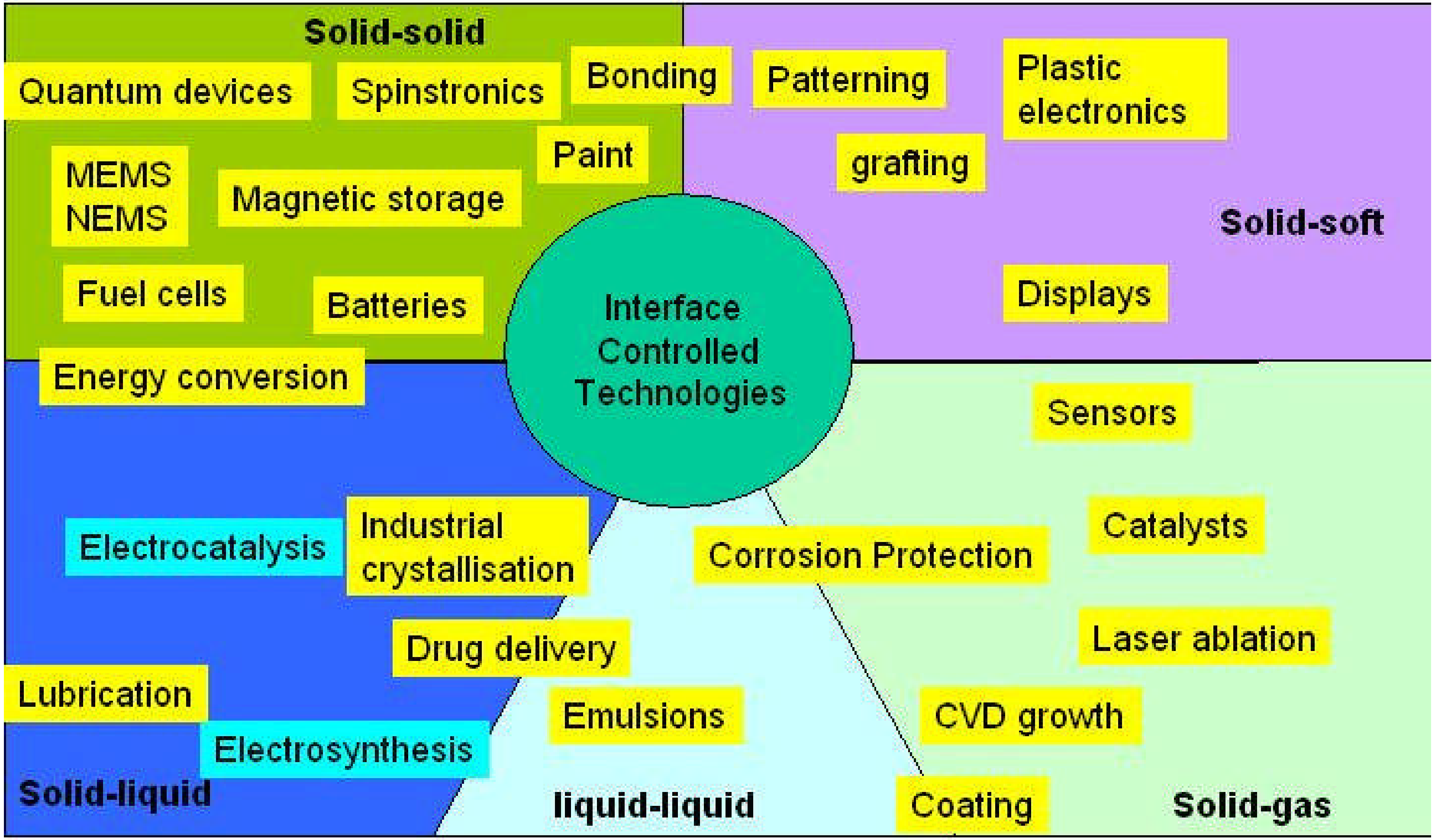
Workshop on In-Situ Characterization of Surface and Interface Structures and Processes

September 8-9, 2005

Advanced Photon Source
X-Ray Operations & Research
Center for Nanoscale Materials

