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UNITED NATIONS EDUCATIONAL, SCIENTIFIC AND CULTURAL ORGANIZATION
INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS
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SMR/872- 7

WORKSHOP ON MATERIALS SCIENCE AND
PHYSICS OF NON-CONVENTIONAL ENERGY SOURCES
18 September - 6 October 1995

"Current Status of R&D Photovoltaics & Related Technologies at NREL"

S. K. DEB
NREL
Golden, Colorado
USA

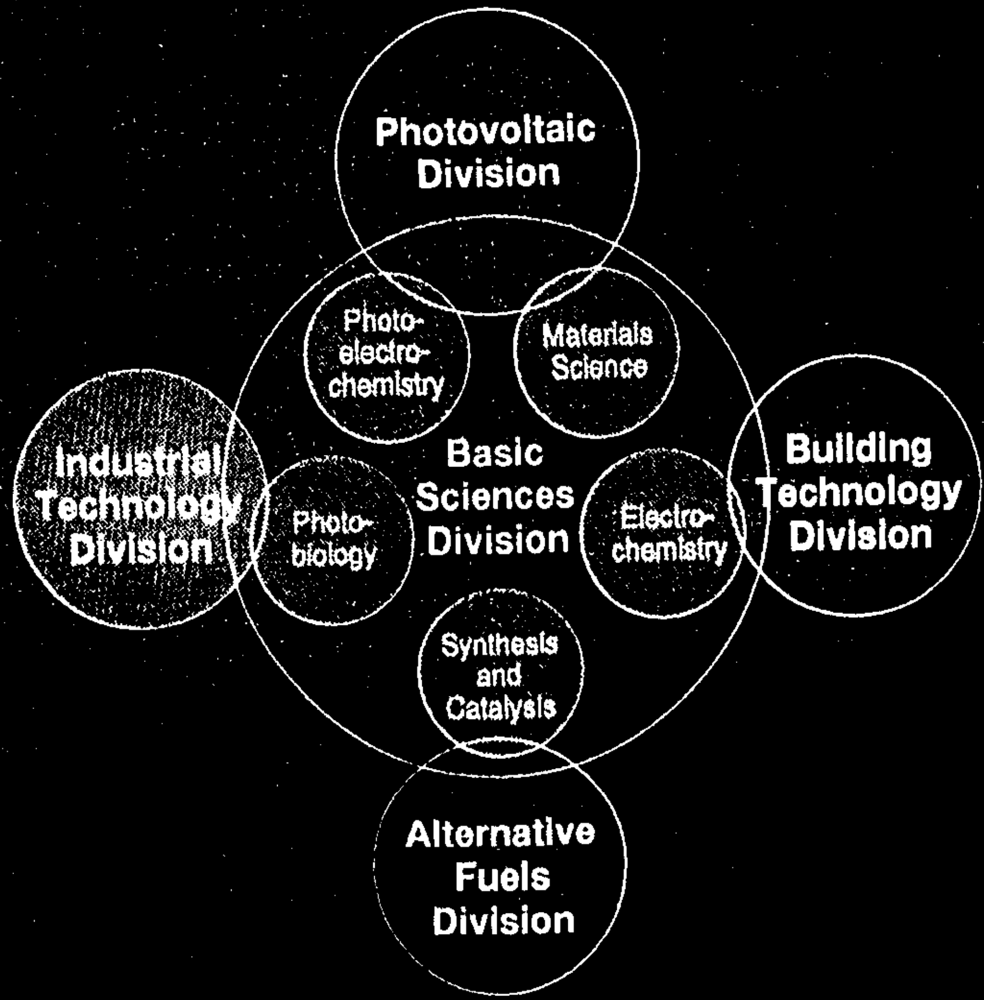
Please note: These are preliminary notes intended for internal distribution only.

Current Status of R&D in Photovoltaics and Related Technologies at NREL

Satyen K. Deb
National Renewable Energy Laboratory
Golden, Colorado, USA

September, 1995

Basic Sciences Division Interactions



Basic Sciences Division

Basic Disciplines	Functions, Services, and Products
Materials Science Chemistry Solid State Physics Photochemistry/Photophysics Electrical and Electronics Engineering Electrochemistry Microbiology Biochemistry	Research and Technology Development - Amorphous Silicon - Crystalline Silicon - III-V Compounds - Superconductivity - Hydrogen - Photoconversion - Photobiology - Photochemistry - Synthesis and Catalysis - Photoelectrochemistry - Liquid Crystals - Interfacial Photochemistry - CVI - Electrochromics Program Management Project Management Technical Assessments

[illegible] Sciences Division
Satyen Deb
Director

Chemical Sciences Program
A J Nozik
Senior Research Fellow

Senior Administrative Assistant
Melody Albrandt

Materials Science Branch
David Staebler
Manager

Photoconversion Branch
Mike Seibert
Manager

...ience Branch
...Staebler

...Crystalline Materials & Advanced Concepts Proj.s
John Benner

- High Efficiency Photovoltaics
- Crystal Growth
- Material & Device Analysis
- University Programs
- New Ideas/ Advanced Conc.
- Aerospace Programs

...ystal Growth
Ted Ciszek

- Single Crystal Silicon
- Solar Cell Device Fabrication
- Structural, Optical, & Electrical Characterization
- Compound Semiconductor Growth (I-II-V, I-III-VI_2, III-V)
- Growth & Characterization of Crystalline Silicon Thin Films
- Hydrogen

Amorphous Silicon
Richard Crandall

- Novel Deposition Methods
- Microstructural & Film Properties
- Improved Deposition/ Characterization
- Light Induced Degradation Effects
- Alloy Materials (a-SiC:H, a-SiGe:H)
- Device Fabrication & Modeling
- Joint PV & Electrochromics Project

III-V Materials and Devices
Jerry Olson

- OMCVD Growth of III-V Materials and Solar Cell Devices
- Order-Disorder Phenomenon in III-V Semiconductors
- Structural, Optical, & Electrical Characterization
- High Efficiency Cascade Cells ($GaInP_2$/GaAs)

Solid State Theory
Alex Zunger

- Alloy Phase Diagram & Thermodynamics
- Stability of Ultrathin Superlattice
- Charge Density Maps for III-V Materials
- Direct Gap Superlattice from Indirect Gap Material
- Band Structure & Charge Density Maps of Semiconductors
- Coherent Epitaxial Effect

...State ...troscopy
...ngelo Mascarenhas

- Laser Raman Spectroscopy
- Luminescence Spectroscopy

Crystal Growth Research Group

Materials Science Branch, Basic Sciences Division

NREL

National Renewable Energy Laboratory
Golden, CO 80401 USA

R&D Activities:

- High purity, low-defect silicon crystal growth via float zone (FZ) method
- Study of defect and impurity effects in Si using FZ as an R&D tool
- Thin-layer multicrystalline Si growth on substrates for PV use
- Origination of new methods for Si crystal growth
- Crystal growth of chalcopyrite ($CuInSe_2$-type) materials
- Crystal growth of experimental materials (high-T_c, $CuAlS_2$, WO_3, etc.)
- Crystal analysis (X-ray topography, lifetime, spreading resistance, etc.)
- Silicon PV device fabrication
- Hydrogen storage and generation materials

Si Float Zone (FZ) Crystal Growth

A High Purity R&D Tool:

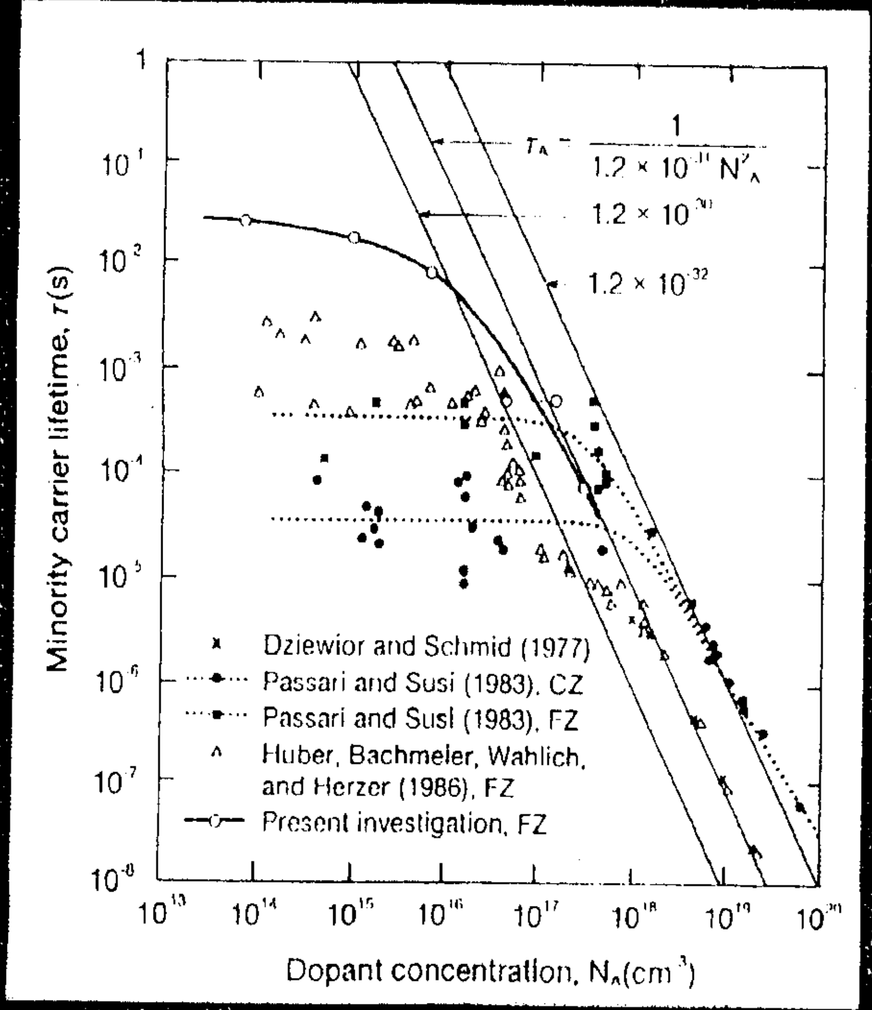
- Liquid Si in contact only with solid Si
- Cold wall environment
- RF generates heat within the Si (no "hot" heaters)

Applications:

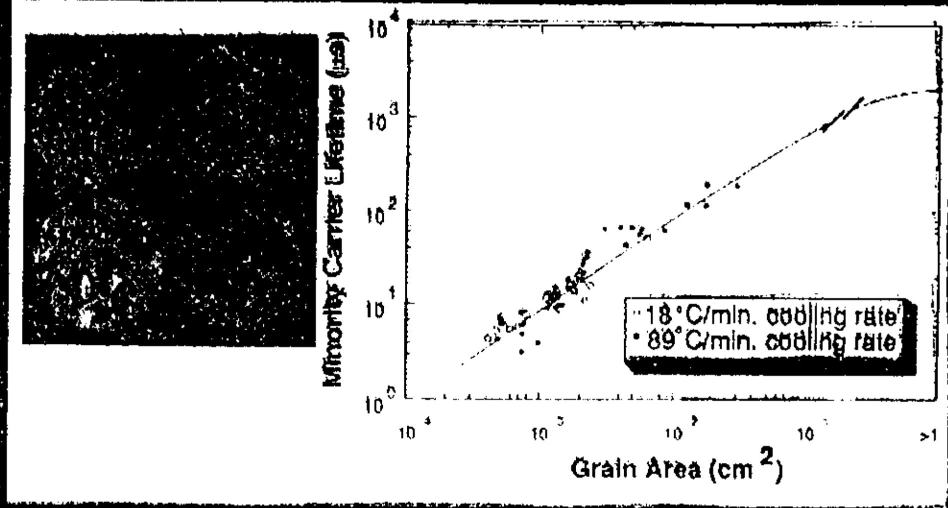
- Dislocation-free Si single crystals with:
  - High purity
  - High minority charge carrier lifetime
  - High resistivity
- Experimental studies with:
  - Defects (Si interstitials, vacancies, grain boundaries, dislocations, etc.)
  - Impurities (O, C, N, metals, dopants)

