



Sandia  
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Laboratories

# Technoscience Search: Opportunities & Challenges for Human & Artificial Intelligences

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## Outline

- The Technoscientific Method
- Engineering Search: Design vs Invention
- Science Search: Hypothesis vs Data Driven

Co-Design for Materials Discovery, Reliability, and Extreme Environments  
November 15-17, 2022

THE GENESIS OF  
TECHNOSCIENTIFIC  
REVOLUTIONS

RETHINKING THE NATURE AND  
NURTURE OF RESEARCH

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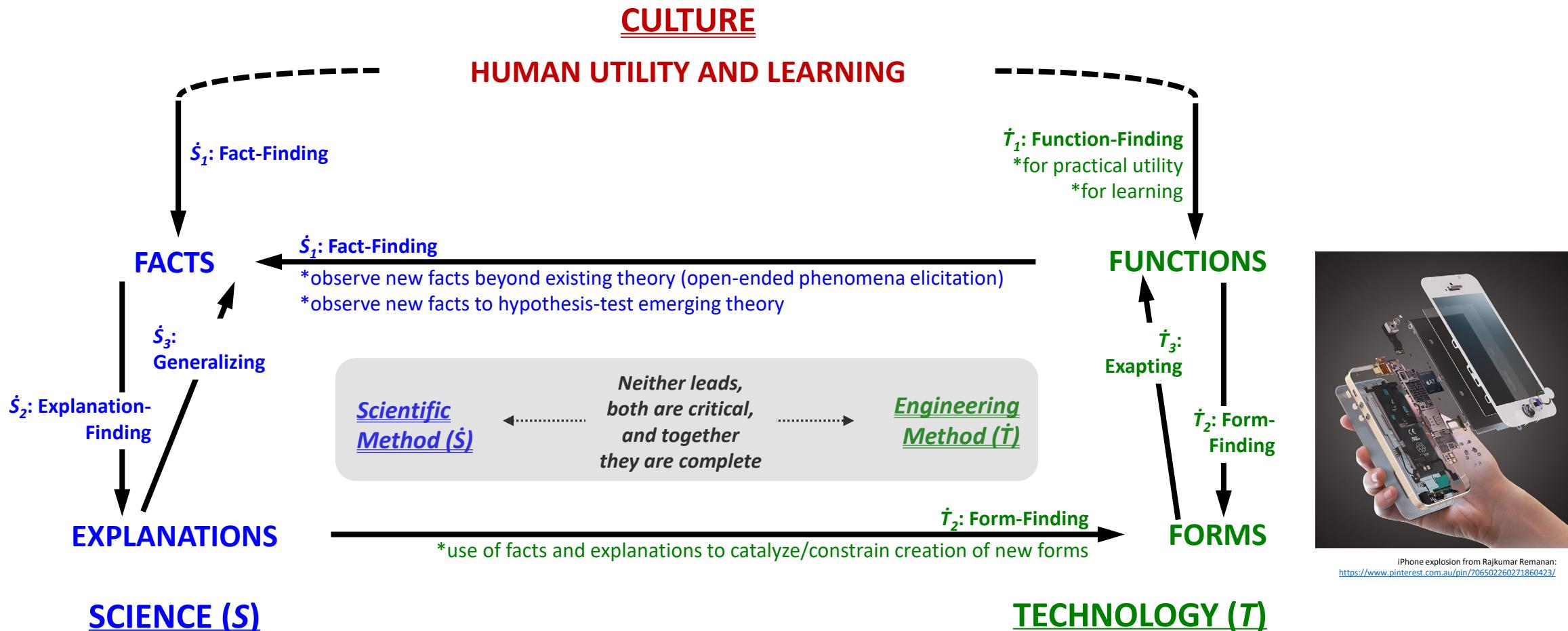


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Case Study of InGaN



# The Technoscientific Method (as practiced by humans)



iPhone explosion from Rajkumar Remanan:  
<https://www.pinterest.com.au/pin/706502260271860423/>

## SCIENCE (S)

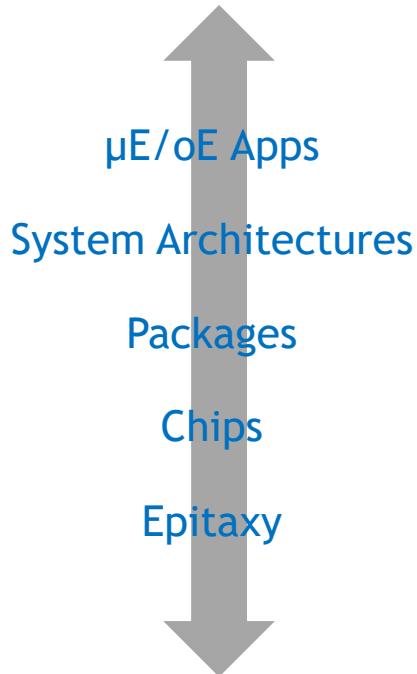
## TECHNOLOGY (T)