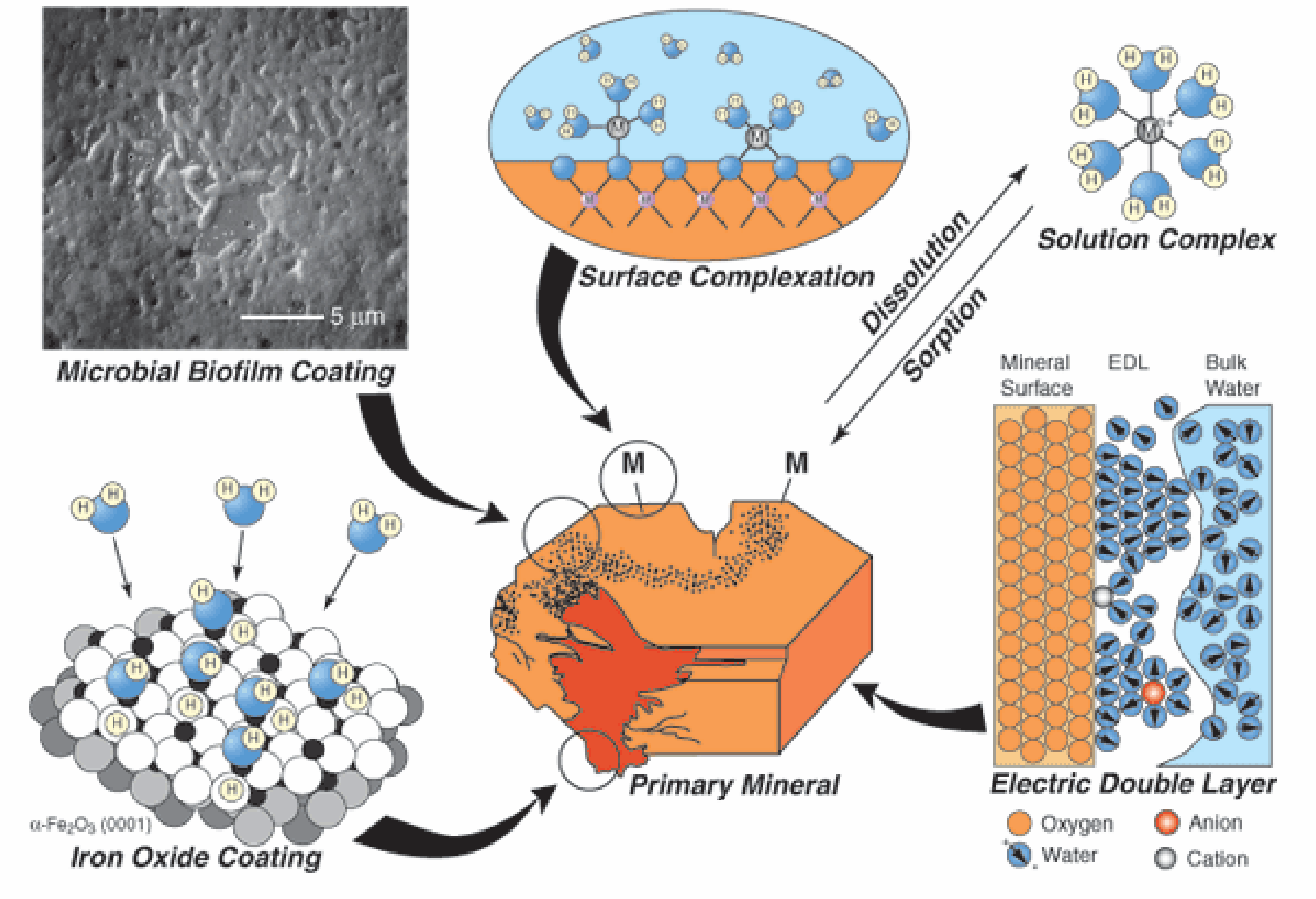
Argonne National Laboratory
Argonne, Illinois



Structure ⟺ Function

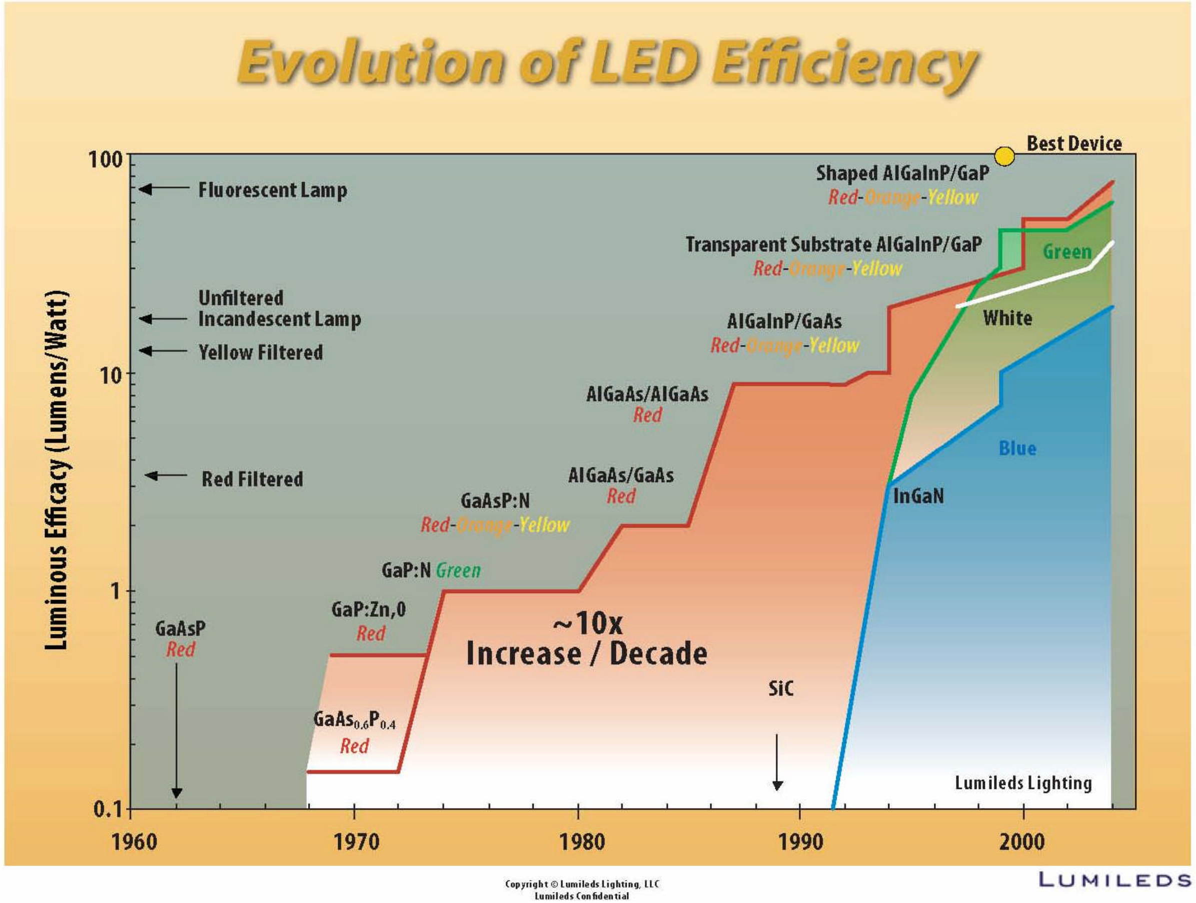
Mineral-water interfacial interactions

Geochemical reactions



G.E. Brown, Jr. (2001) How minerals react with water, *Science* 294, 67-69.