Examples of FZ Experimental Studies

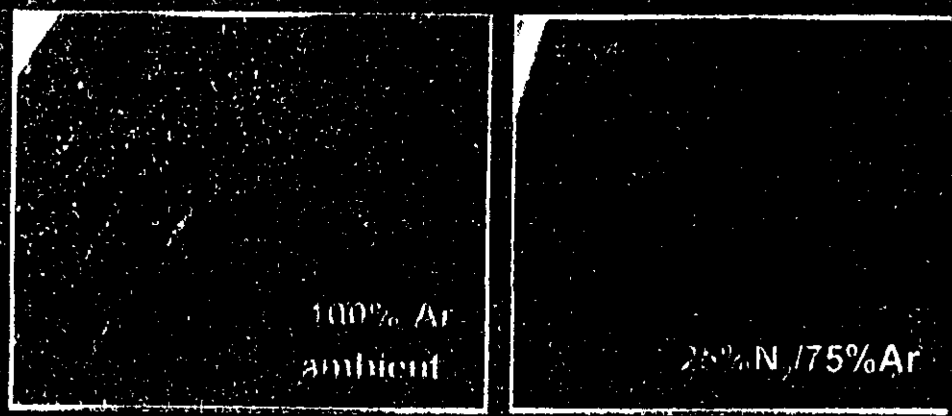
High minority charge carrier lifetime



Grain boundary effects on lifetime

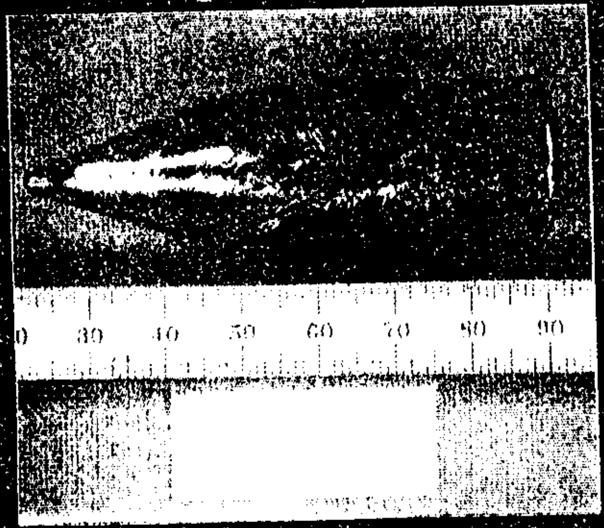


Nitrogen effect on microdefects

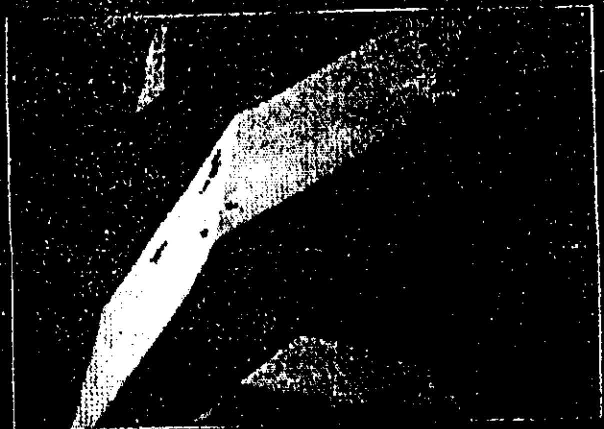


Some Other Crystal Growth Activities

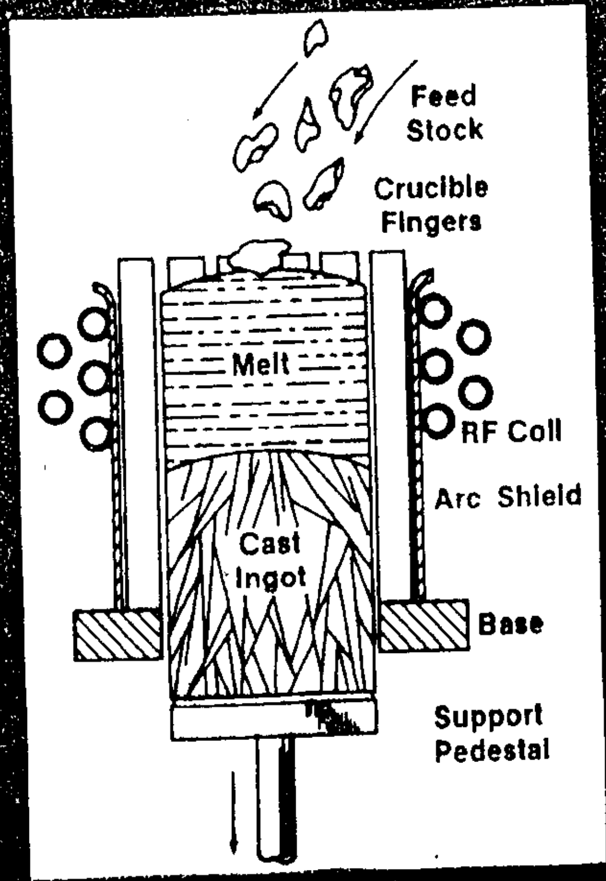
$CuInSe_2$ crystal growth

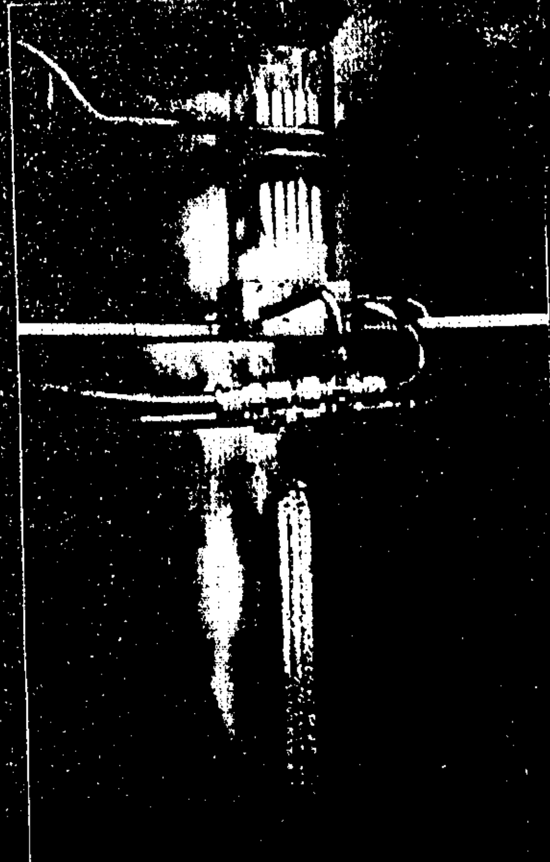


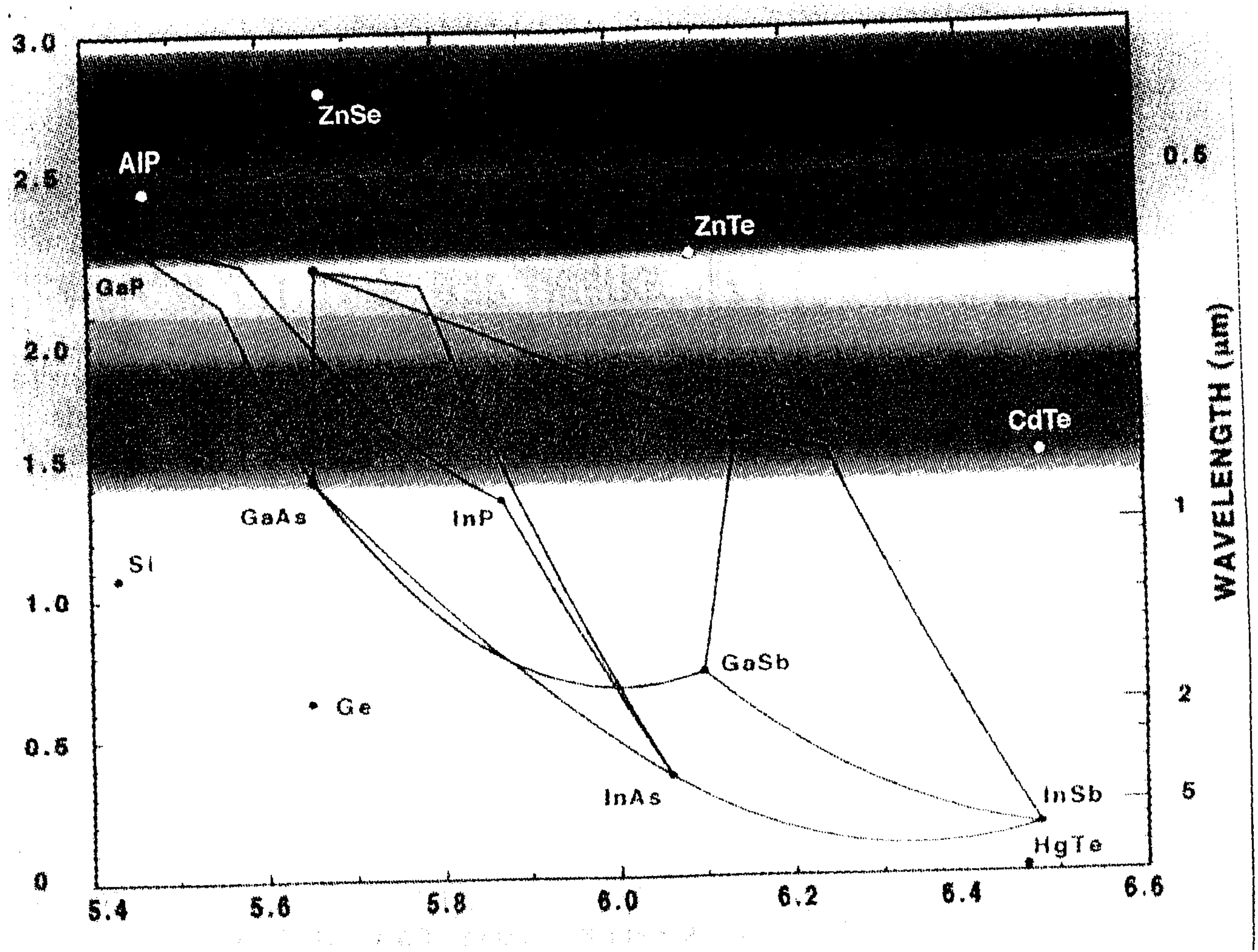
WO_3 crystal growth



Electromagnetic cold-crucible continuous casting



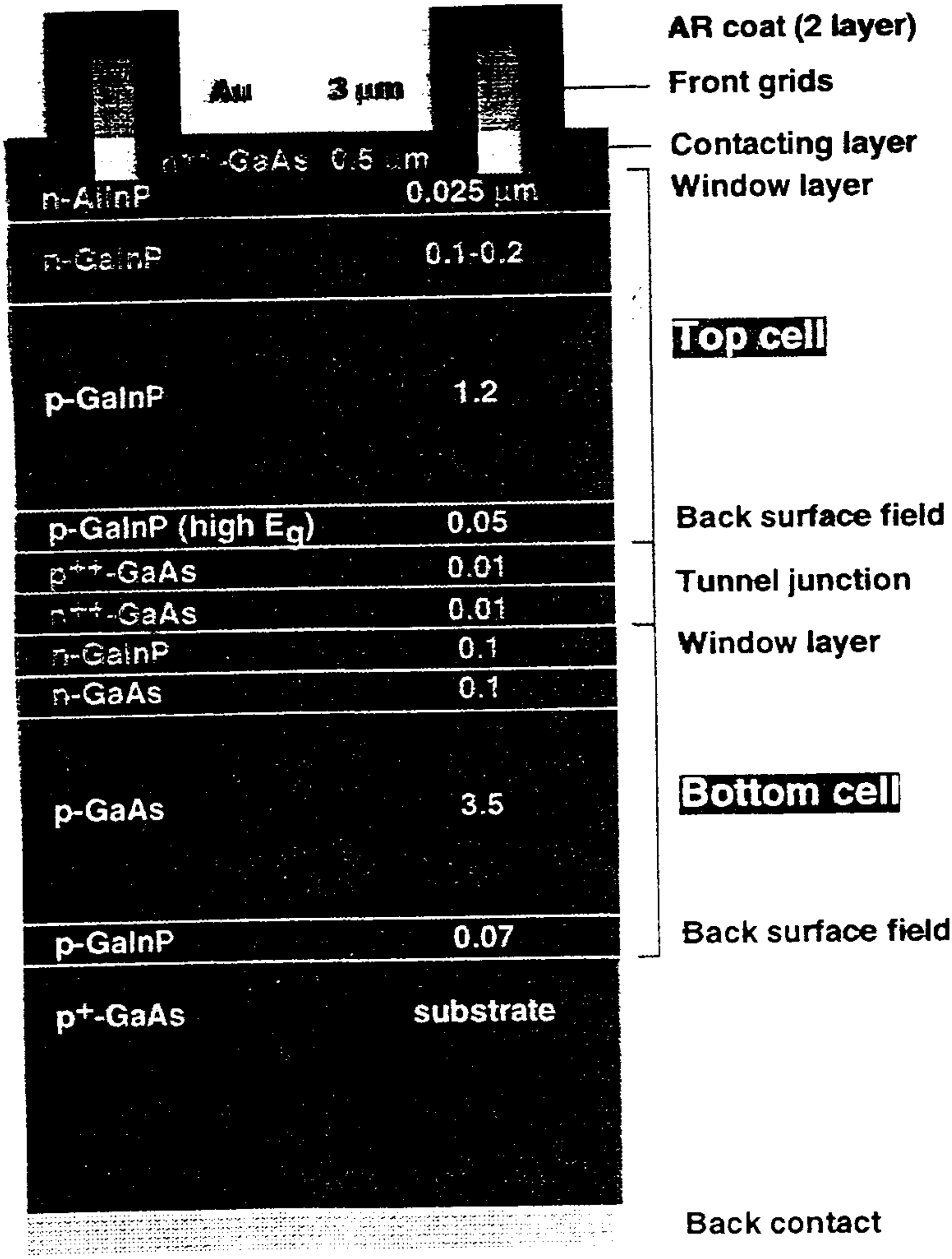




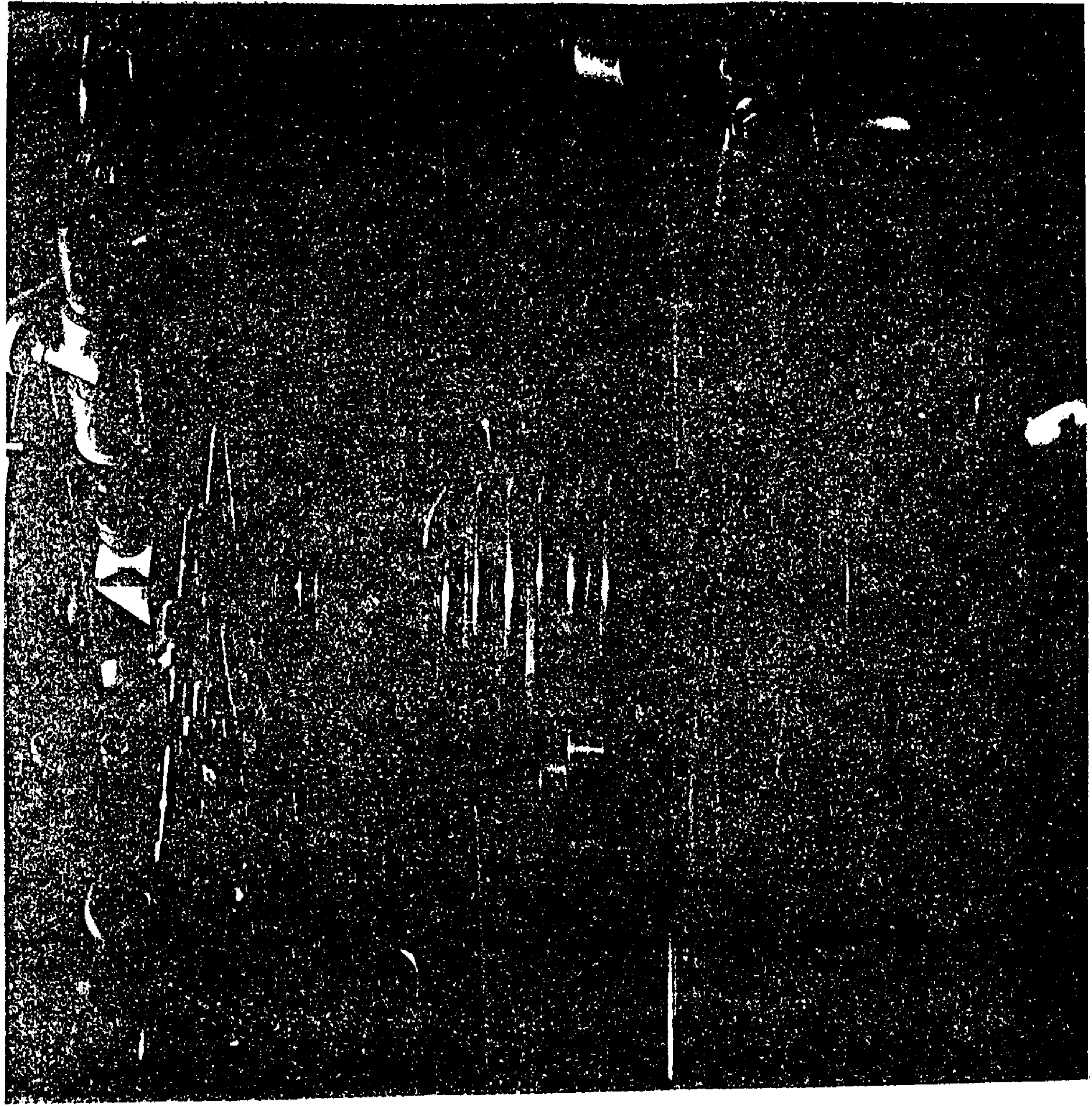
3.0
2.5
2.0
1.5
1.0
0.5
0
5.4
5.6
5.8
6.0
6.2
6.4
6.6
0.6
1
2
5
WAVELENGTH (µm)
ZnSe
