Light-induced crystallization of thin Si films

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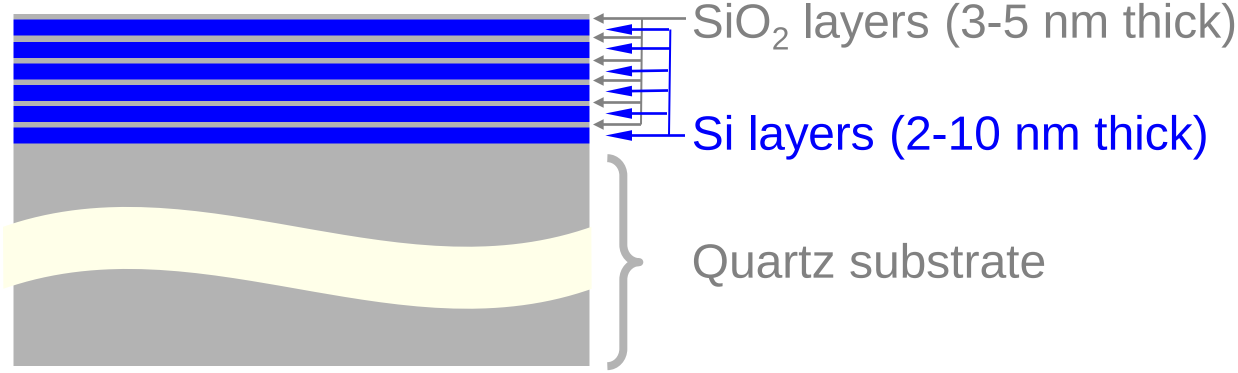
Outline

- Motivation
- Experiments with light-induced crystallization
- Model, calculations, results and discussion
- Summary

Motivation

High crystal quality Si/SiO_2 MQW on cheap substrate:



Fabrication:

- Subsequent deposition of a-Si and SiO_2 layers on a quartz substrate;
- Crystallization of Si layers.

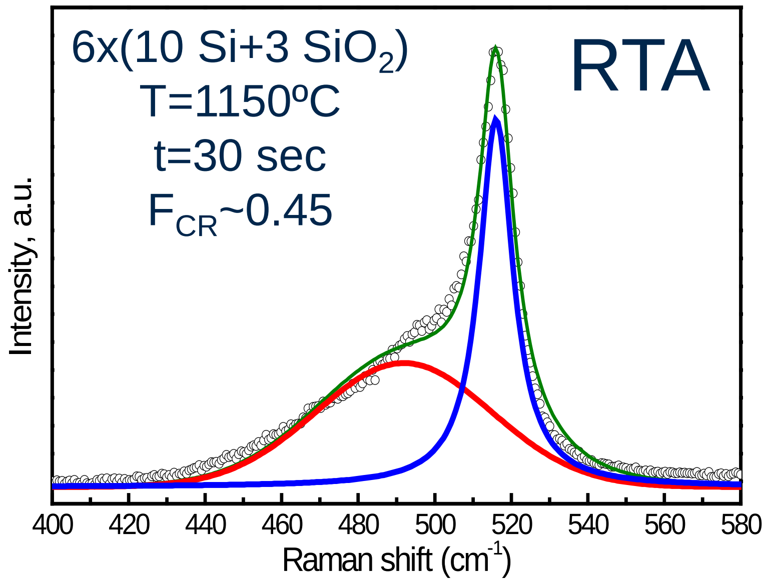
Possible future applications:

- Tandem solar cells
- 3^{rd} generation PV materials
- Photonics
- Device apps, nanoelectronics
- …

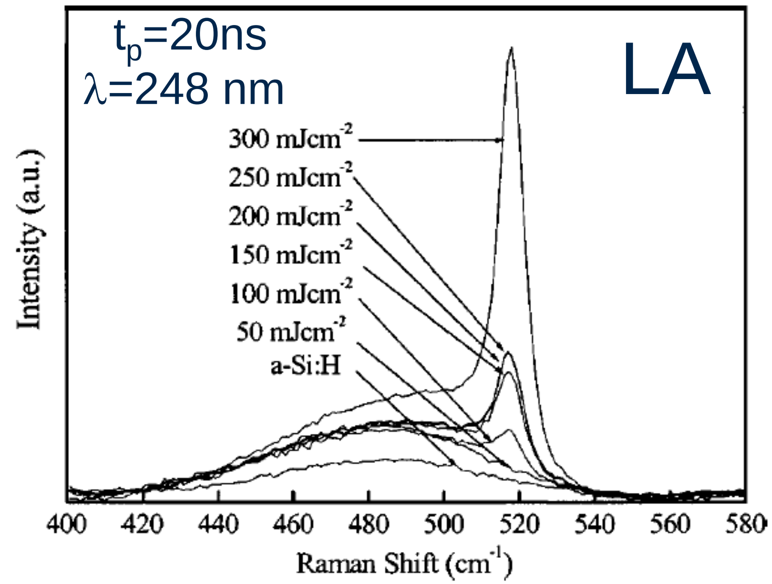
High crystal quality of Si-nc layers is crucial!