A. Munkholm, Lumileds Lighting - MOCVD of (Al,In,Ga)N for Lighting



Lighting accounts for ~20% of global electricity consumption.

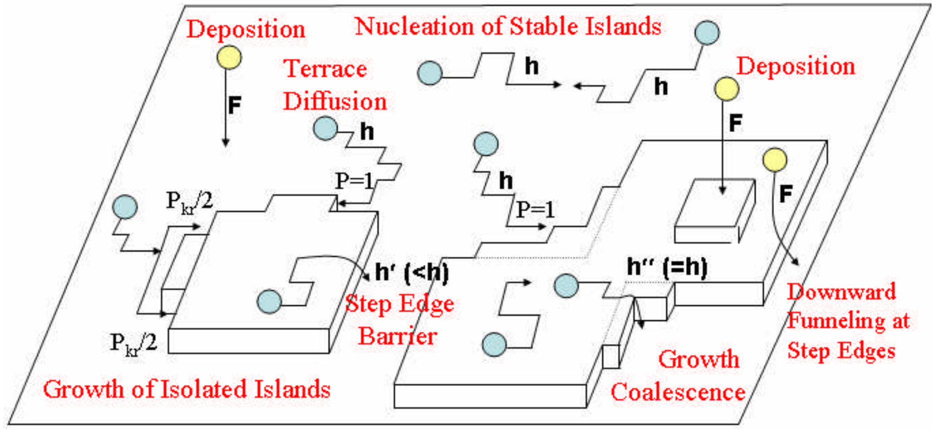
Potential 10% reduction in global electricity consumption

- ~1000 TWh/year in energy (or $100B/year in cost)
- 200M tons/year global carbon emissions

INTEGRATED MODELING OF HOMOEPITAXIAL THIN FILM GROWTH

Jim Evans – Iowa State University

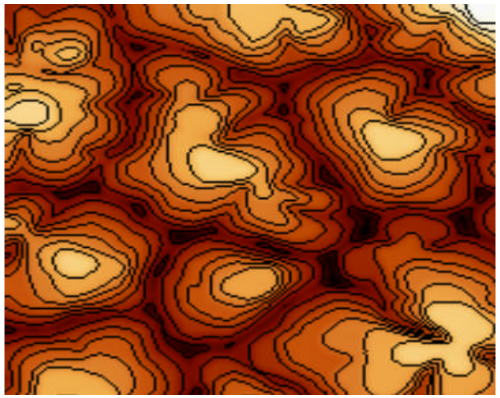
MULTILAYER GROWTH OF AG/AG(111): EFFECT OF STEP EDGE BARRIER

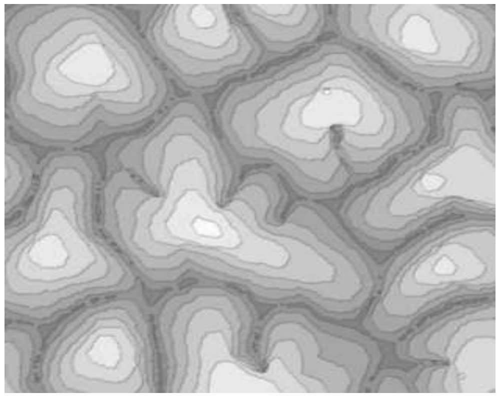


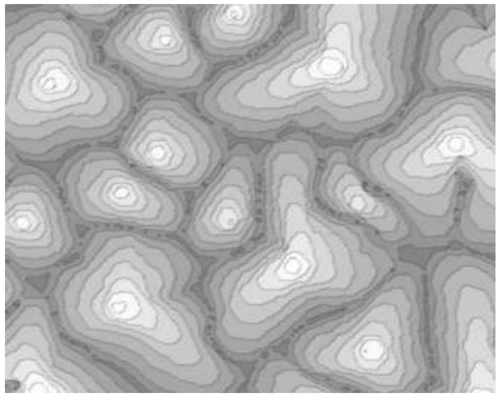
STM IMAGE: 3ML @ 150K
Note flat tops of mounds
(large size of top islands)

KMC SIMULATIONS: 3 ML @ 150K … with E_d = 0.10 eV

E_{ES} = 0.15 eV $\nu = 10^{12}$/s	**E_{ES} = infinity**
(finite ES barrier)	**(no interlayer transport)**