AlP
ZnTe
GaP
CdTe
GaAs
InP
Si
GaSb
Ge
InAs
InSb
HgTe

GaInP/GaAs Tandem Cell

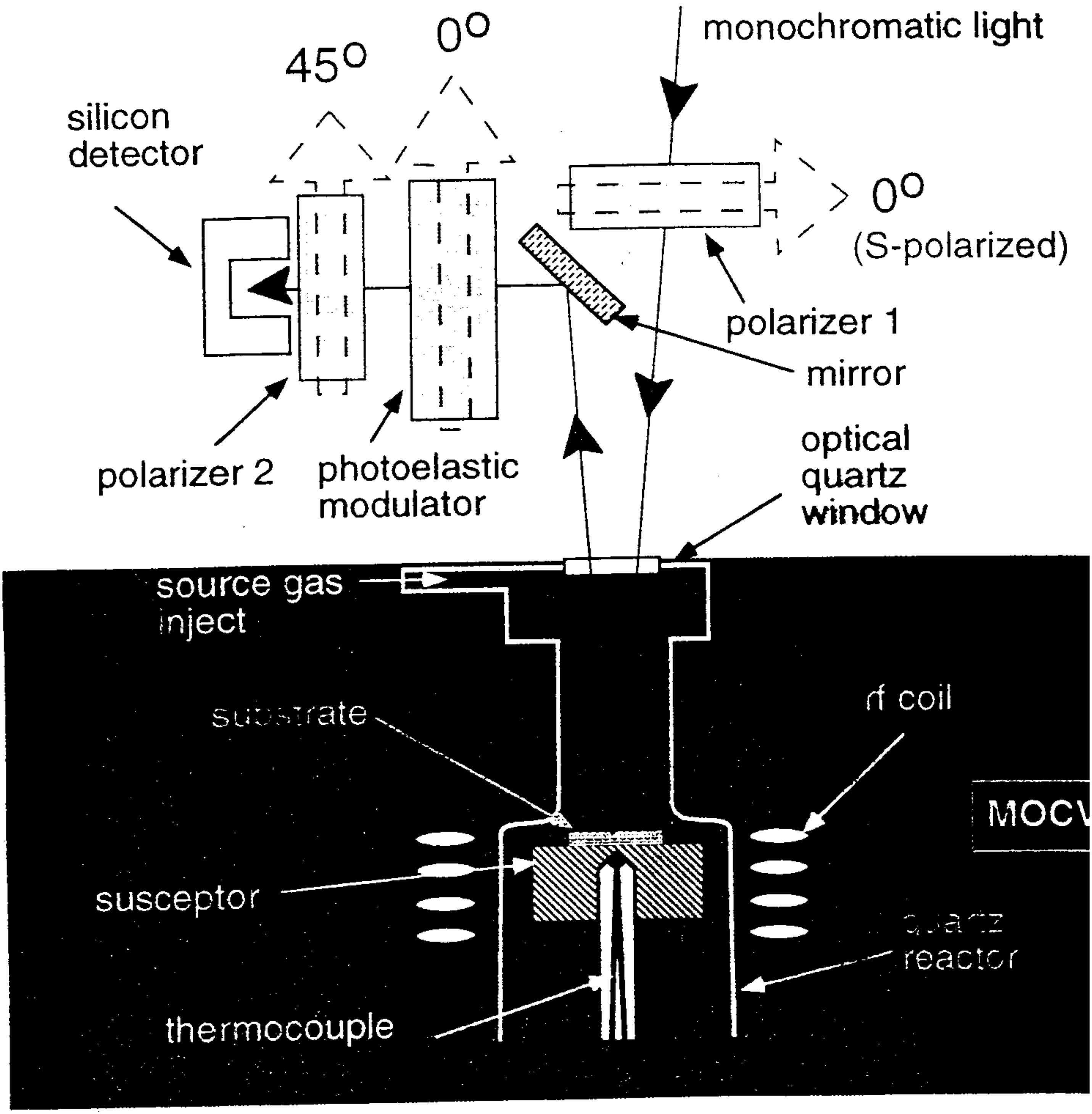
(Adapted for concentrator)



U.S. Department of Energy
Office of Energy Research
Office of Basic Energy Science
Division of Materials Science



In situ REFLECTANCE DIFFERENCE SPECTROSCOPY (RDS)



U.S. Department of Energy
Office of Energy Research
Office of Basic Energy Science
Division of Materials Science

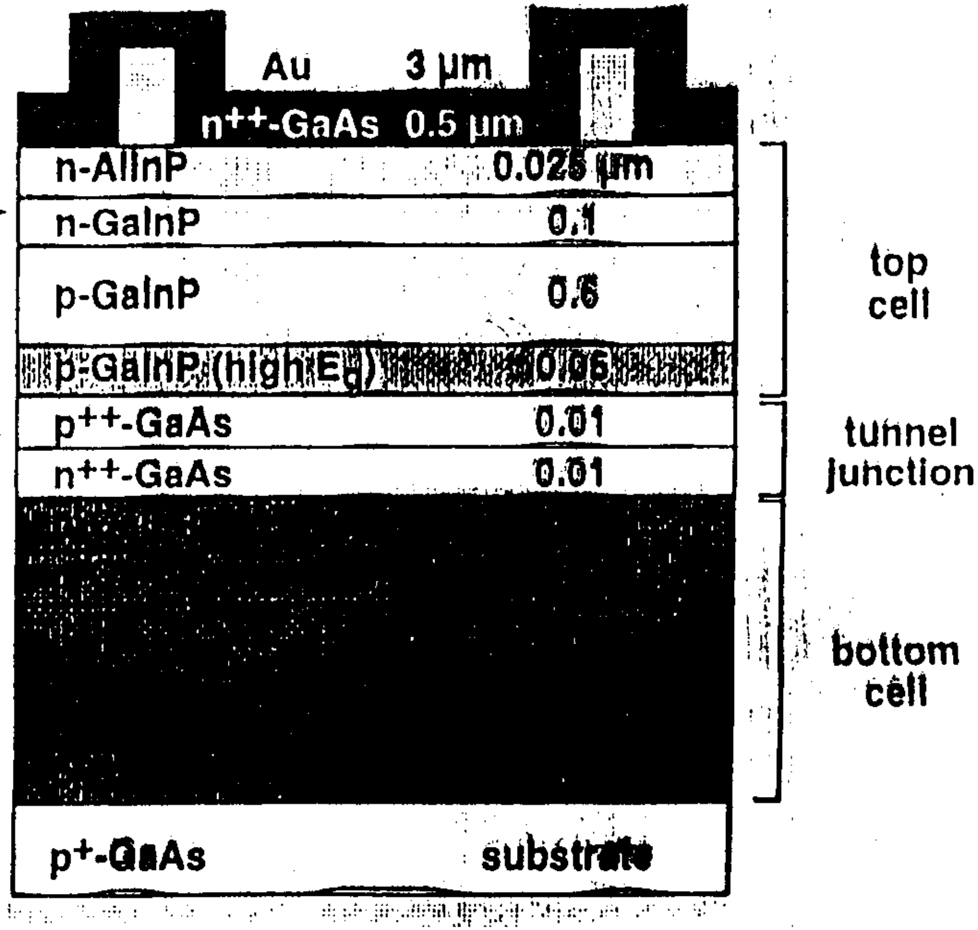
GaInP/GaAs Tandem Cell

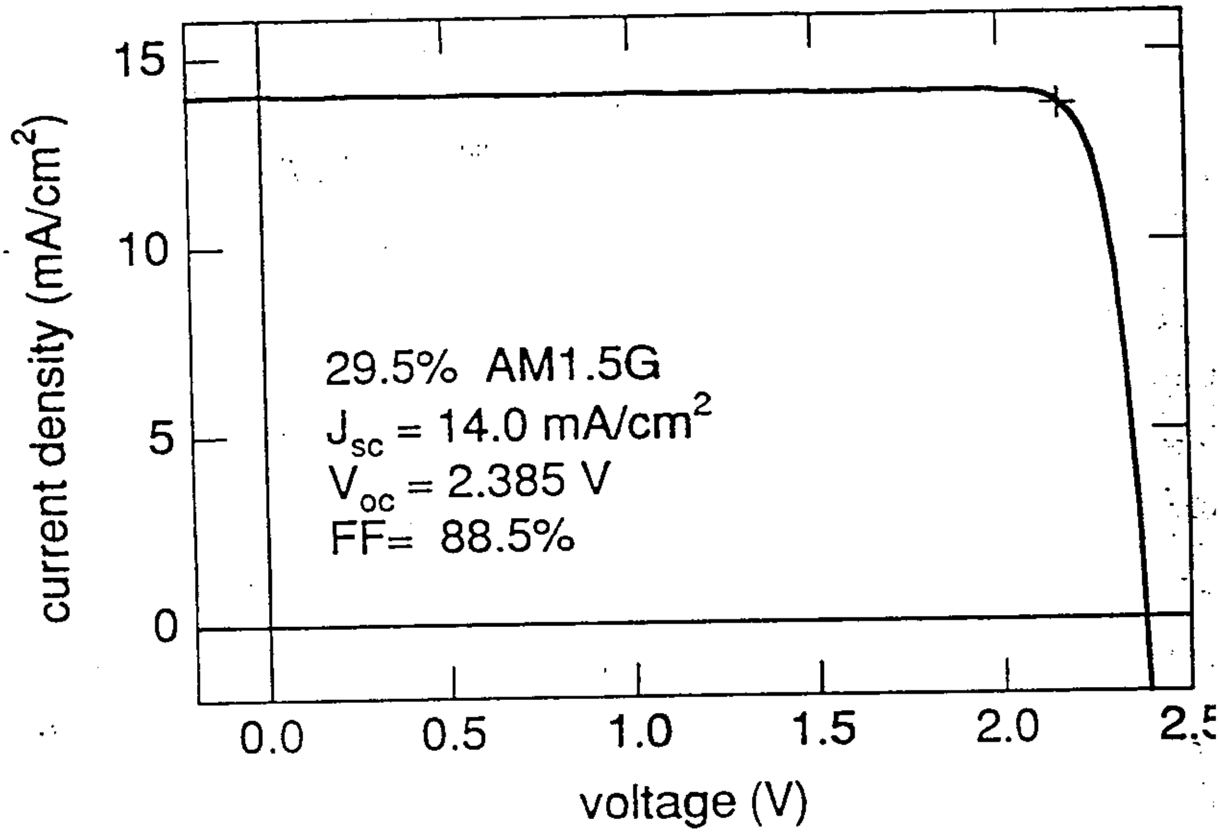
- Several record efficiencies:
  29.5% AM1.5G (flat plate),
  30.2% from 140x to 180x , 29.1% 425x AM1.5D (concentrator),
  25.7% AM0, 19.5% AM0 post-irradiation (space)