Problems with crystallization of Si/SiO_2 MQW

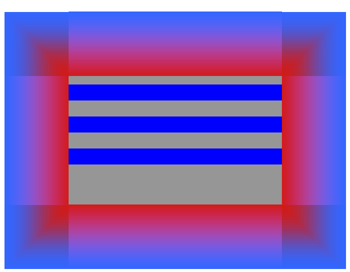
[T. Mchedlidze, et al.
Thin Solid Films **516**, 6800 (2008)]



[A. Adikaari and S. Silva
J. Appl. Phys. **97**, 114305 (2005)]



- $F_{CR}=I(Si_{CR})/I(Si_{TOT}) < 0.7$
- High residual compressive stress



“Bulk” heating:

High level of crystallization (>80%) *impossible*.

Reasons: Si melting, mismatch in the thermo-physical properties of MQW components.

Smart light-induced crystallization

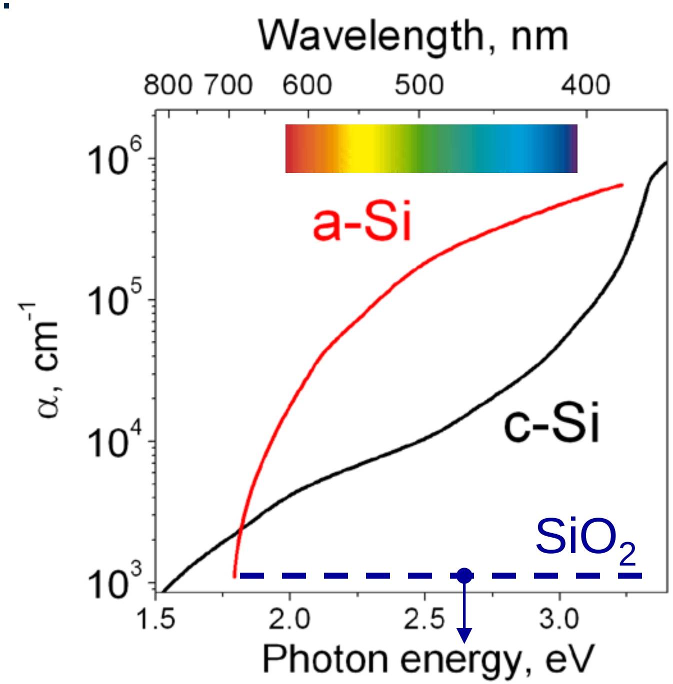
What to do:

- Preferential heating of a-Si layers;
- Avoid a-Si melting ►solid phase transition;
- Input proper amount of energy.

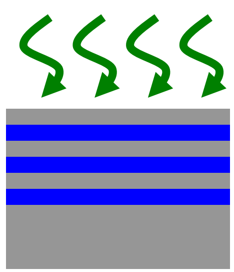
Concept:

Employ differences in light absorption between a-Si, Si-nc, SiO_2 and a substrate;

- Self-regulated crystallization process.



Realization:



Convert a-Si to Si-nc using proper light flux @ ~500 nm.