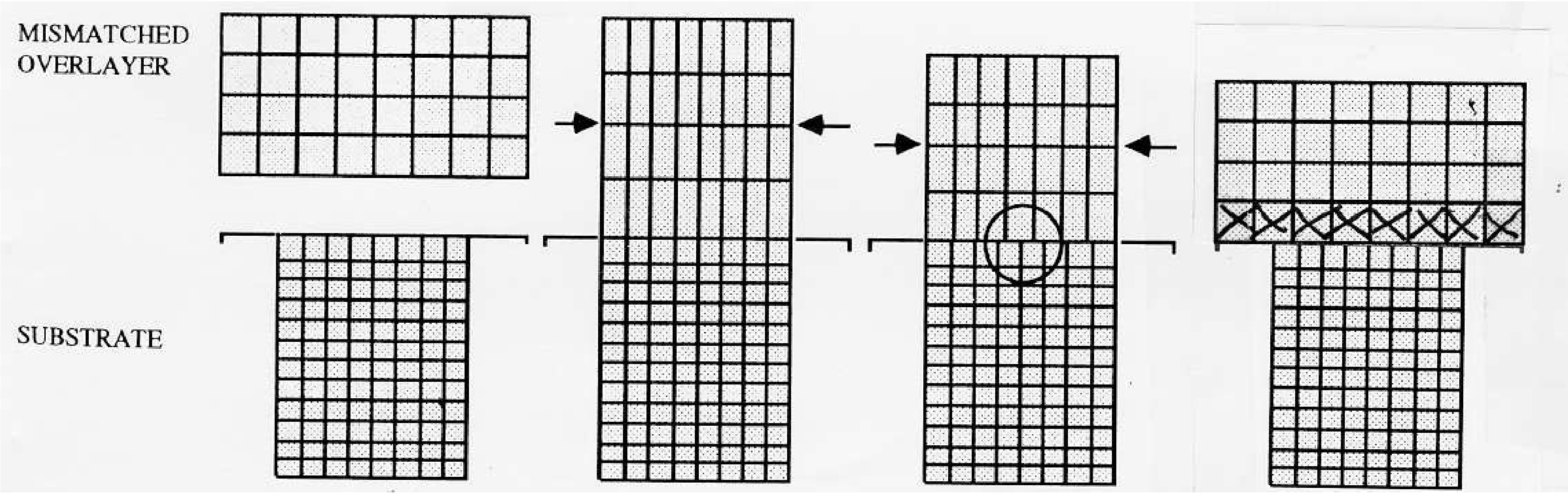




Images = 95 × 95 nm^2 *Maozhi Li, P.-W. Chung, et al. (ISU)*

Engineering the Band gap with lattice mismatch, strain & dislocations

Jim Harris, Stanford University

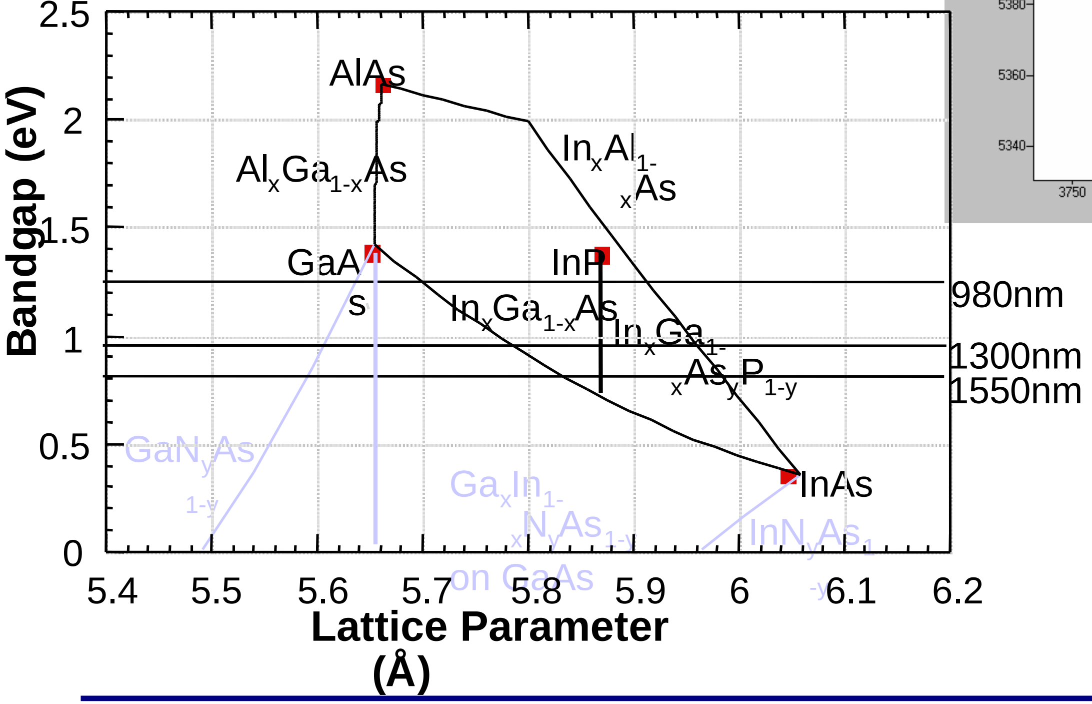


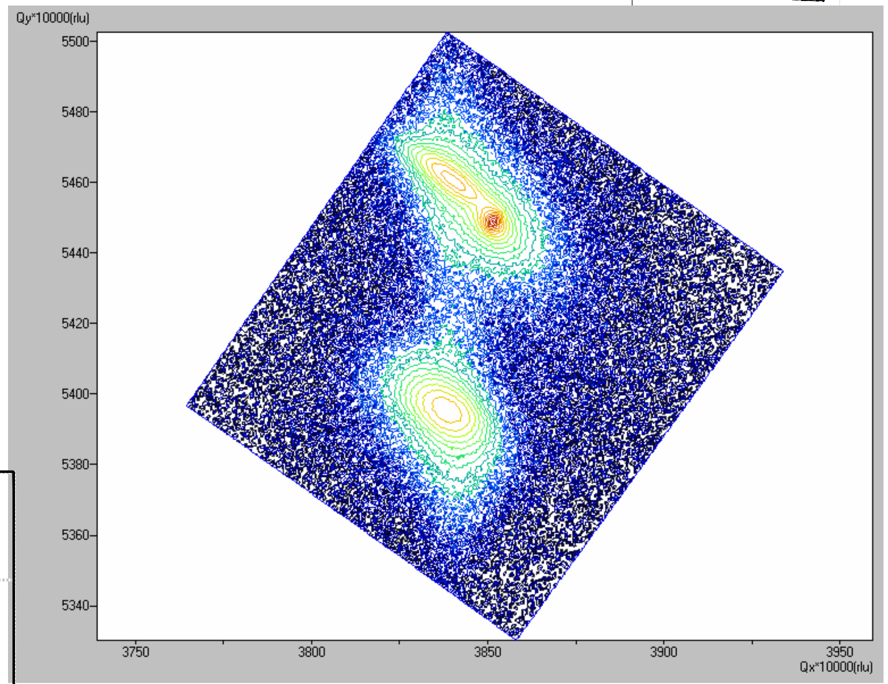
Bulk Materials | Coherent (Strained) | Incoherent (Partially Relaxed) | Unstrained (Completely Relaxed)

The degree of strain and introduction of dislocations depends upon epitaxial layer lattice mismatch and thickness--if the strain energy is less than required to create a dislocation, the layer remains strained, if not, it is relaxed with dislocations.