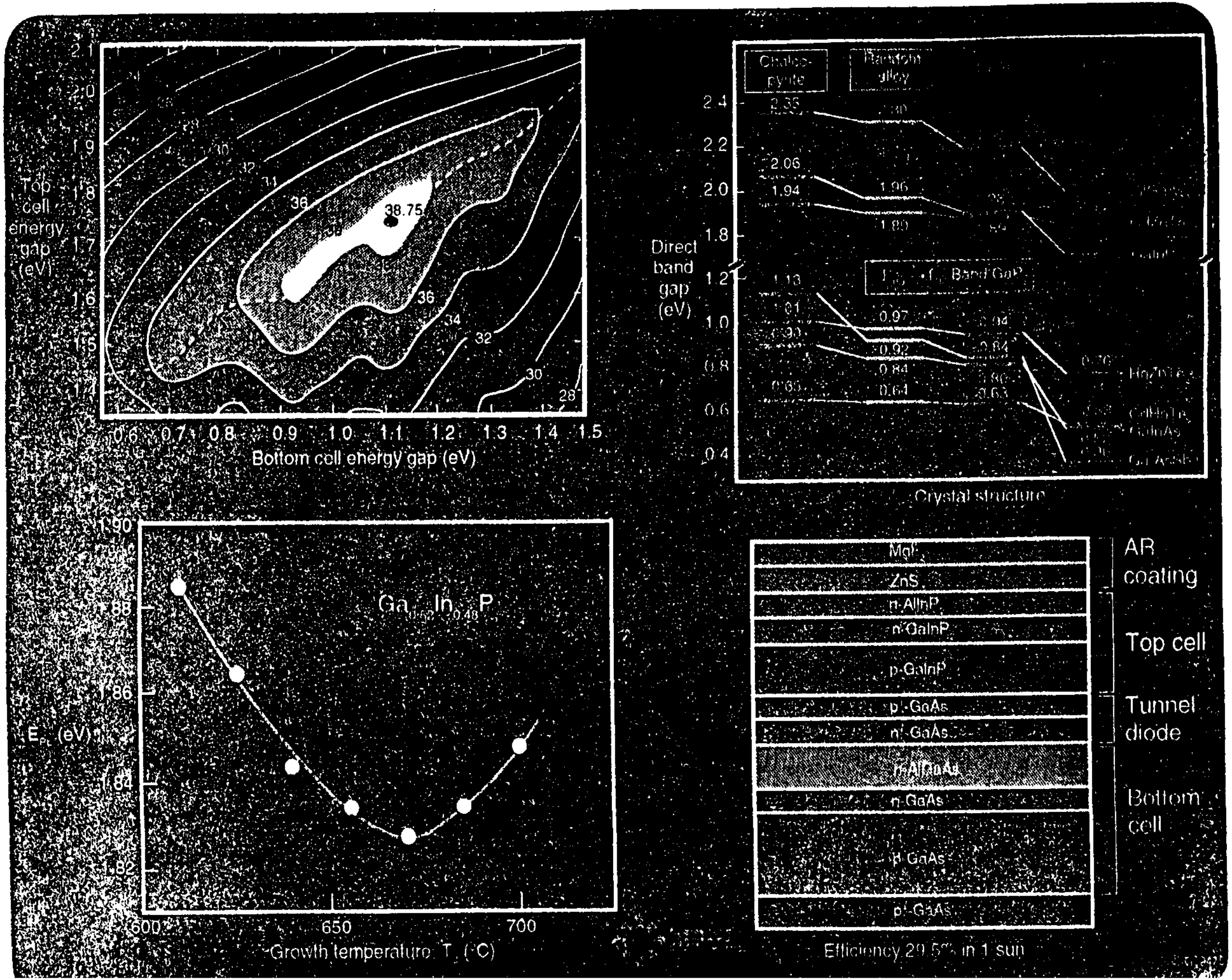
Ordering-induced anisotropy in conductivity important for emitter sheet resistance (concentrators)

Change in degree of ordering used to make passivating layer

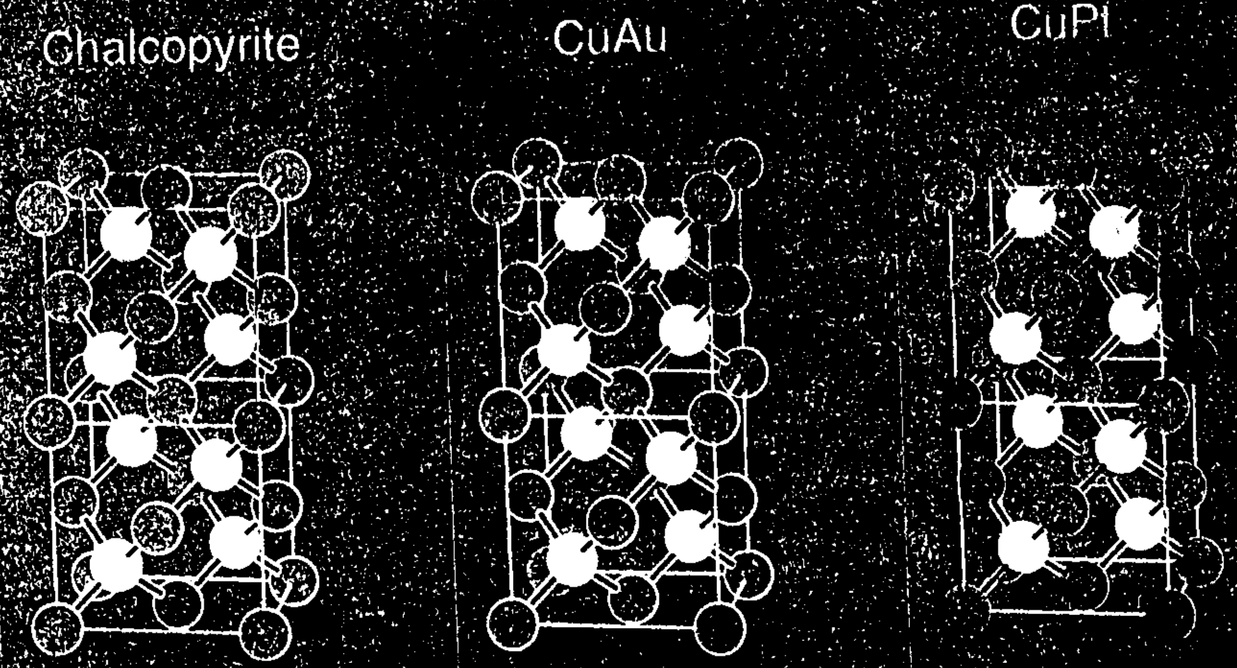
Series connection → maximum efficiency by balancing number of photons absorbed in each cell
→ need to know/control top cell band gap by controlling degree of ordering




current density (mA/cm2)
15
10
5
0
0.0
0.5
1.0
1.5
2.0
voltage (V)
29.5% AM1.5G
Jsc = 14.0 mA/cm2
Voc = 2.385 V
FF= 88.5%

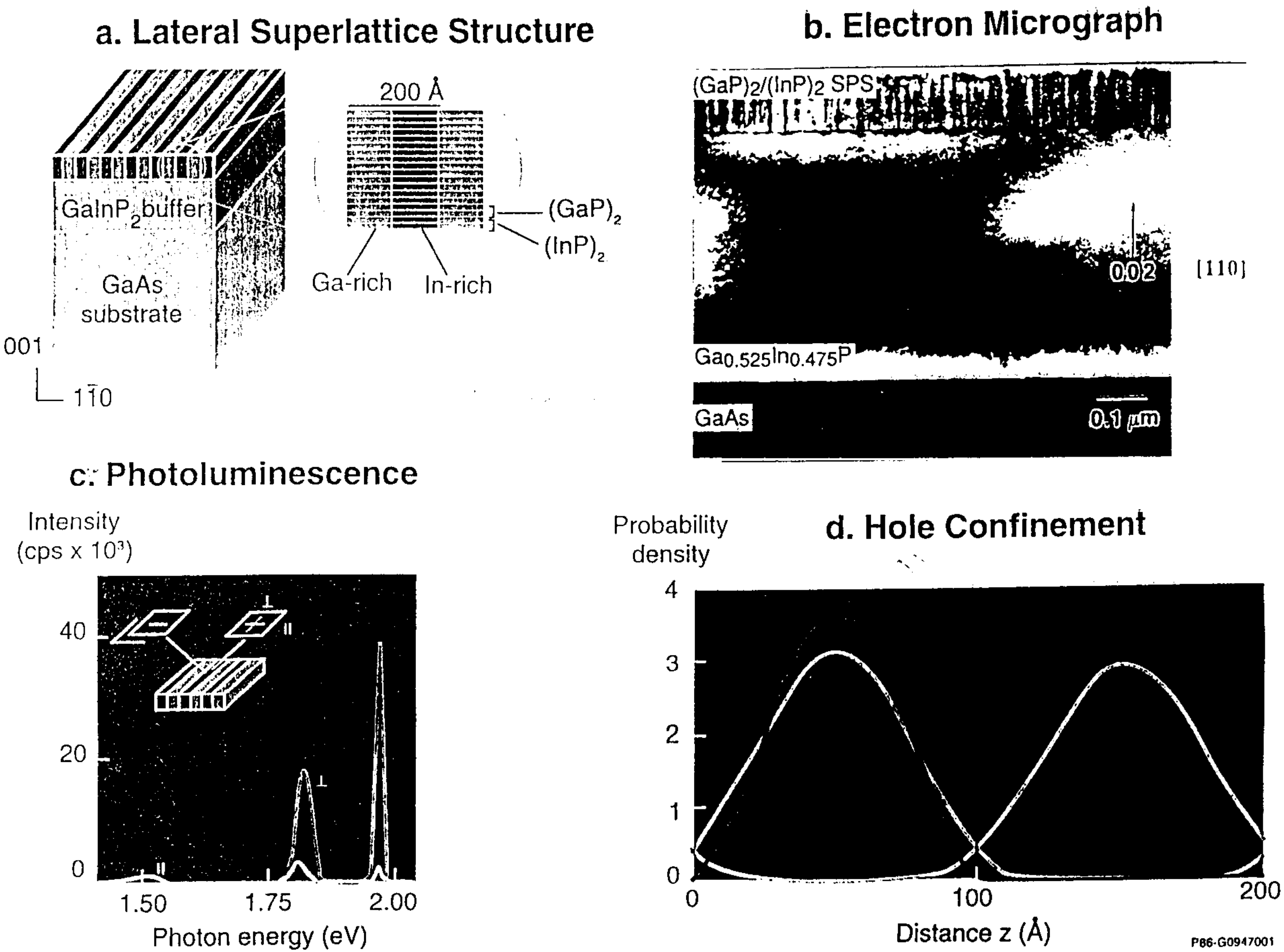

Top cell energy gap (eV)
Bottom cell energy gap (eV)
38.75
Chalco-pyrite
Direct band gap (eV)
Crystal structure
Ga0.52In0.48P
Growth temperature
MgF
ZnS
n-AlInP
n-GaInP
p-GaInP
p-GaAs
n-GaAs
p-GaAs
p-GaAs
AR coating
Top cell
Tunnel diode
Bottom cell
Efficiency 29.5% in 1 sun

Semiconductor Alloy Structures



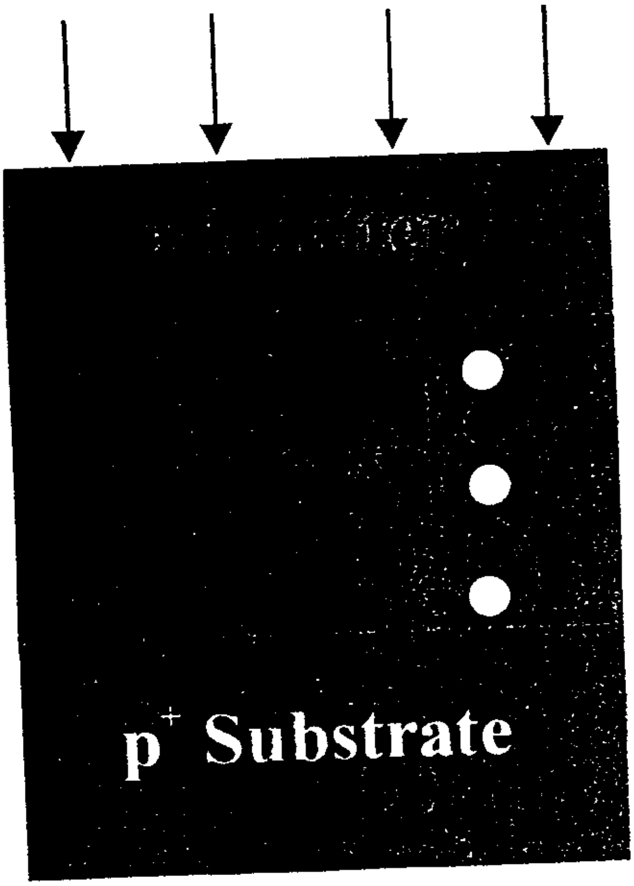
Solid State Theory

- Alloy phase stability (metals and semiconductors)
  - alloy phase diagrams
  - short-range order
- Electronic properties of III-V and II-VI alloys
  - vs. constituents and composition
  - effects of long and short range order
- Electronic properties of semiconductor superlattices
  - properties of 1-D random superlattices
  - effects of interface non-abruptness
- Electronic properties of quantum dots, wires, and films
  - III-V and II-VI materials
  - free-standing and embedded
- Semiconductor surfaces
  - structural and electronic properties of ideal surfaces, steps, and defects
  - surface-induced ordering of alloys
  - surface segregation in alloys
- Methods for electronic structure modelling of large, mesoscopic size systems
  - semiempirical pseudopotentials
  - k-dot-p like methods (first-principles based and empirical)


a. Lateral Superlattice Structure
200 Å
GaInP2 buffer
GaAs substrate
001
1$\bar{1}$0
Ga-rich
In-rich
(GaP)2
(InP)2
b. Electron Micrograph
(GaP)2/(InP)2 SPS
0.02
[110]
Ga0.525In0.475P
GaAs
0.1 µm
c. Photoluminescence
Intensity (cps x 10³)
40
20
0
1.50
1.75
2.00
Photon energy (eV)
d. Hole Confinement
Probability density
4
3
2
1
0
0
100
200
Distance z (Å)
P86-G0947001