### Nuances

- The S&T repositories of knowledge are organized as loosely modular hierarchies of questions and answers
- Particular results of every mechanism of the technoscientific method will have various degrees of “surprise”

# Engineering Search: The Modular/Amodular and The Exploitative/Exploratory

## III-V Materials & Applications Value Chain “Stack”



	EXPLOIT THE KNOWN	EXPLORE THE UNKNOWN
AMODULAR CO-SEARCH	<p><b>Co-Design</b> 1990s: Distributed Feedback (DFB) Lasers</p>	<p><b>Co-Invention</b> 2000s: InGaN Blue LEDs</p>
MODULAR SEARCH	<p><b>Design</b> 1980s: Vertical-cavity surface-emitting lasers (VCSELs)</p>	<p><b>Invention</b> 1970s: Molecular Beam Epitaxy (MBE)</p>
	<ul style="list-style-type: none"> <li>Enabled by “technology headroom”</li> <li>Enhanced by science</li> </ul>	<ul style="list-style-type: none"> <li>Catalyzed by “reverse salients”</li> <li>Enhanced by contrariness</li> </ul>

# Engineering Invention: The Key Role of Surprise and Informed Contrariness

## Visible Light Emitters Search Space

Common Scientific Wisdom Says II-VIs are Possible  
(false positive)

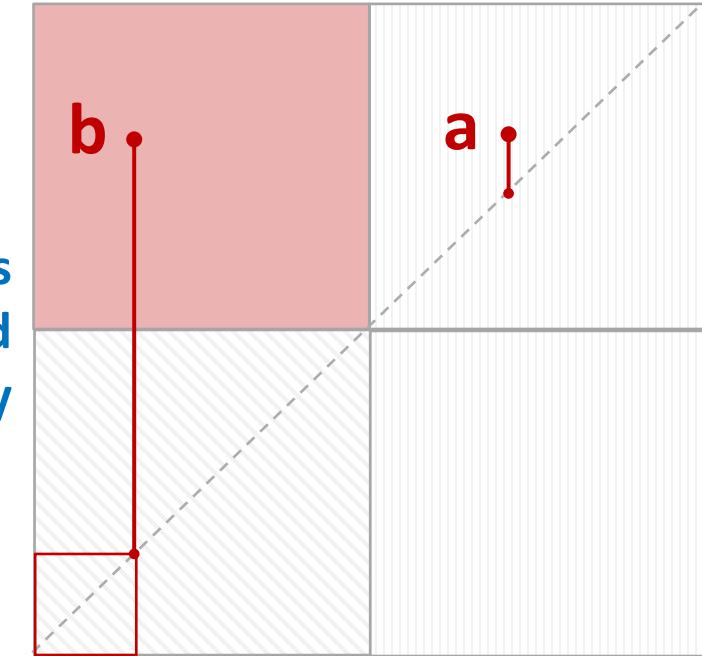
Conventional Scientific Wisdom Says III-Vs are  
Impossible (false negative)

1 Seeming  
impossibility of  
high quality GaN  
epitaxial films

2 Seeming  
impossibility of p-  
type doping of GaN

## Informed Contrariness

Researcher's  
Informed  
Utility



Common Wisdom Utility

# Science Search: Fact & Explanation Elicitation & Finding

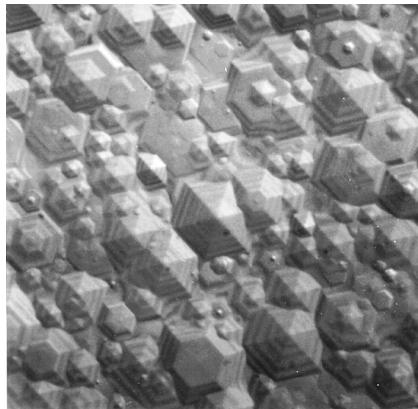


## Akasaki & Amano:

Complex sequence of growth/annealing/growth of AlN/sapphire reduces roughness and defect density