Smart light-induced crystallization

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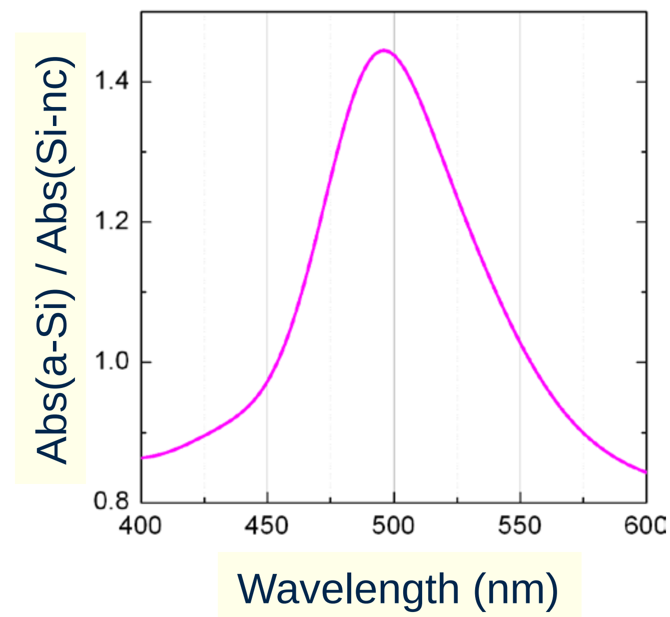

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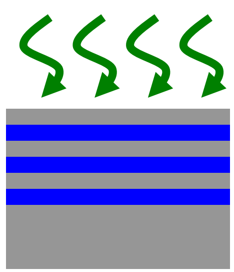
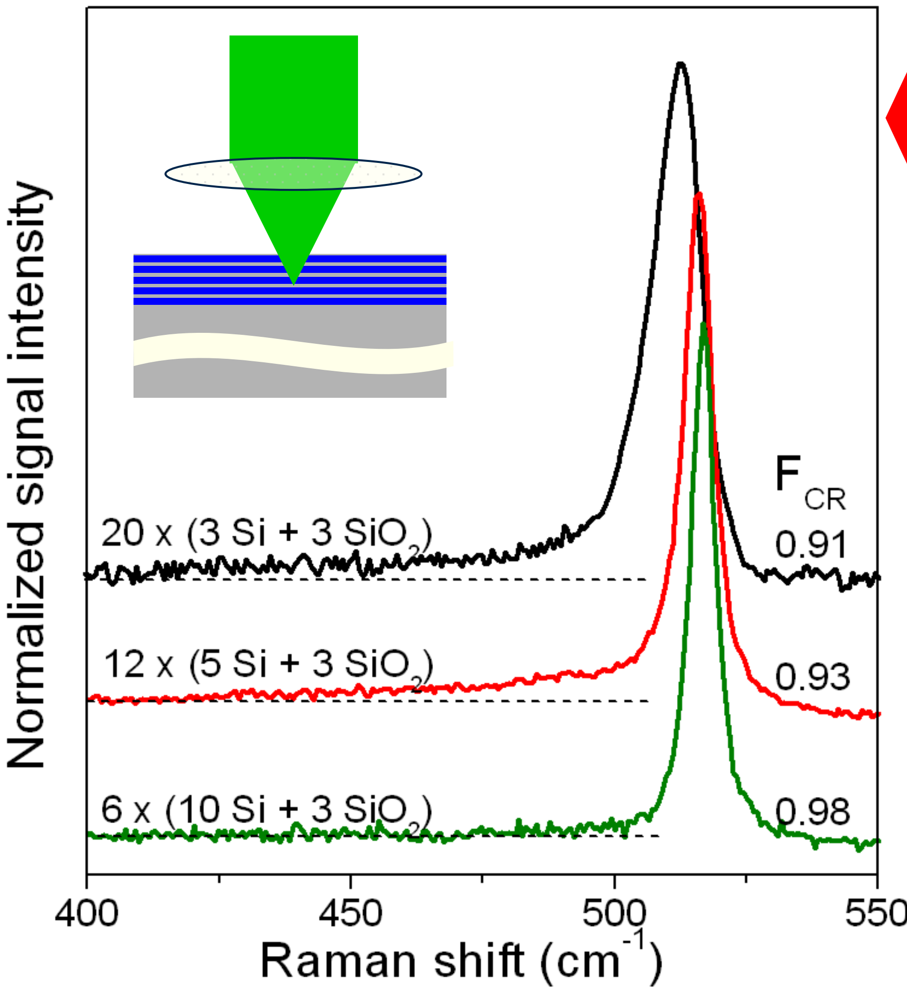