Relaxed GaInNAsSb film – J. Harris

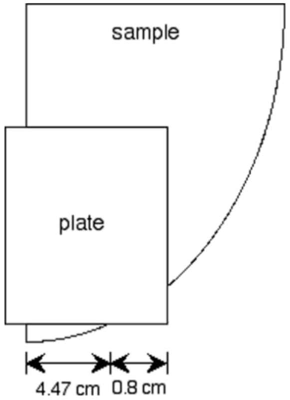
GaInNAsSb 1 μm film on GaAs

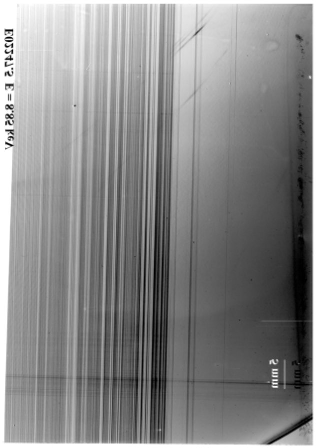


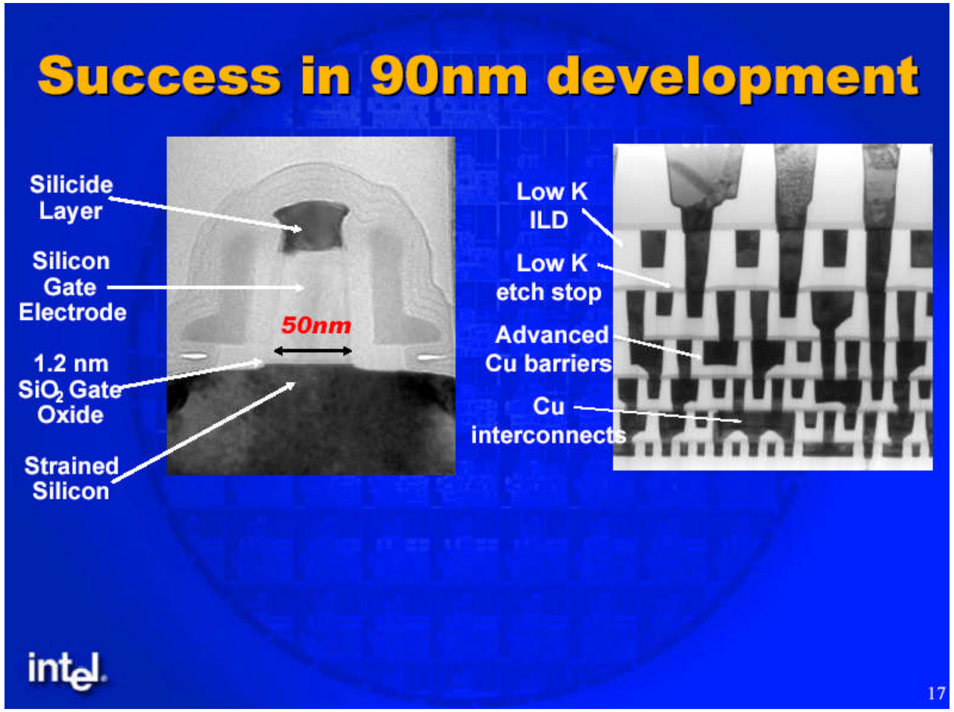


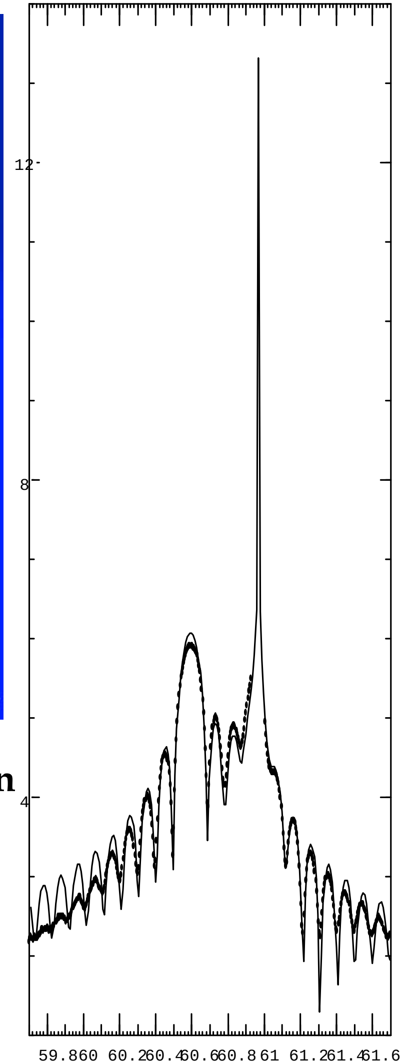
- (224) RSM of a relaxed film
- Need higher resolution to examine relaxation parameters more accurately

Strained Si on SiGe Films

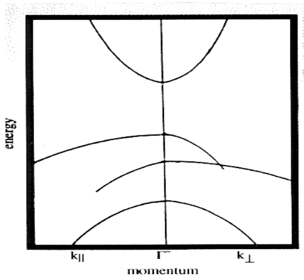


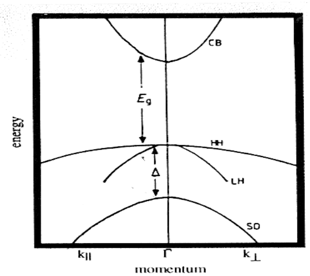


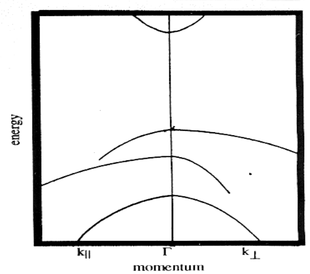




Biaxial Tension **Unstrained** **Biaxial Compression**







Workshop Goals

- Identify scientific and technological opportunities in the area of in-situ characterization of surface and interface structures and processes,
- Assess the applicability of existing and future x-ray tools to these fields, and
- Appraise the interest of the research community in developing dedicated facilities for in-situ x-ray characterization at the Advanced Photon Source.