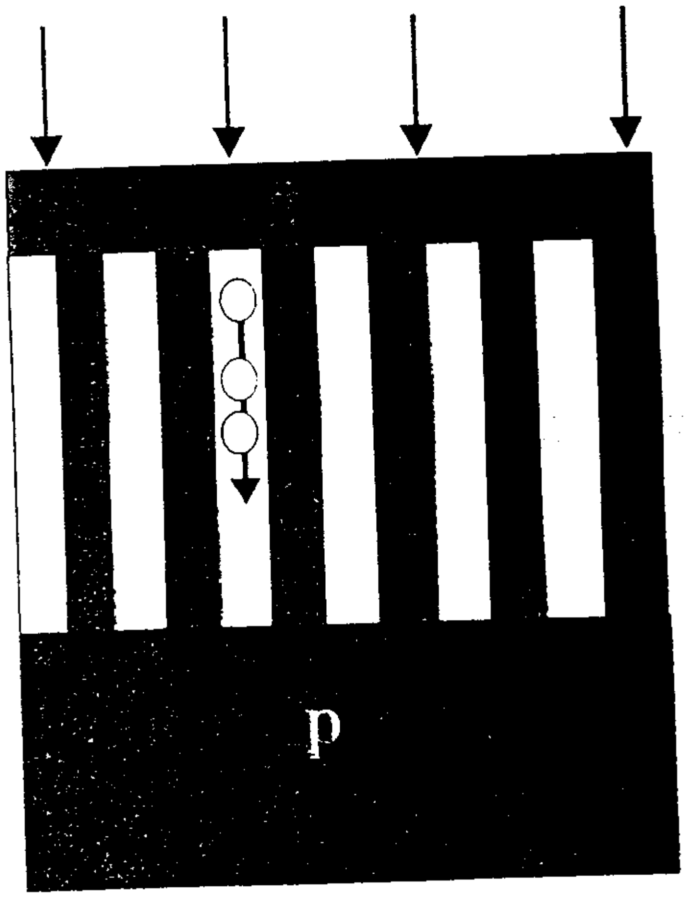
Solar Cells with Enhanced Minority Carrier Lifetime

Conventional Cell



electrons and holes often recombine before being collected

Lateral SL Cell



spatial separation of the carriers enhances the minority carrier lifetime

[illegible]ersion Branch

[illegible] Seibert

Photobiology
Mike Seibert, P.I.
Paul Weaver, P.I.

- Photosynthetic water splitting function
- Reaction center structure & function
- Membrane surface topology
- Photobiological H_2 production
- Bioremediation
- Biological conversion of gasified biomass to thermoplastics

Synthesis and Catalysis
Dan DuBois, P.I.
Calvin Curtis, P.I.

- Catalyst synthesis & charcterization
- Electrochemcial CO_2 concentration
- Homogeneous & electrocatalysis
- CO_2 & CO reduction chemistry
- Semiconductor precursors

Interfacial Photochemistry
Arthur Frank, P.I.

- Semiconductor & catalyst materials research
- Polymer-modified, colloidal, & particulate semiconductors
- Modified semiconductor electrodes

Molecular Semiconductors
Brian Gregg, P.I.

- Molecular semiconductor processes
- Liquid crystal PV

Photoelectrochemistry
John Turner, P.I.

- Novel PEC structures
- Surface Passivation
- Water-splitting catalysts
- Modeling chemical dynamics and semiconductor carrier kinetics

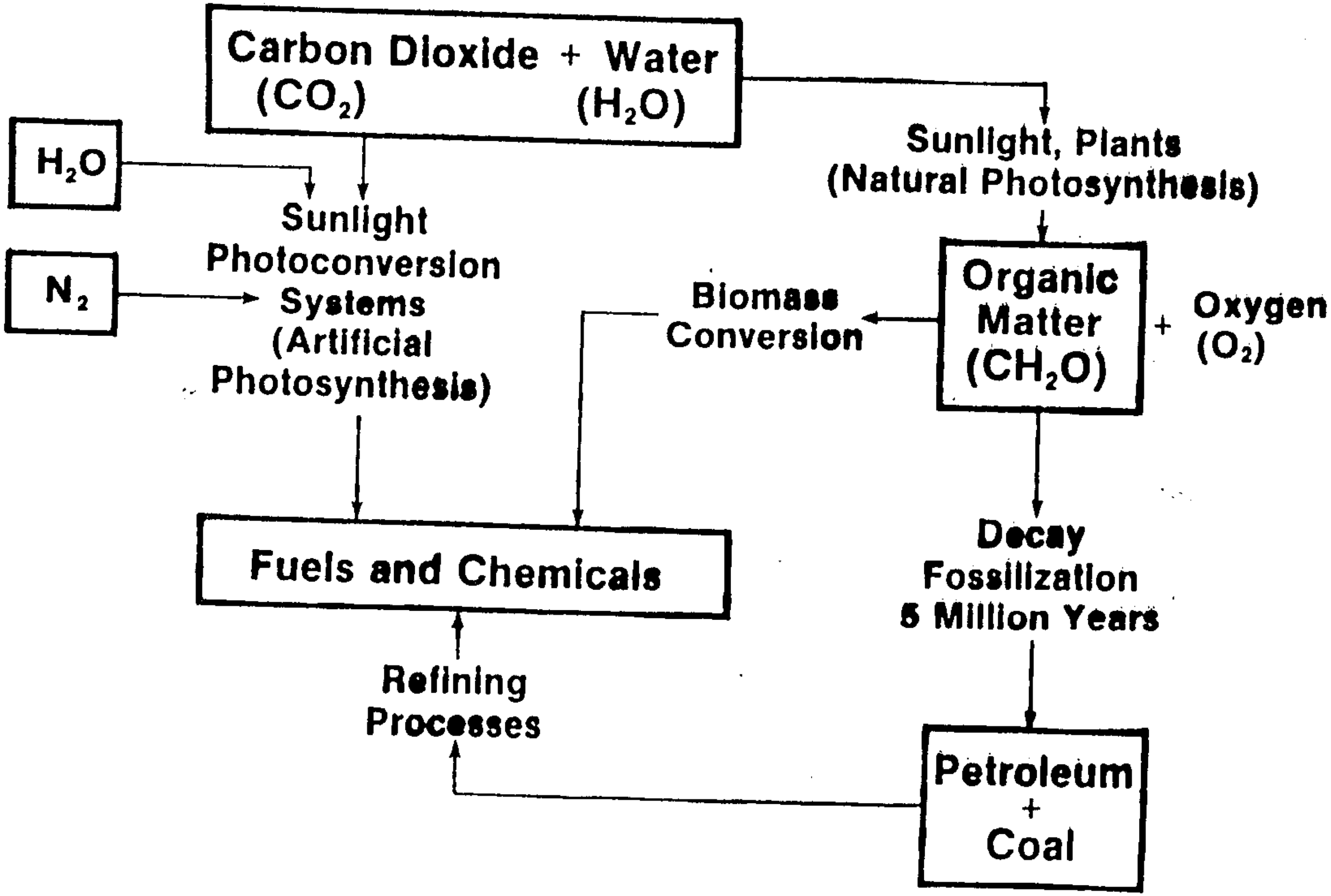
[illegible]

[illegible], P.I.

- Electrochromic-solar controlled windows
- Lithium, rechargeable batteries
- Vacuum insulated auto batteries & catalytic converters

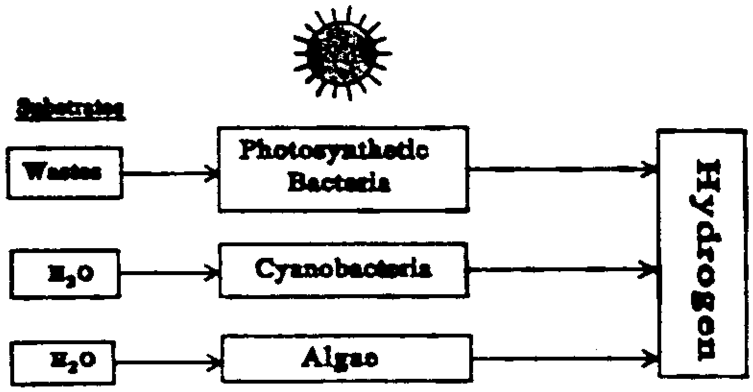
PHOTOCONVERSION

Research in this area encompasses all quantum-conversion processes, other than photovoltaics, that lead to the direct production of useful fuels or chemicals.



Carbon Dioxide + Water
(CO_2) (H_2O)
H_2O
N_2
Sunlight
Photoconversion
Systems
(Artificial
Photosynthesis)
Sunlight, Plants
(Natural Photosynthesis)
Organic
Matter
(CH_2O)
+ Oxygen
(O_2)
Biomass
Conversion
Fuels and Chemicals
Decay
Fossilization
5 Million Years
Refining
Processes
Petroleum
+
Coal

Photobiological Hydrogen Production



- Background:

  - Photosynthetic bacteria are the most studied, however they do not split water.

  - Cyanobacteria and algae split water with alternating dark light cycles, O_2 while illuminated, H_2 in the dark.

  - However, the H_2 evolving systems in cyanobacteria and algae are deactivated by O_2 and N_2.

  - Some strains of photosynthetic bacteria have been found with O_2 tolerant H_2 evolving systems.

- Approach:

  - Move the genetic coding for the O_2 tolerant H_2 evolving system from photosynthetic bacteria to algae.

GOALS

Longer Term: To develop new science in photoconversion-related areas to the point that new generations of solar and renewable energy technologies can be considered for ultimate use by the Nation.

Nearer Term: To demonstrate technical and economic feasibility of photoconversion-related processes and devices that could have short-term impact in aiding U.S. industry and national competitiveness.

[illegible] Program

- Administrative Support
  (K. Kimbro)

Hot Carrier Solar Cells

- Solar Cell Device Fabrication
  (M. Hanna)
- Structural, Optical, & Electrical Characterization
  (Z. Lu)

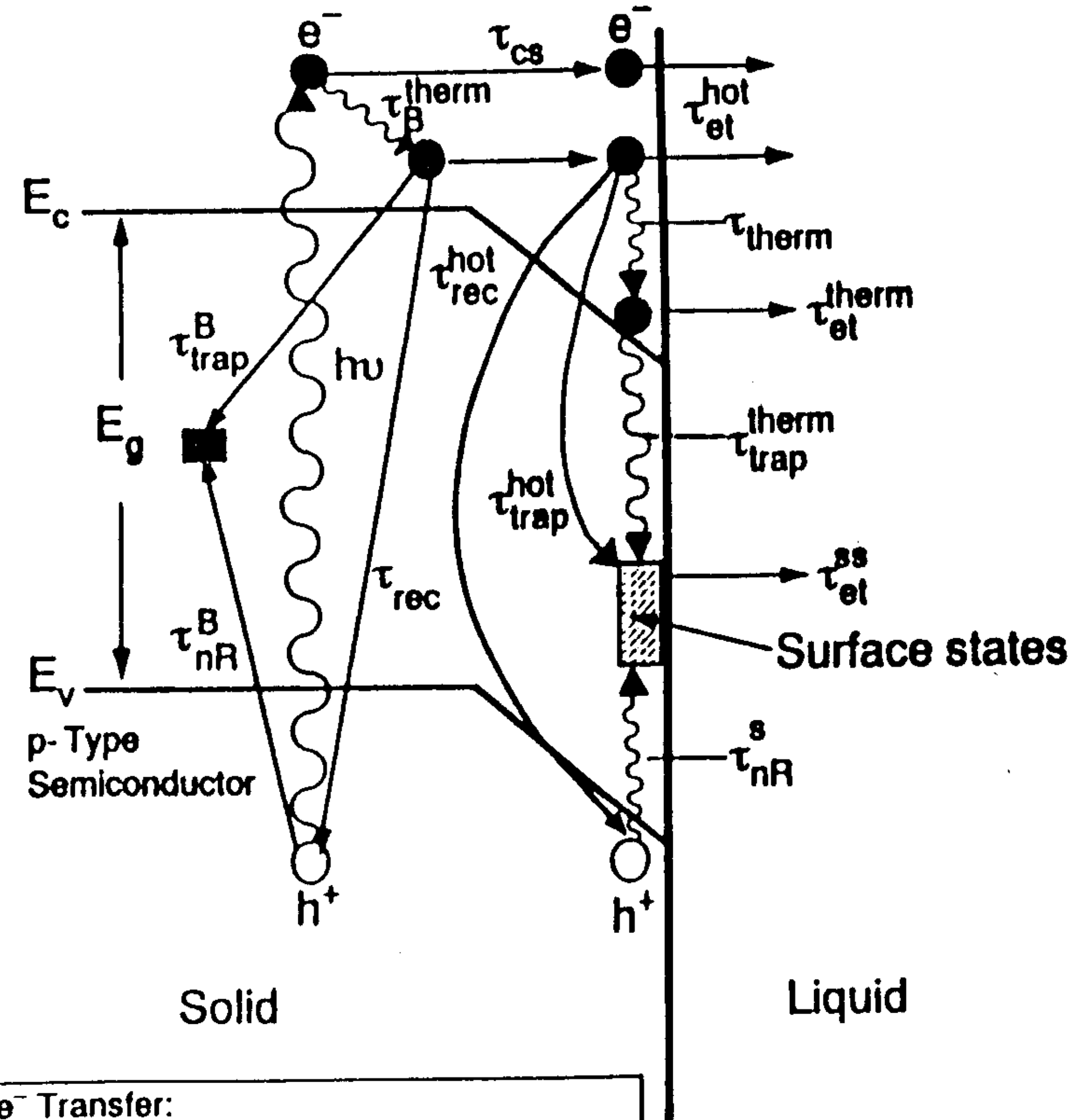
Basic Research on Semiconductor-Liquid Interfaces