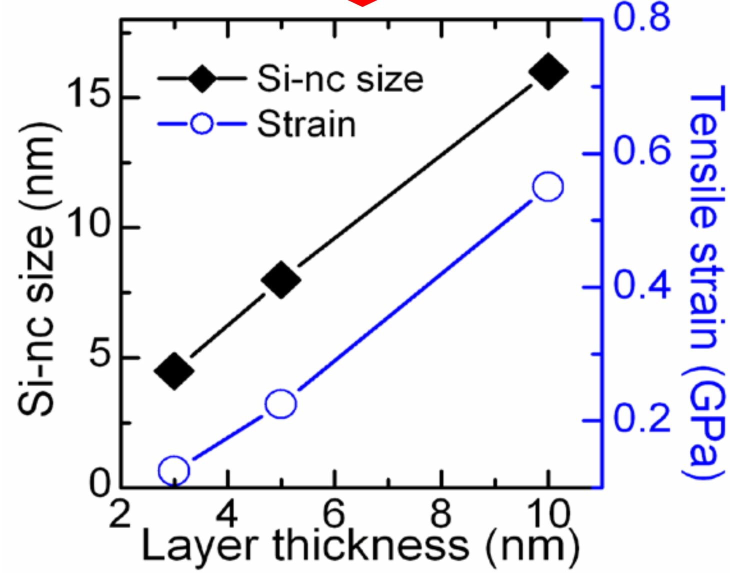
Convert a-Si to Si-nc using proper light flux @ ~500 nm.

Light induced crystallization: static mode



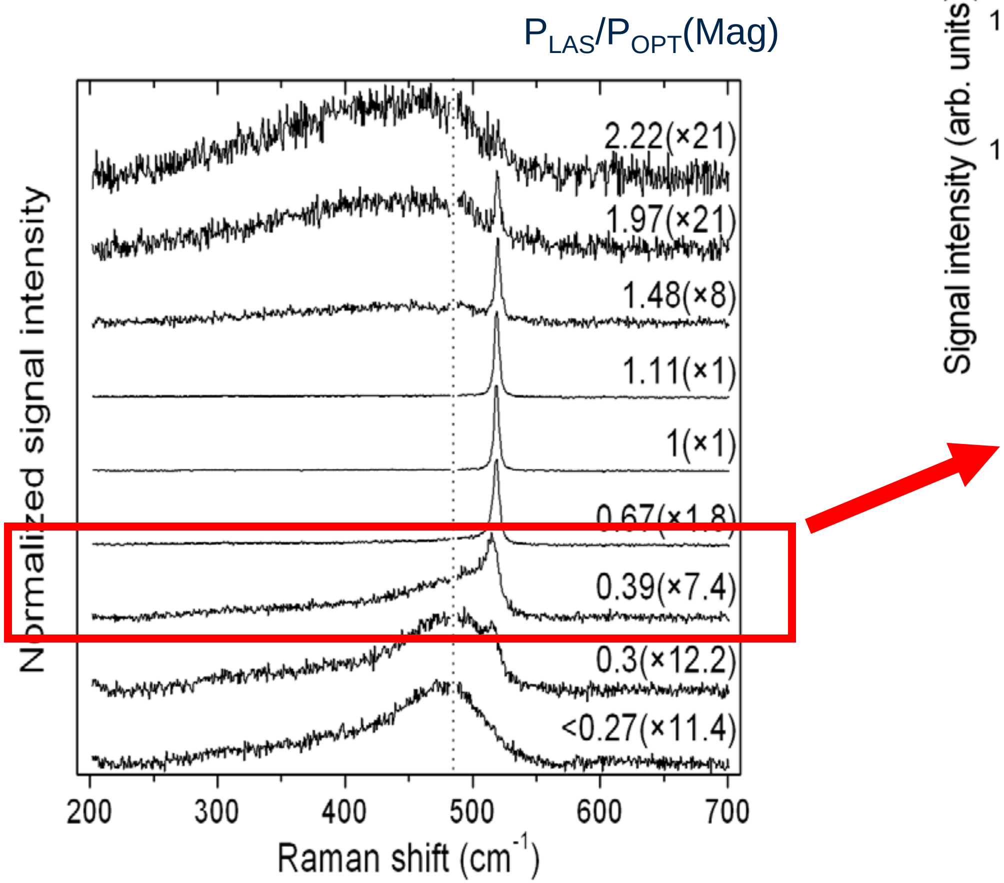
Raman spectra detected from various MQW crystallized in nearly optimal conditions of light flux @ 532 nm.