Workshop Science Program

Broad Topical Categories

a. Surfaces, interfaces and nanostructures

b. Thin film growth processes

c. Interfaces in catalytic and geological environments

d. Electrocatalysts and electrode surface chemistry

Expert X-ray developers/users

J. F. van der Veen, Swiss Light Source

I. K. Robinson, University of Illinois at Urbana-Champaign

G. E. Brown, Jr., Stanford University

K. Ludwig, Boston University

T. Chiang, University of Illinois at Urbana-Champaign

A. Munkholm, Lumileds

C-H. Hsu, National Synchrotron Radiation Research Center

M. J. Bedzyk, Northwestern University

P. F. Lyman, University of Wisconsin, Milwaukee

Y. Yacoby, The Hebrew University

R. Felici, European Synchrotron Radiation Facility

D. Fong, Argonne National Laboratory

C. Park, Argonne National Laboratory

Others whose science benefits from advanced x-ray tools

N. M. Markovic, Lawrence Berkeley National Laboratory

R. Hull, University of Virginia

G. Eres, Oak Ridge National Laboratory

D. Schlom, Penn State University

K. Wahl, Naval Research Laboratory

R. J. Hamers, University of Wisconsin, Madison

S. Sibener, University of Chicago

J. Evans, Ames Laboratory and Iowa State University

J. S. Harris, Stanford University

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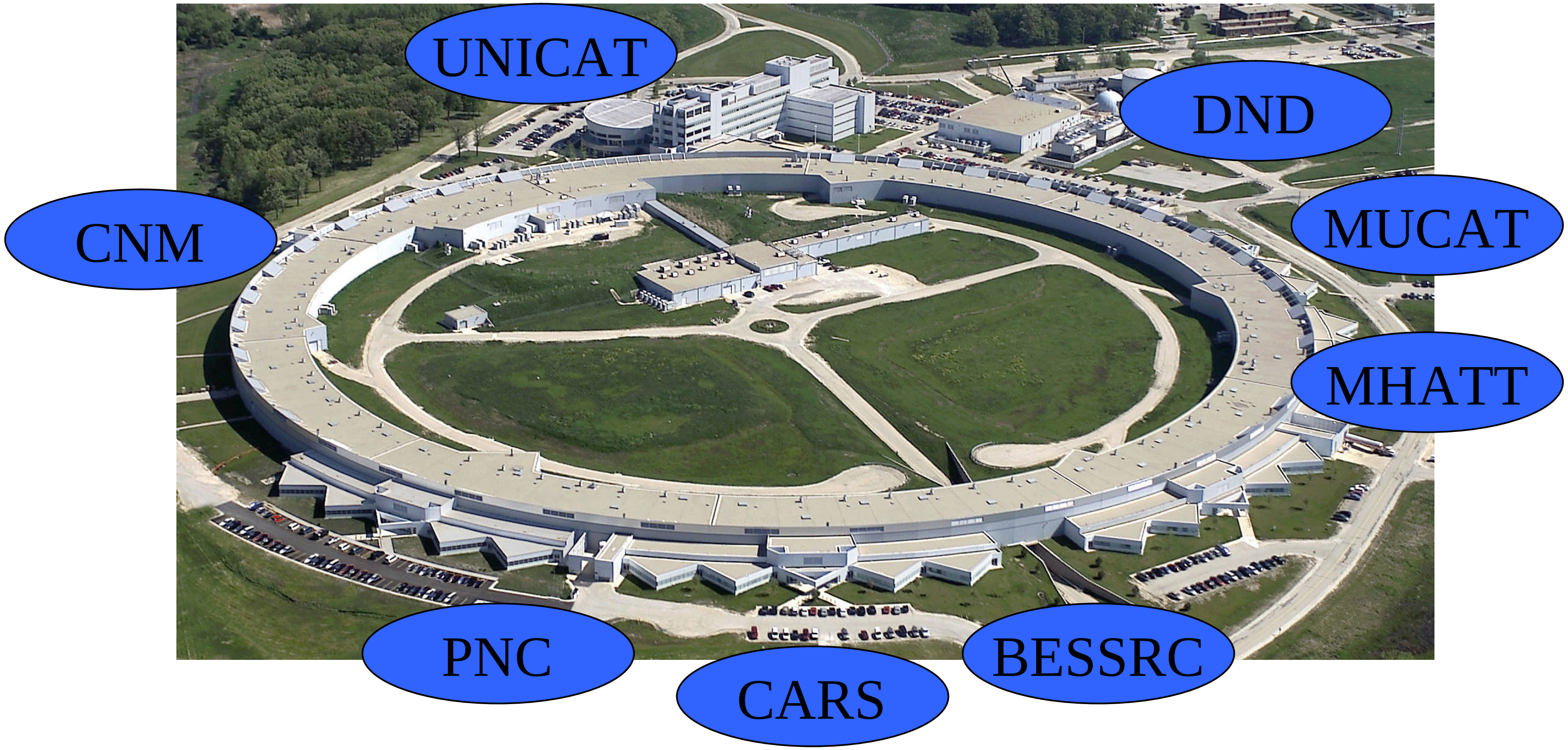
Surface/Interface Science at the APS Today



Surface/Interface Science at the APS Today

Sector 5 – UHV surface chamber

Sector 6 – UHV surface chamber, thin film deposition

Sector 7 – COBRA

Sector 11 – Electrochemical and geochemical interfaces

Sector 12 – MOCVD, standing waves, electrochemistry, geochemistry, oxidation

Sector 13 – General Purpose/surface diffraction

Sector 20 – MBE capable surface xafs, reflectivity, standing wave chamber, COBRA

Sector 33 – UHV chamber/thin film growth, PLD system

Sector 34 – UHV chamber/coherent diffraction

Other Reflectivity, GISAXS, liquid surface scattering and General Purpose scattering capabilities throughout