- Theory
  (B. Smith)
- Quantum Dots
  (J. Machol, O. Micic)
- Measurements of Carrier Dynamics
  (R. Ellingson)
- Photoelectrochemical Characterization
  (B. Thacker)

[illegible] Solar Cells

- Dynamics of Electron Transfer Dyes to Semiconductors
  (J. Sprague)

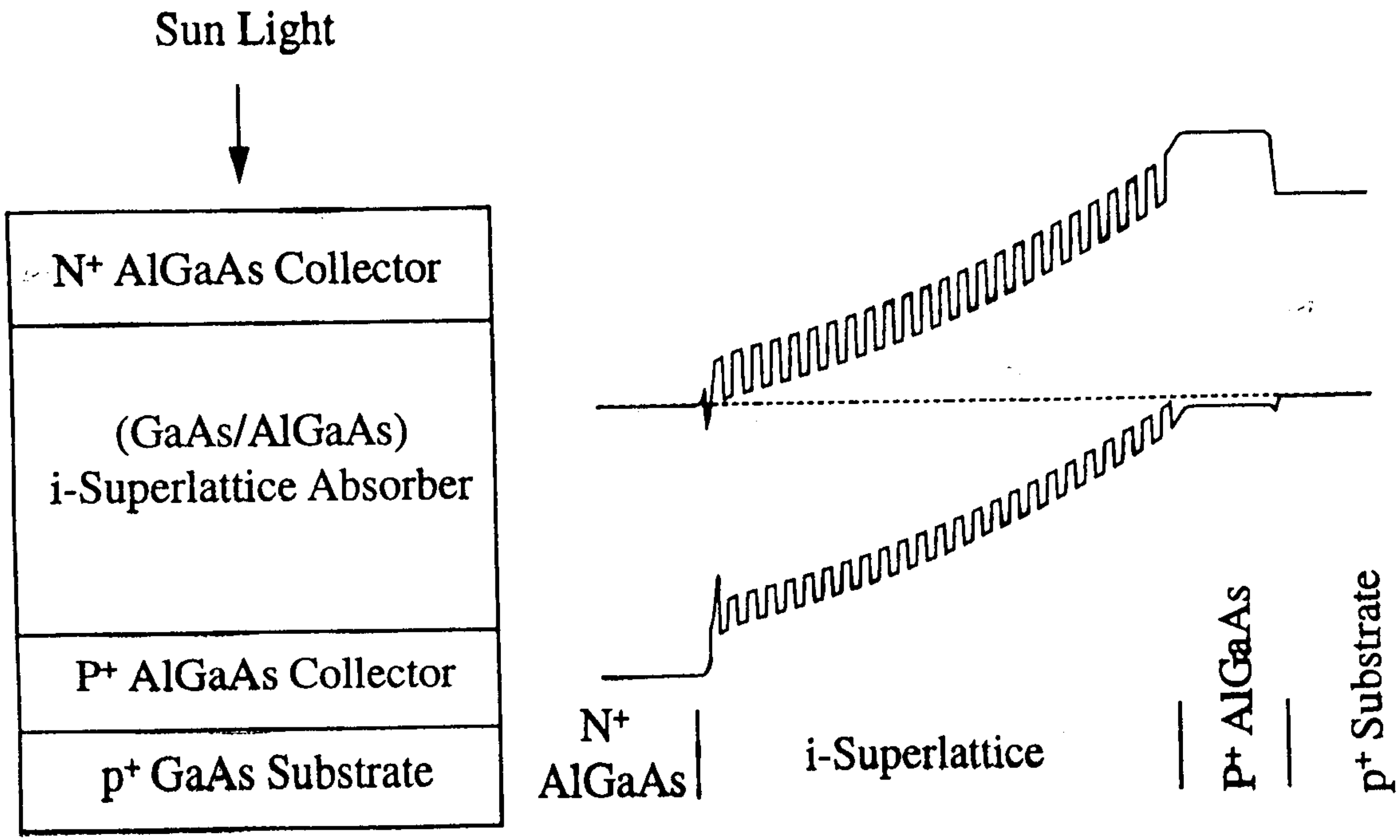
Dynamics of Photogenerated Charge Carriers



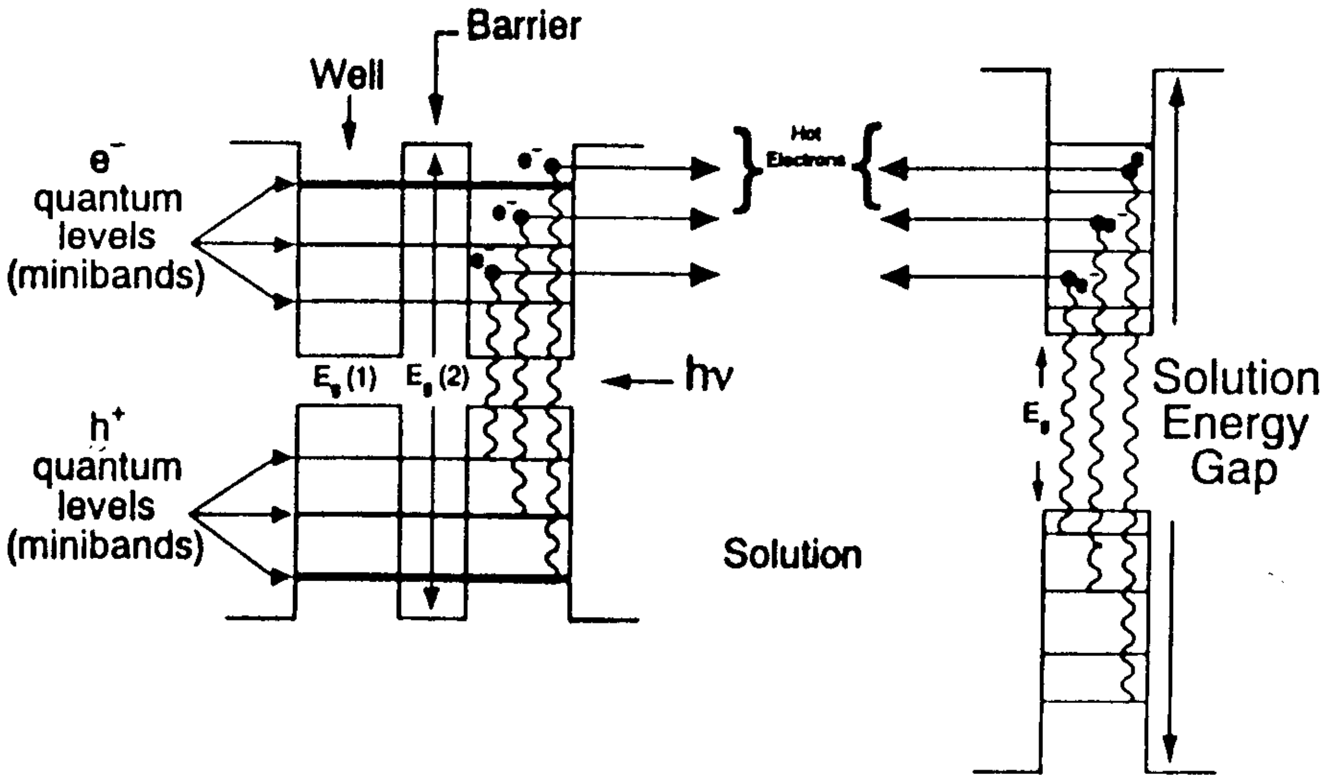
For Hot e⁻ Transfer:

$$\tau_{et}^{hot} < \tau_{therm}, \tau_{trap}^{hot}, \tau_{rec}^{hot}, \tau_{nR}^{B}, \tau_{rec}$$

Hot Carrier Solar Cell
Device Structure/Band Diagram



Quantization Effects in Photoelectrochemistry

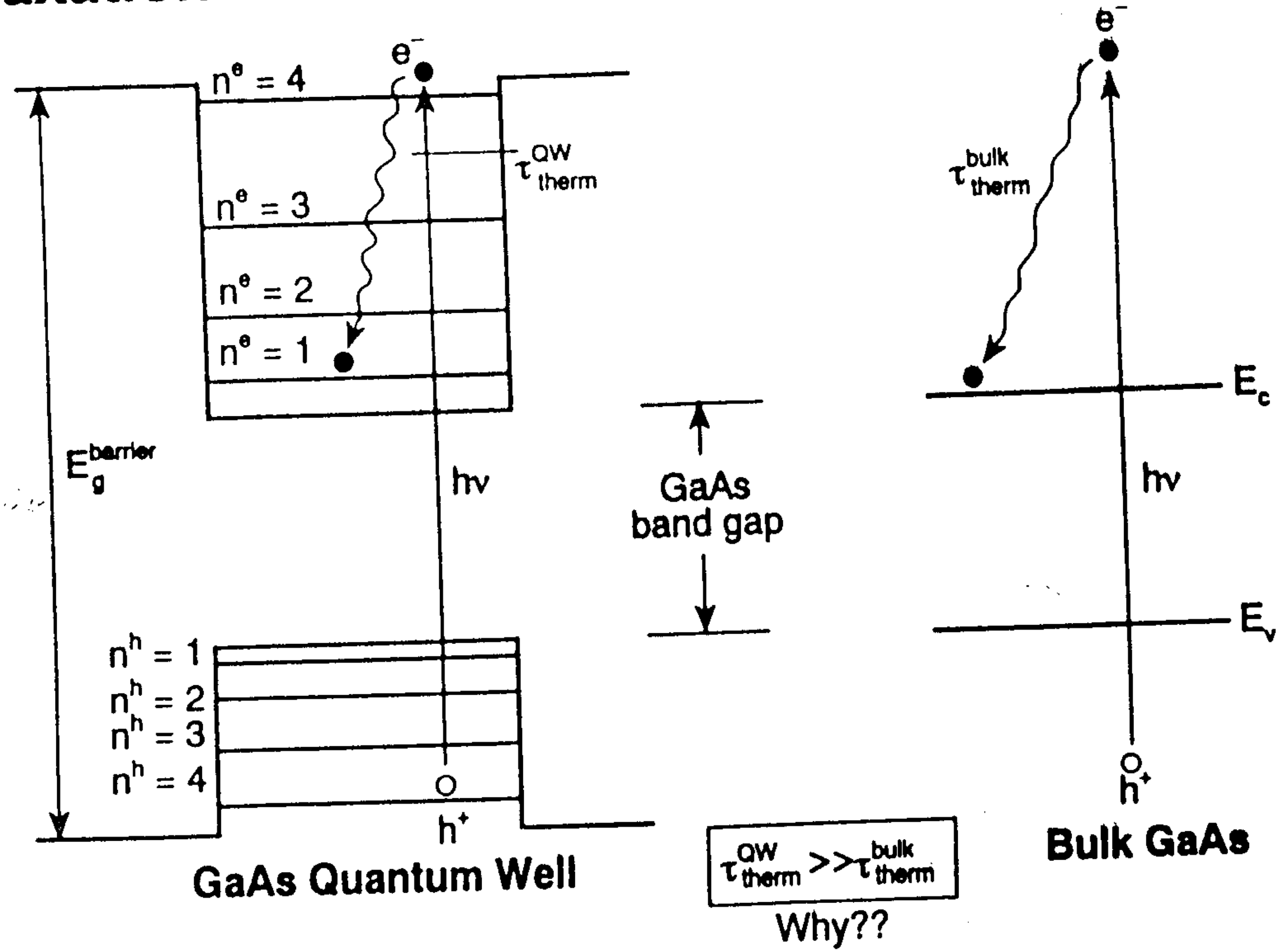


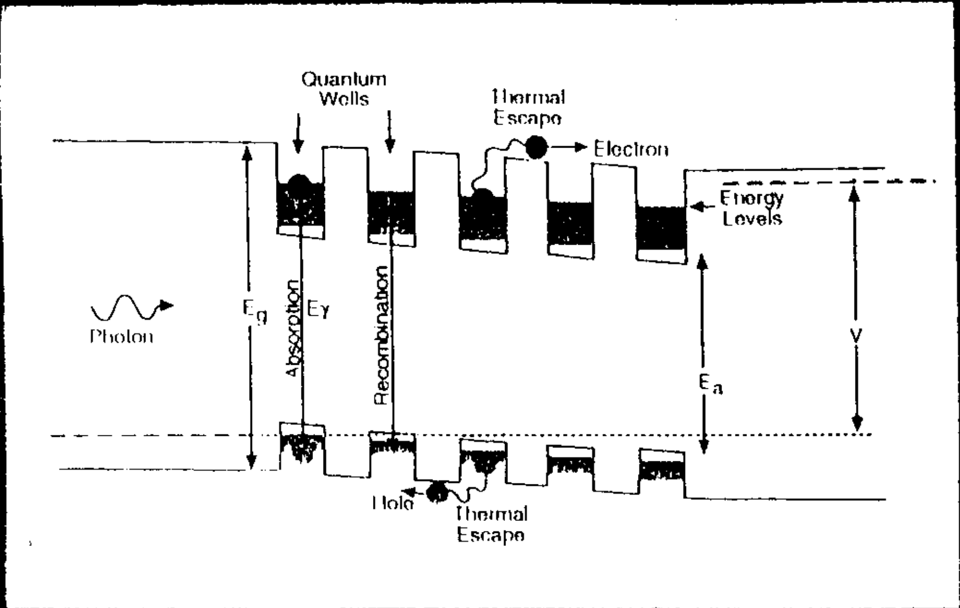
Superlattice Photoelectrodes   Quantum Dots