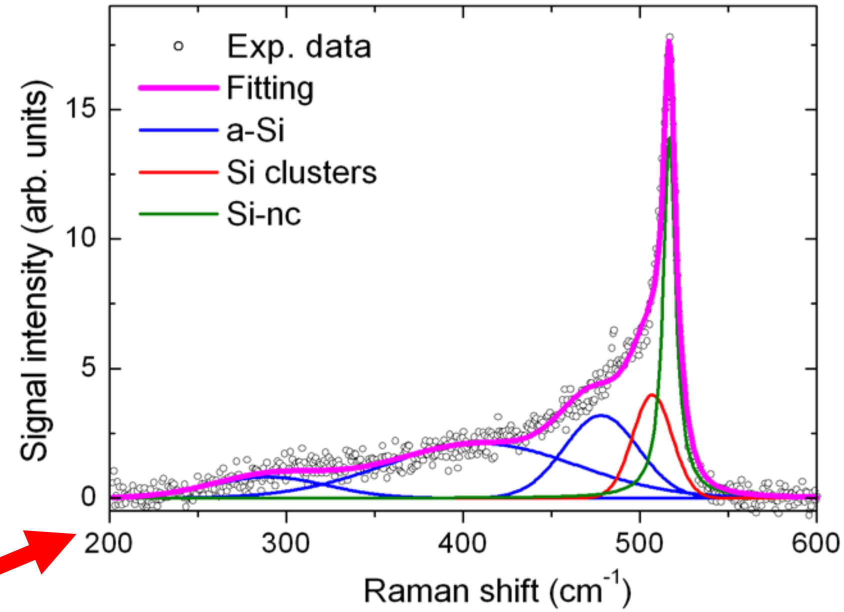
Sizes of Si-nc crystallites and strain in the MQWs estimated from Si-nc peak characteristics.



[T. Mchedlidze, et al., Phys. Rev. B **77,** 161304(R) (2008)]