Census of Surface/Interface Programs at the APS*

Sector	Specialized In-situ Surface/interface (% of beamtime)	General Purpose In-situ Surface/interface (% of beamtime)	General Purpose Ex-situ Surface/interface (% of beamtime)
5 ID	3.5	6.5	4.8
6 ID	10		
7 ID		3	18
10 ID			
11 ID		35.5	
12 ID	29	20	
13 ID		21.5	
20 ID	15	0	9.5
33 ID	25.1		6
34 ID	20	10	
Totals	102.6	96.5	38.3
		Total % Usage	
		237.4	
		# undulators**	
		3.2	

*Usage numbers averaged over the past 2 years

**# undulator beam lines

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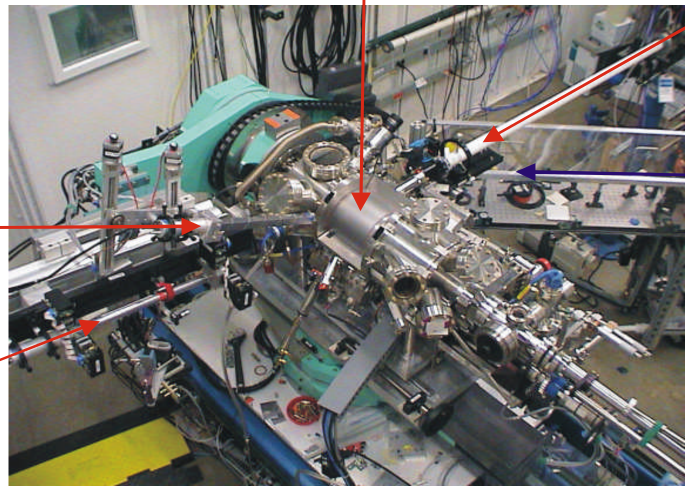
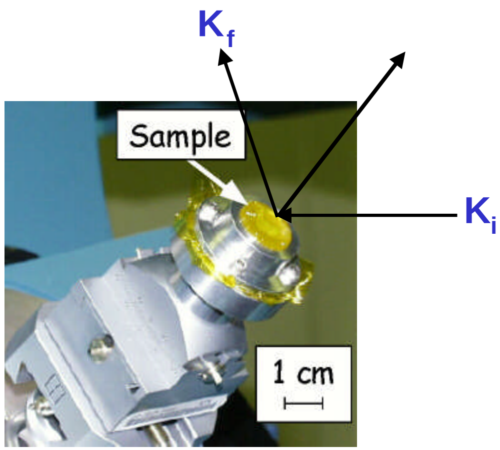
Observations - Facility Requirements

- Need flexible scattering systems which are permanently available
  - Get new programs started
  - Get rapid turnaround on novel and routine problems
  - Integration with other techniques (e.g. AFM)
  - Standard interfaces for small to medium sample chambers
- Major Instruments (e.g. growth systems, UHV systems)
  - Regular beamtime
  - Toxic gas and material handling
  - Integration with other techniques (eg. RHEED, PEEM, XPS…)
  - Supporting laboratory space
  - Access to instrument when beam not available
  - Wide range of synchrotron techniques (diffraction and spectroscopy) useful
- Development and support of
  - Detectors
  - Data collection and analysis systems
- Need staff and facilities doing research in this area full time

Observations

• Some experiments require specialized end station equipment and chambers





•Many experiments that study liquid-solid or high pressure gas-solid interfaces use “snap-on” chambers or cells that mount to general purpose scattering diffractometers

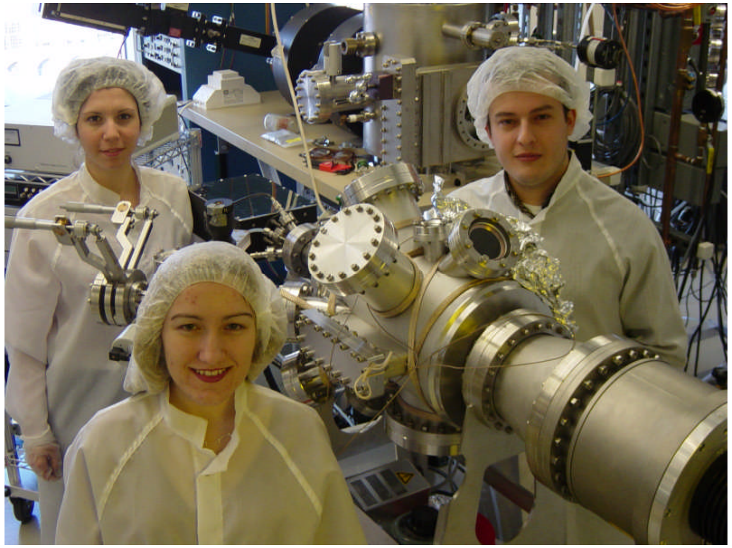
• Through operational experience we find many experiments are run at the same energy each time. So, fixed energy beam line branches are possible.