- **Quantization effects may permit hot electron transfer in superlattices and quantum dots**
- **Band gap of absorber can be tuned by controlling size of semiconductor layers or particles**

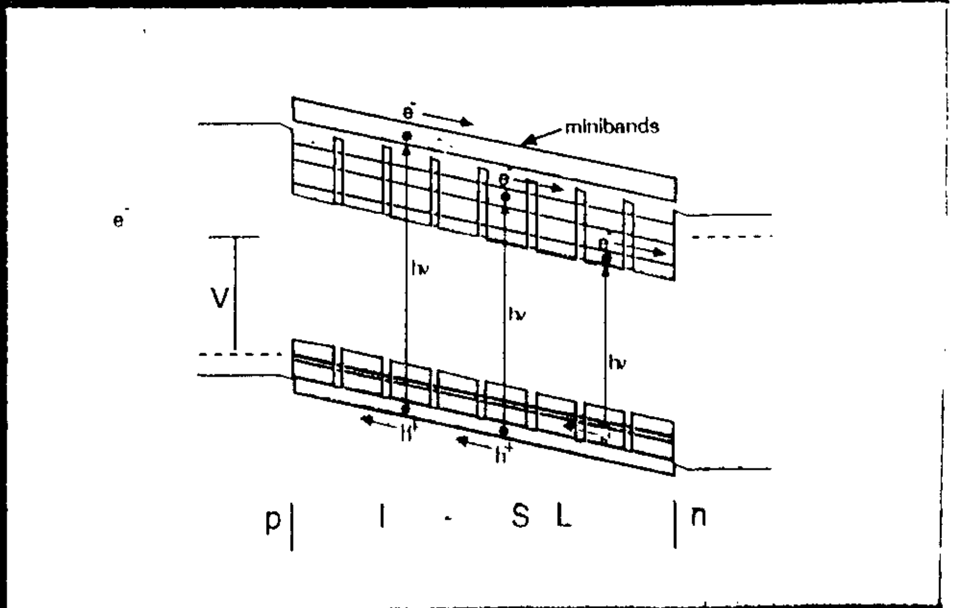
P109-G0933209 B&W

Relaxation Times in GaAs Wells vs Bulk GaAs





Quantum Well Solar Cells



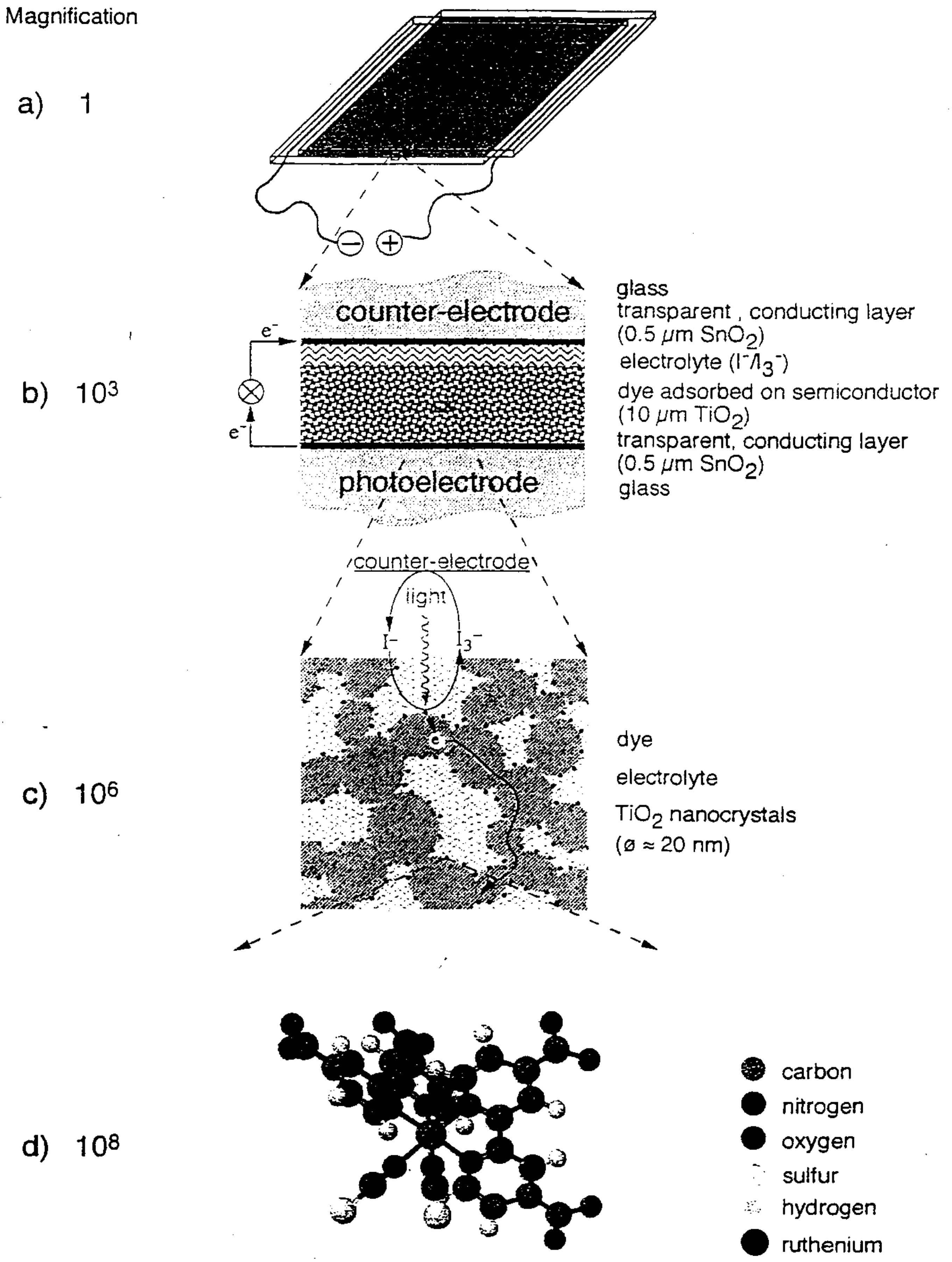
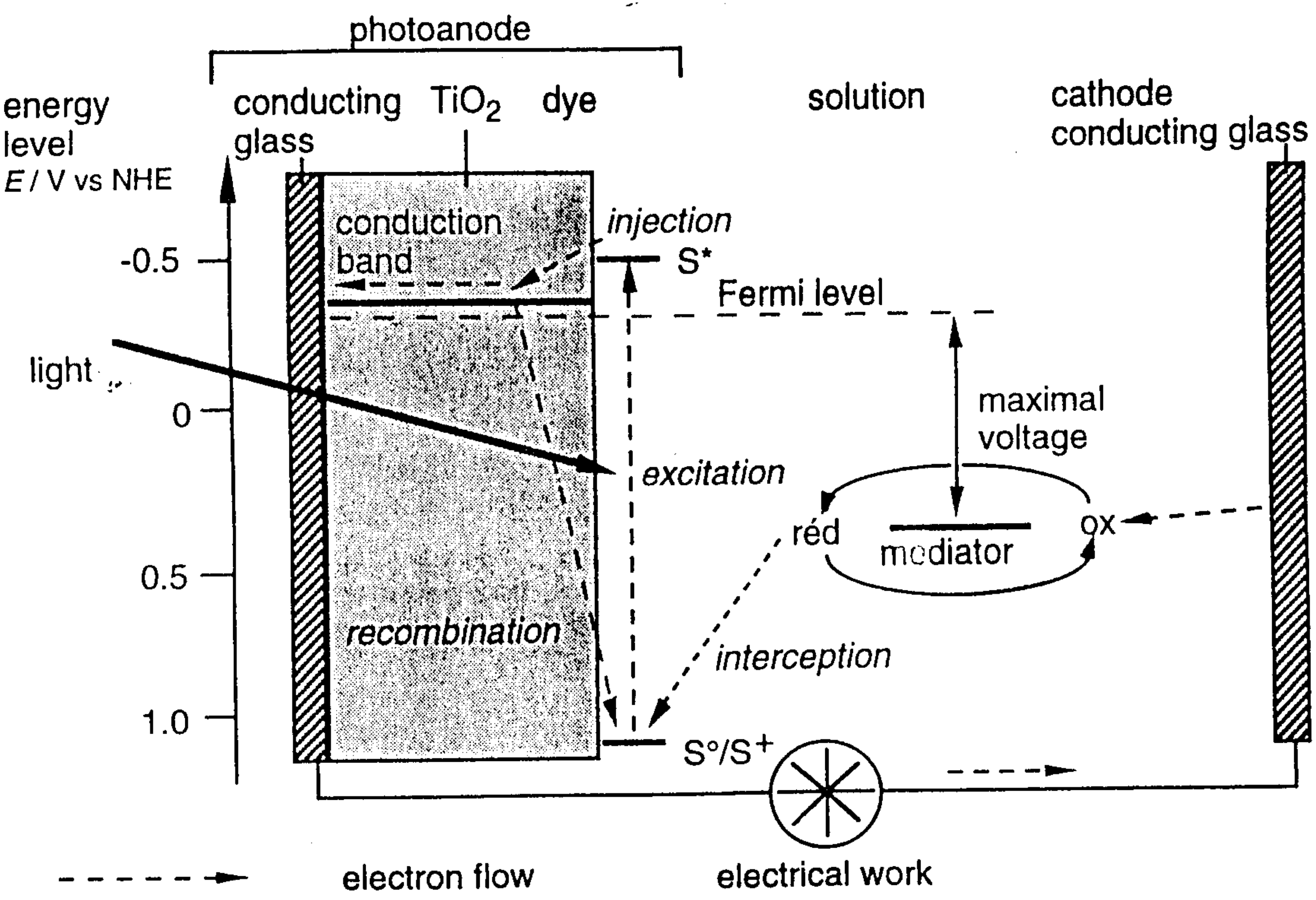


Fig.4 : Schematic view of the dye-sensitized, nanocrystalline solar cell and its components. a) general view; b) cross section; c) blow-up of the nanocristalline photoanode; d) the cis-$(NCS)_2$ bis(4,4'-dicarboxy-2,2'-bipyridine)-ruthenium(II) dye (1).


photoanode
energy
level
E / V vs NHE
conducting
glass
TiO2
dye
solution
cathode
conducting glass
conduction
band
injection
-0.5
S*
Fermi level
light
0
maximal
voltage
excitation
réd
mediator
ox
0.5
recombination
interception
1.0
S°/S+
electron flow
electrical work

Basic Sciences Division Hydrogen Program Research

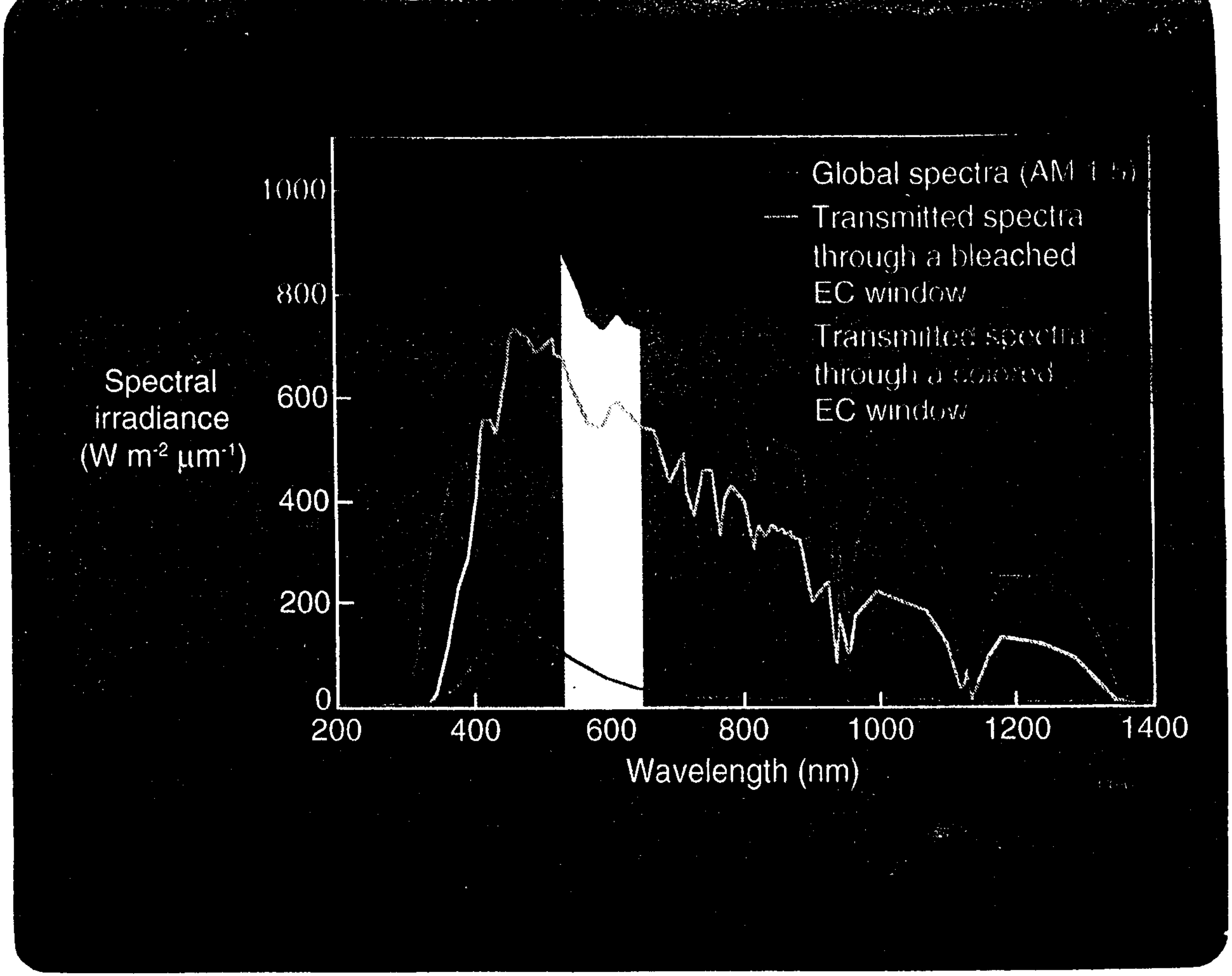
Goal: *Development of advanced hydrogen production and hydrogen storage technologies.*

Hydrogen Production by Direct Conversion.