Influence of light flux value



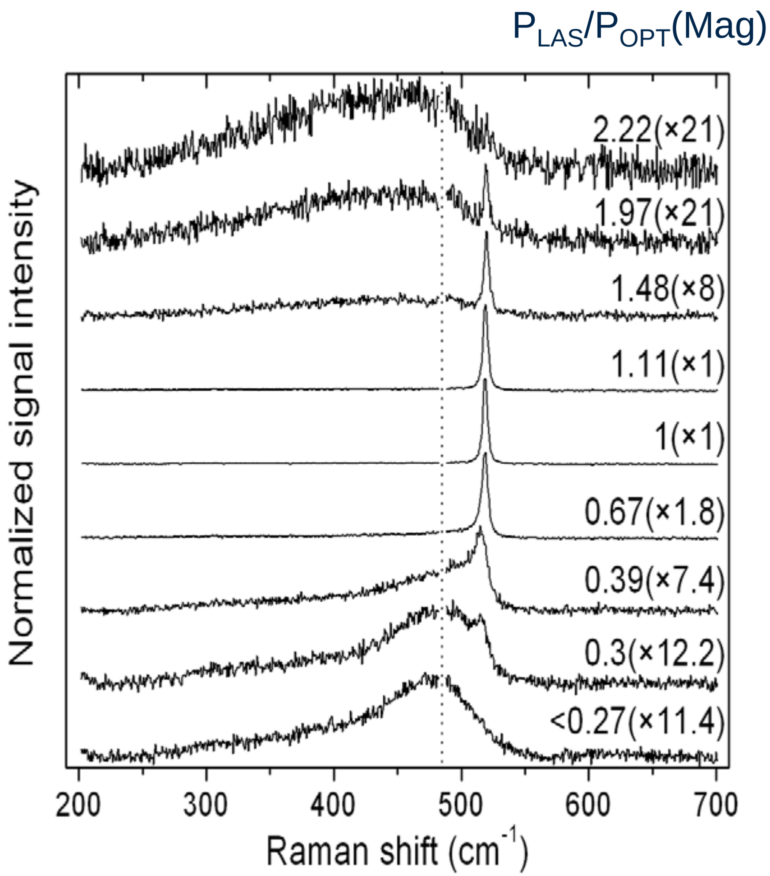


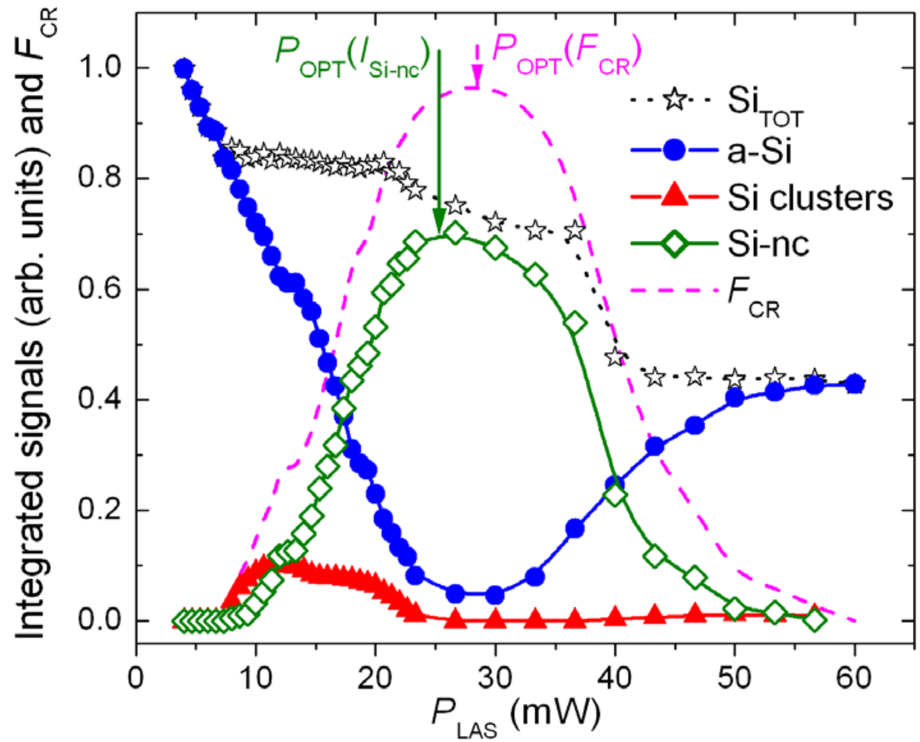
$I_{Si\text{-}nc}$

$F_{CR}=I_{Si\text{-}nc}/I_{Si}$

[T. Mchedlidze, et al., J. Appl. Phys. 107, 124302 (2010)]

Influence of light flux value



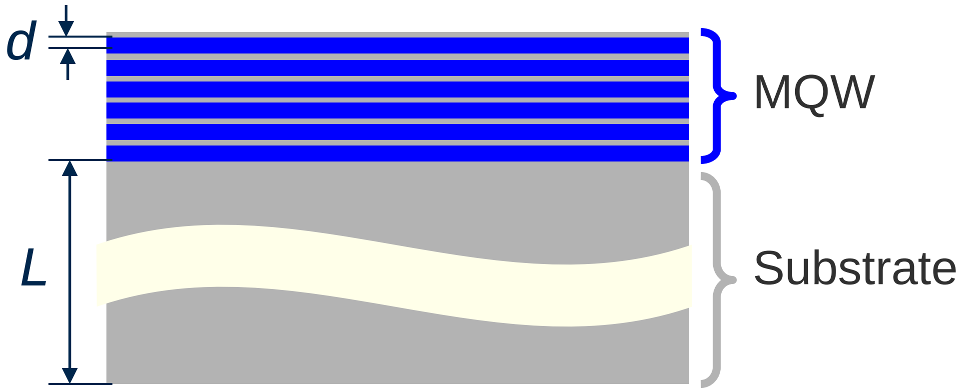


$$\eta = \left[\frac{I_{Si-nc}}{P_{LAS}} \right]$$

$$PR = \frac{P_{OPT}(I_{Si-nc})}{P_{OPT}(F_{CR})}$$

[T. Mchedlidze, et al., J. Appl. Phys. 107, 124302 (2010)]

Heating of MQW by light: assumptions



(a) Light is absorbed “only” in the Si layers of MQW

since @ λ_{LAS}= 532 nm

$\alpha_{QUARTZ} << \alpha_{Si\text{-}nc} < \alpha_{a\text{-}Si}$

(b) Heat transfer is determined by the properties of the substrate

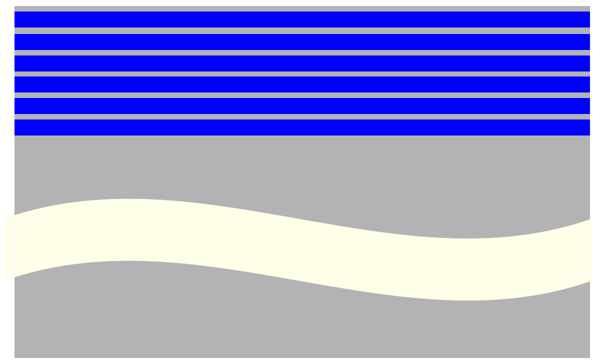
due to $n \cdot d << L$ and negligible lateral heat transfer in MQW layers

(c) consider heat transfer only perpendicular to the MQW surface

since beam radius >> $n \cdot d$

(d) Optical interference in MQW layers and **temperature dependences of the material properties could be neglected**.