X-ray Studies of Materials with Analysis in Real Time (XSMART) Facility

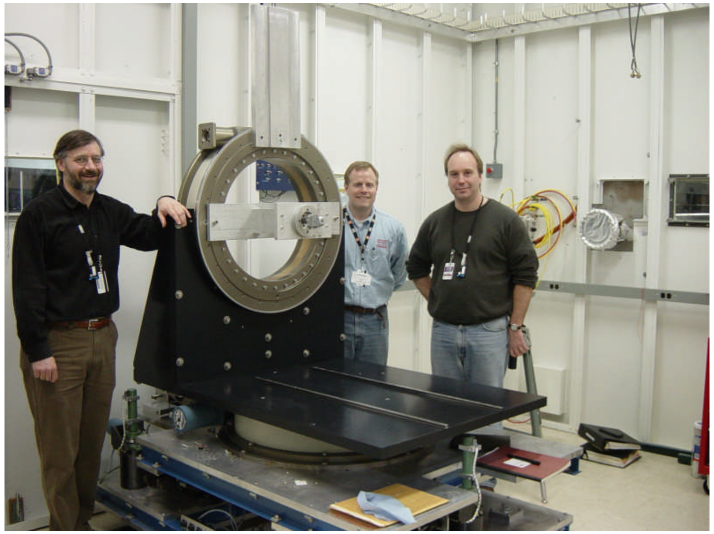
Karl Ludwig, Boston University

NSLS insertion device beamline X21 back hutch

Experimental conditions can be optimized in chambers at the home laboratory …



… the chambers can then be rolled onto the base diffractometer permanently installed at NSLS



Observations

- Specialized endstation equipment such as MBE, PLD or MOCVD systems are different. These:

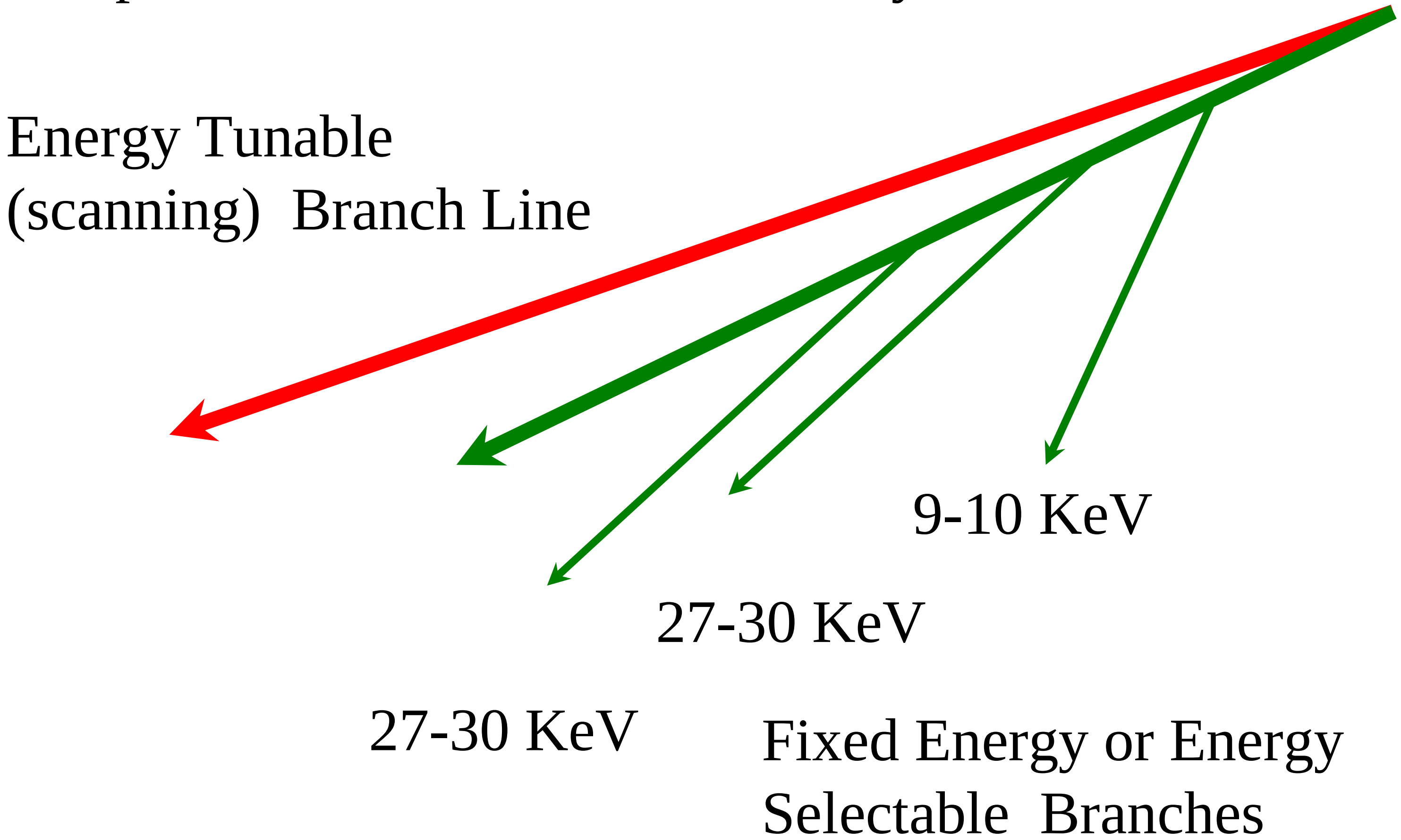
  - require substantial investments

  - are not well suited to conventional general user access

  - are not always easily made transportable

  - require off-line access

Concept for a Canted Undulator facility



Strategic Planning at APS

Surface and Interface Scattering…

Recommendations that emerge from the workshop will help direct decisions regarding how an existing sector could be reconfigured to serve this community, or whether a green field facility might be required.

Tactical Plan for X-Ray Operations and Research at the APS (2005-2015) Rev 10a

Gabrielle Long, 27 June 2005

Workshop Summary – What's Next?

Written Workshop Report – Including:

Specific Recommendations

Exploration of new access modes

Assessment of needs for dedicated facilities

Encourage APS research & staffing in this area

Encourage detector and data analysis development

Workshop Summary – What's Next?

surface-interface@anl.gov

http://surface-interface.aps.anl.gov/2005workshop/

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Suggestion Form

Please use this form to submit suggestions for things you think should be considered in the course of developing of *in situ* characterization capabilities at the APS.

The information will be e-mailed to the three workshop organizers: Paul Fenter, Paul Fuoss, and Paul Zschack. Please identify yourself to the extent you feel comfortable. The form does not collect information from your browser session.

Suggestions:

Name/contact info (optional):

Have you ever used the APS (optional)? Yes No