## Nakamura:

Ditto for GaN/sapphire



*GaN/sapphire  
before Akasaki,  
Amano, Nakamura*



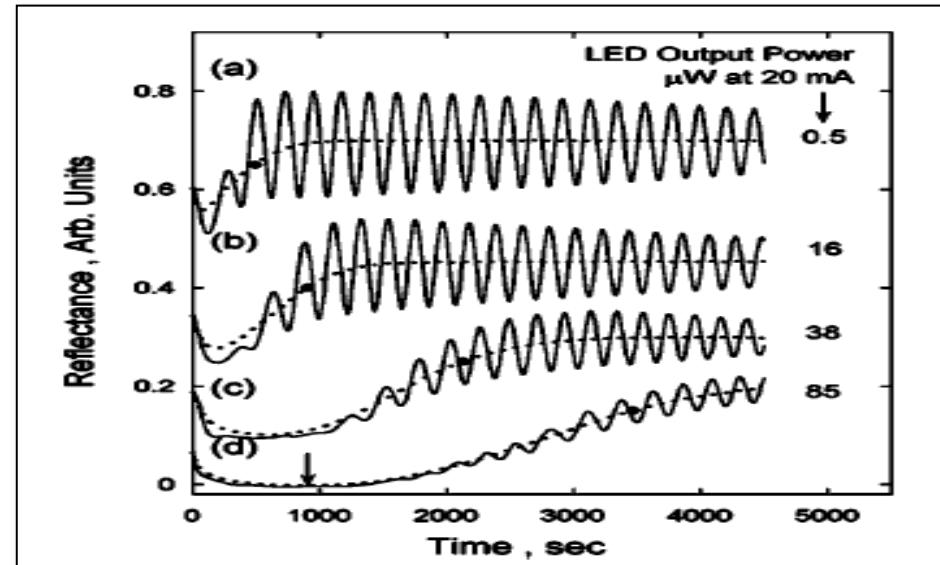
*GaN/sapphire after  
Akasaki, Amano,  
Nakamura*

## Han & Breiland:

Used *in situ* reflectance to show that severe roughness *must* precede smoothness

## Koleske, Coltrin & Mitchell:

Imagined that grain ripening enables sparse nucleation followed by epitaxial lateral overgrowth



*0 Scientific fact based on an engineered form that fulfills a function*

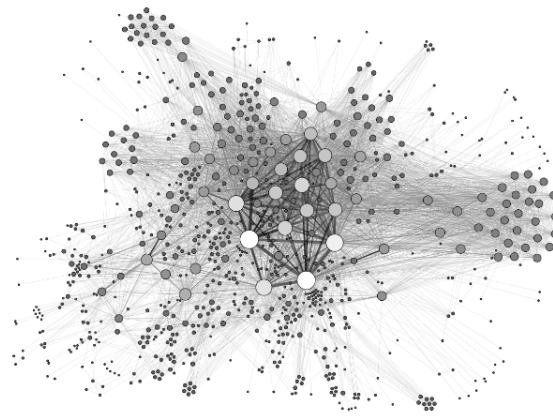
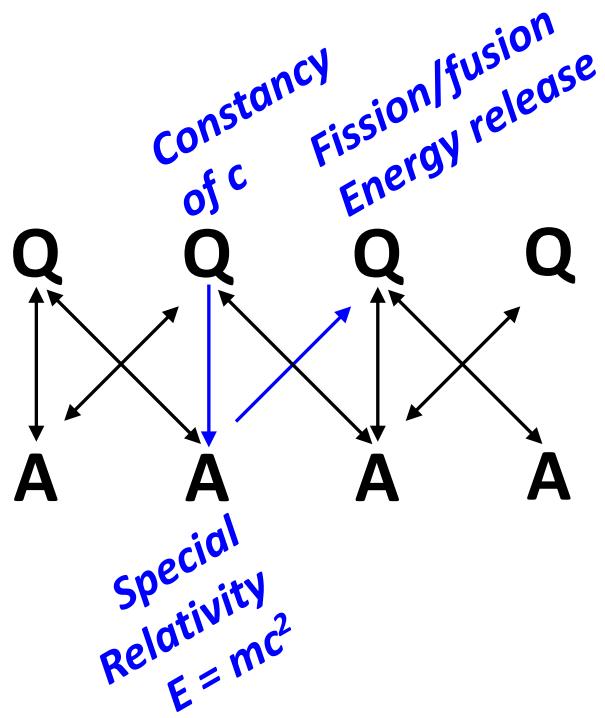
*1 Imagined overarching explanation (hypothesis)*

*2 Auxiliary measurements to stimulate (not test) more detailed explanations (hypotheses)*

*3 Detailed explanations (hypotheses) and verifications*

# Science Discovery: The Key Role of Analogy-Making and Generalizability

## Science



Phil Anderson's  
“Seamless Web of Knowledge”

PW Anderson, “Science: A ‘Dappled World’ or a ‘Seamless Web’?” *Stud. Hist. Phil. Mod. Phys.* 32, 487-494 (2001).

## Technology