Heating of MQW by light: modeling



Light absorption: α, R

Heat transfer: k, κ

≈ Heating of semi-infinite metal slab, by light beam having power: $P_{ACT} \approx n \cdot d \cdot \alpha \cdot P_{LAS}$

$$\Delta T(\tau) = \frac{\alpha P_{ACT} \beta^2 \kappa (1-R)}{\pi k} \int_0^\tau \frac{\exp(\alpha^2 \kappa t)\,\mathrm{erfc}(\alpha \sqrt{\kappa t})}{1 + 4\beta^2 \kappa t} dt$$

[B. J. Bartholomeusz, J. Appl.Phys. **73**, 1066 (1993)]

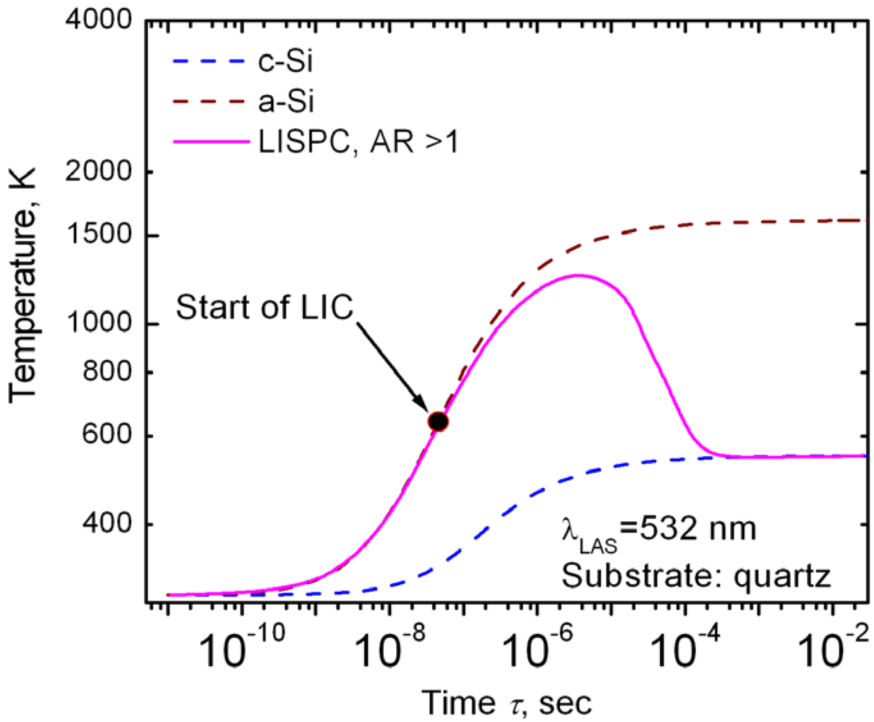
α is absorption coefficient, k is thermal conductivity, κ is thermal diffusivity, R is reflectance, $\beta = 1/\sqrt{2}\sigma_{eff}$, with σ_{eff} an irradiance radius of the laser spot.

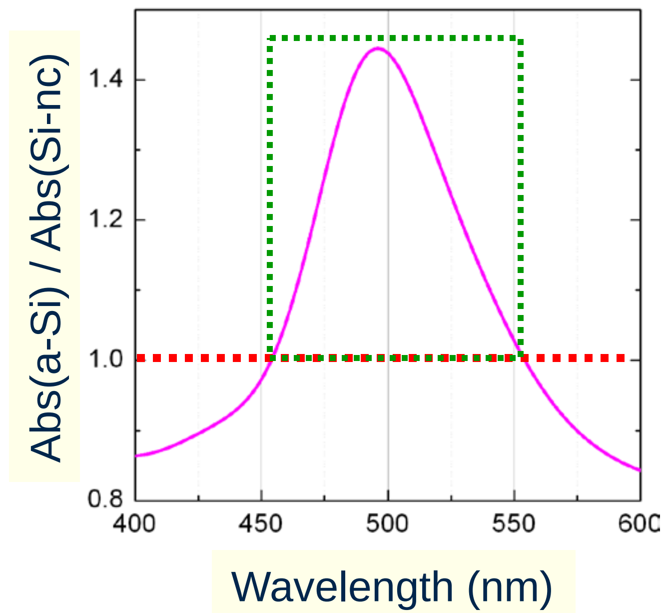
All parameters could be found in publications.