Photoelectrolysis : *The combination of a photovoltaic system and an electrolyzer into a single monolithic system.*

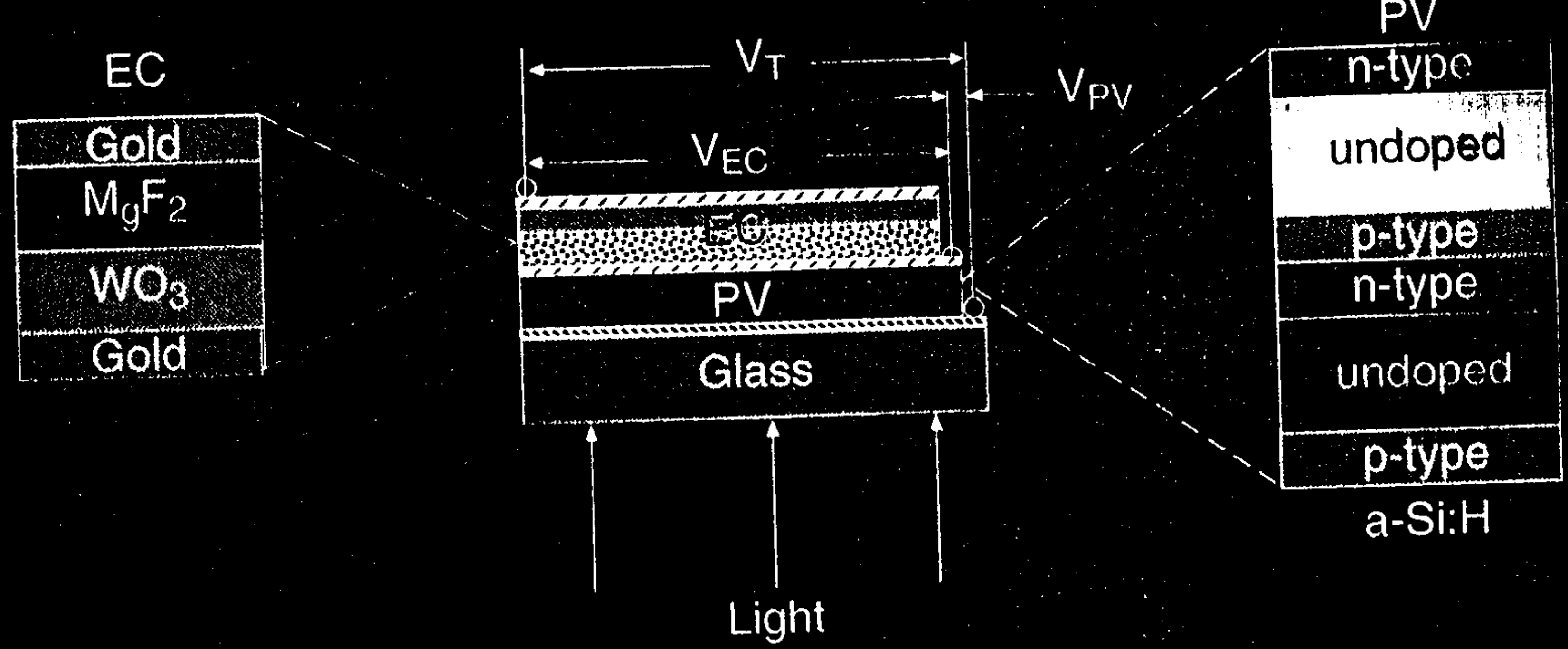
Photobiological: *Photosynthetic organisms producing hydrogen from water and wastes.*

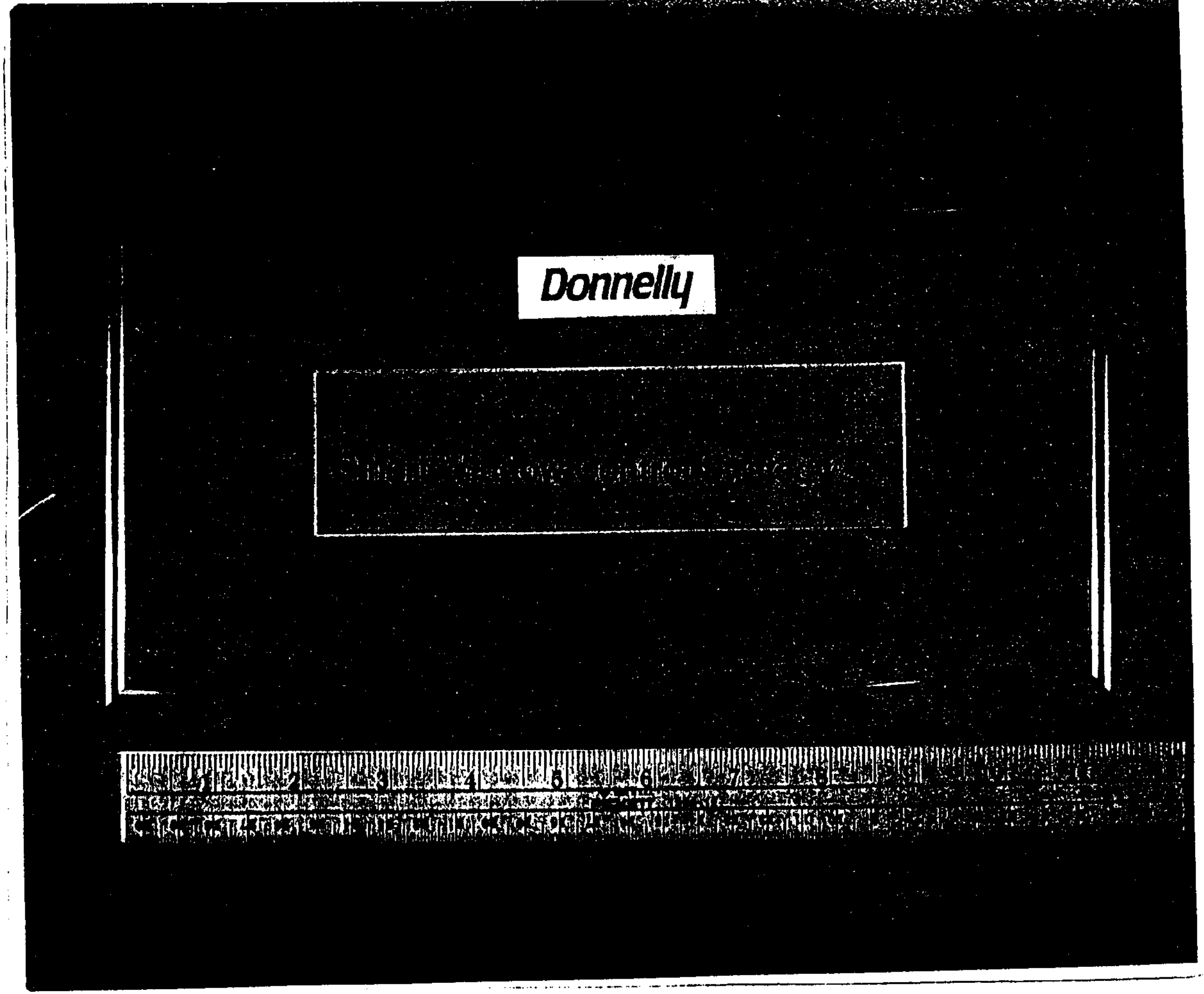
Hydrogen Storage: *Identify and investigate new hydrogen storage options with the potential for dramatic improvement over currently available technologies.*

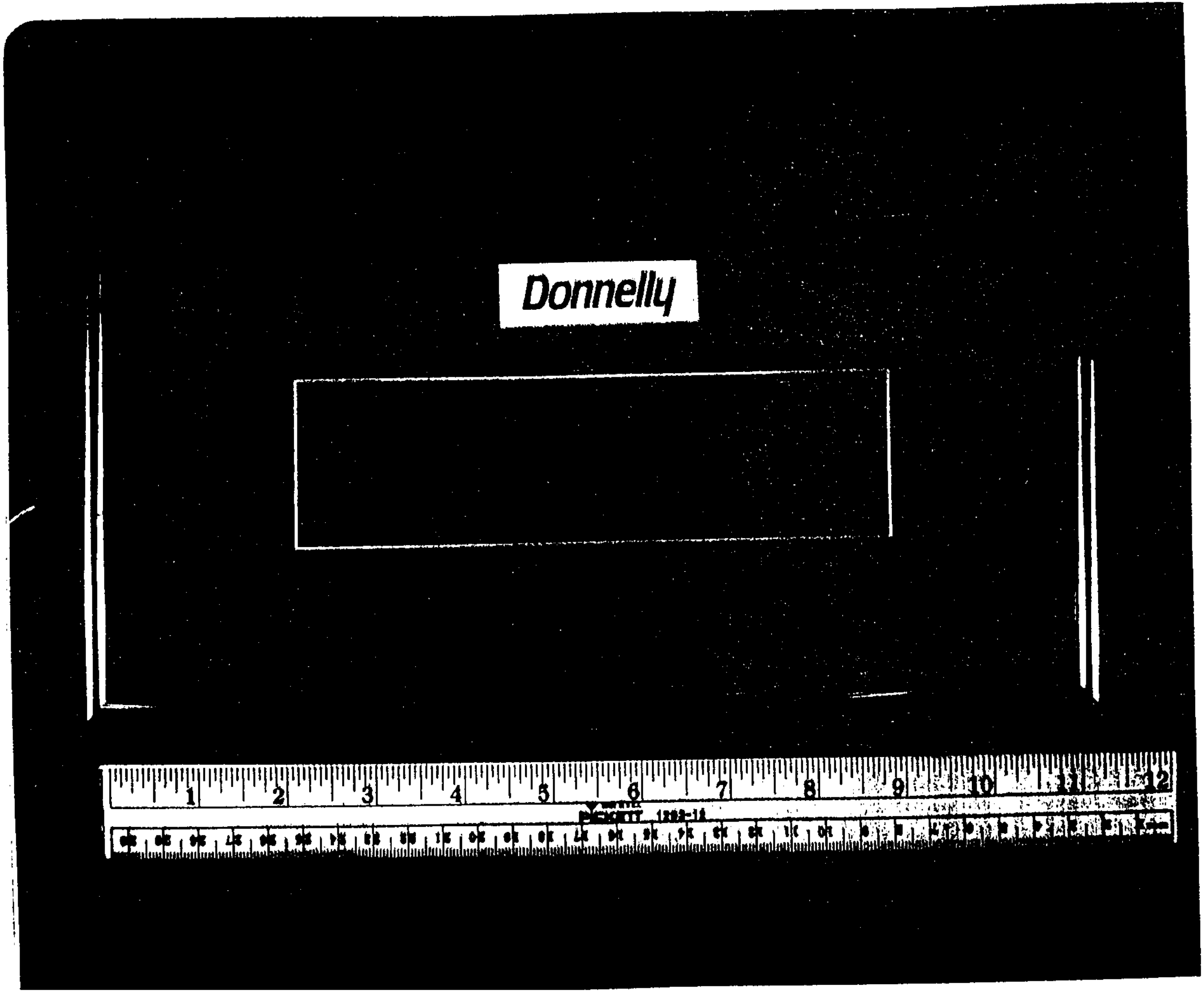


Global spectra (AM 1.5)
Transmitted spectra through a bleached EC window
Transmitted spectra through a colored EC window
Spectral irradiance (W m-2 µm-1)
1000
800
600
400
200
0
200
400
600
800
1000
1200
1400
Wavelength (nm)

PV/EC Proof of Concept Demonstration




Donnelly


Donnelly

PV/EC Compatibilities

	PV [a-Si]	EC [WO [illegible]]
Voltage (V)	0.85	1.5
Current (A/m^2)	60	10

EC Switching OD = 0.48 (T = 33%)

Energy 150 J/m^2 Time 10 s

Power 15 W/m^2

PV area and the time required
*under 600 W/m^2 solar at 6% efficiency

Area	Time
0.1m^2	49 s
0.01m^2	490 s

Construction

both multilayer films

Fabrication

both sputtering and PECVD

Automotive Applications of Electrochromics