bell, Science 2, 242-253 (1881)

INNOVATIONS AT THE SMALL SYSTEMS LABORATORY IN PHOTOMECHANICS

- At the Small Systems Laboratory, we have made photons to mechanical motion one of the core research subjects.
- To date, we have used nanomaterials with polymers and used the light induced Thermo-mechanical effect for wide variety of applications.
- Cantilever actuators¹, micro-mirrors², micro-grippers³ and world's first nanopositioners based on graphene photomechanics⁴ have all been developed at our laboratory.
- The next generation of photomechanical systems are currently being developed.

¹ Lu et al., **Nanotechnology** 16 (11) 2548, 2005 ; Lu et al., **Applied Physics Letters** 88 (25) 253107, 2006. ²Lu et al., **JMEMS** 16 (6) 1515-1523, 2007; Lu et al., ³ Lu et al., **Nanotechnology** 18 (6) 065501, 2007 ⁴ Loomis et al., **Scientific Reports**, 3 1900, 2013.

PHOTONS TO MECHANICAL MOTION: NANOTUBE COMPOSITE FOR LIGHT DRIVEN ACTUATION

MICRO-OPTO-MECHANICAL SYSTEMS

PICKING AND PLACING OBJECTS



Test dynamometer



PHOTOMECHANICAL NANOPOSITIONER



Loomis et al., Scientific Reports, 3 1900, 2013.

PHOTOMECHANICAL NANOPOSITIONER



Positioning accuracy: ~120 nm,

Loomis et al., Scientific Reports, 3 1900, 2013.

www.nature.com/scientificreports

SCIENTIFIC REPORTS

OPEN Chromatic Mechanical Response in 2-D Layered Transition Metal Dichalcogenide (TMDs) based Nanocomposites

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The ability to convert photons of different wavelengths directly into mechanical motion is of significant interest in many energy conversion and reconfigurable technologies. Here, using few layer 2H-MoS₂ nanosheets, layer by layer process of nanocomposite fabrication, and strain engineering, we demonstrate a reversible and chromatic mechanical response in MoS₂-nanocomposites between 405 nm to 808 nm with large stress release. The chromatic mechanical response originates from the *d* orbitals and is related to the strength of the direct exciton resonance A and B of the few layer 2H-MoS₂ affecting optical absorption and subsequent mechanical response of the nanocomposite. Applying uniaxial tensile strains to the semiconducting few-layer 2H-MoS₂ crystals in the nanocomposite resulted in spatially varying energy levels inside the nanocomposite that enhanced the broadband optical absorption up to 2.3 eV and subsequent mechanical response. The unique photomechanical response in 2H-MoS₂ based nanocomposites is a result of the rich *d* electron physics not available to nanocomposites based on *sp* bonded graphene and carbon nanotubes, as well as nanocomposite based on metallic nanoparticles. The reversible strain dependent optical absorption suggest applications in broad range of energy conversion technologies that is not achievable using conventional thin film semiconductors.

Altimetric Score of 90!



New 2D Nanomaterials for Photons to Mechanics

Liquid Phase Exfoliation and Optical Properties

Three types of samples were prepared namely (a) bulk: (b) intermediate: sonicated for 50 hours and centrifuged for 45-120 minutes and layers separated (c) few layers: well characterized commercially available few layers in ethanol was purchased. The samples were characterized for number of layers using an SEM.

Lambert-Beer's law characterized by $A/I = \alpha C$, where A/I is the absorbance per length, α is the extinction coefficient, and C is the concentration,

The two peaks marked A (1.9 eV) and B (2.1 eV) correspond to the direct exciton transition at the K point



Bulk (100-500)

600

800

800

Test dynamometer



Layer by Layer process was used to fabricate actuators.

The few layer based nanocomposites showed the strongest optical absorbance (300 nm to 750 nm) compared to their intermediate and bulk counterparts. The characteristic exciton resonance peak A (\sim 1.9 eV) and B (\sim 2.1 eV) is seen suggesting existence of a direct bandgap inside the nanocomposite.

RESONANT RAMAN SCATTERING



The change in line shape, intensity and peaks with decrease in number of layers/suggest strong electron-phonon coupling. Rahneshin et al., Scientific Reports 6: 34831, 2016

CHROMATIC ENERGY CONVERSION



Power transmitted through the sample and the corresponding photomechanical actuation of nanocomposites at different wavelength of light respectively: (a-b) bulk consisting of 100-500 layers; (c-d) intermediate consisting of 10-30 layers and (e-f) few layers consisting of 1-6 layers. The samples were all 0.1 wt. % nanocomposites using LBL process. No pre-strains were applied for these experiments.

CHROMATIC MECHANICAL RESPONSE



(a) Magnitude of exerted stress as a function of pre-strains for different layered nanocomposites at 405 nm excitation; (b) Magnitude of exerted stress as a function of pre-strains at different wavelengths for the few-layer nanocomposite; insert is the actual temperature in the sample measured using thermocouples placed equidistant from center of the nanocomposite to the clamps; (c) Shift in the Raman vibrational modes $E_{2a} \sim 1.7$ for strain of 10% for the few-layer nanocomposite; (d) Strain enhanced optical power absorption in fewnanocomposite.



FORCE, EFFICIENCY AND LONG TERM RESPONSE

(a) Force versus time at different laser power; (b) Efficiency versus incident photon energy; (c) Long term response of the 2H-MoS₂ few layer actuators operated over ~6 hours (~150 cycles) at 640 nm wavelength suggesting excellent stability.

High efficiency among photo-mobile polymer networks. Twice greater than graphene and 1000 times greater than PVDF.

UNIQUE MECHANISM

- In MoS₂, Ab initio calculations have suggested strong peaks in the visible region suggesting van Hove singularities in JDOS.
- van Hove singularities peaks increase with decrease in number of layers suggesting strong light absorption.
- The valence band consists of 4d orbitals that are responsible for chromatic absorption, sending electrons from the ground state to the excited state in the conduction band depending on the energy of irradiated light.
- The strong covalent bonds (σ bonds) of the chalcogen atom couples this absorbed light due to the superposition of the 4d orbitals of Mo and 3p orbitals of S in the conduction band into an extraordinary thermal effect thus giving rise to this chromatic photomechanical effect.
- This is a unique mechanism not available to sp bonded materials such as carbon nanotubes and graphene, as well as plasmonic metallic gold nanoparticles.

CONCLUSION

- 2D Layered materials are rich areas to explore for energy conversion (photovoltaics, photo-thermal, solar-thermal, photo-mechanics etc)
- The chromatic mechanical response is a new discovery in TMD based nanocomposites not available in graphene and nanotubes.
- Potential applications include micro-optomechanical and nanopositioning systems with chromatic mechanical response.
- The photo-thermal mechanism is unique due to the overlap of the d and p orbitals. d-electron physics in action!

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