Heating of MQW by light + LIC

Optimal light flux, λ=532 nm

$$AR(\lambda) = \frac{Abs(a-Si)}{Abs(Si-nc)}$$



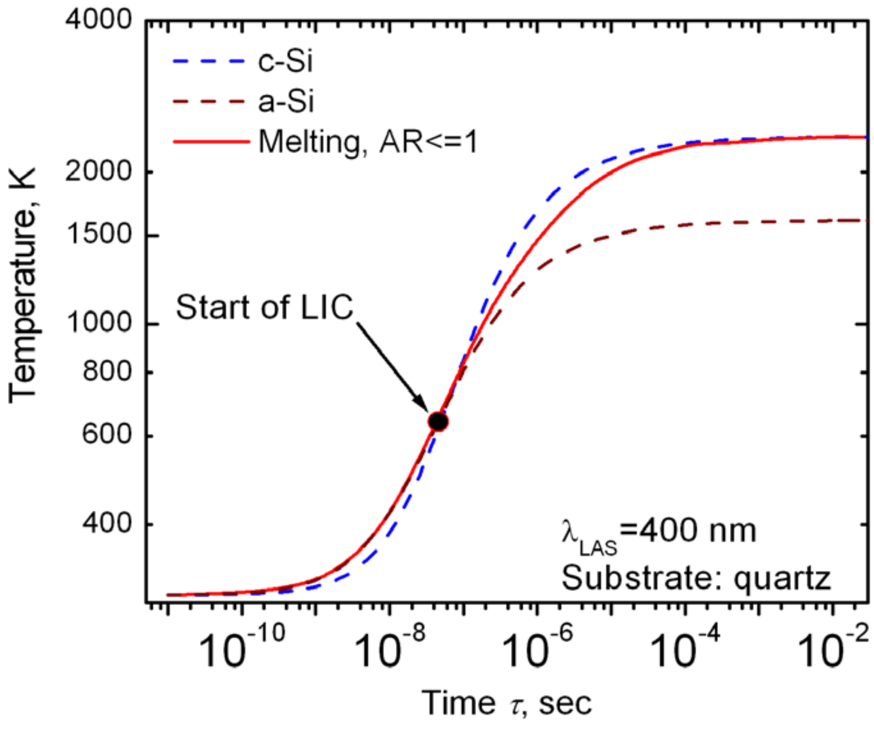


Wavelength dependence of LISPC was obtained experimentally

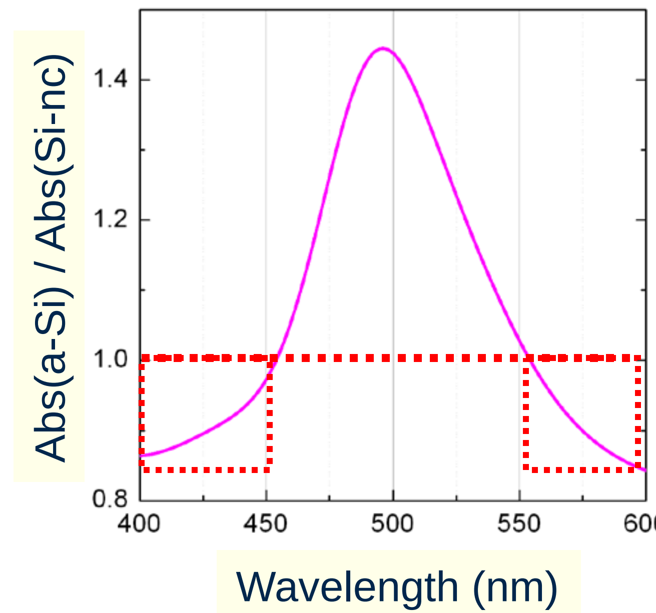
[T. Mchedlidze, et al., J. Appl. Phys. 107, 124302 (2010)]

Heating of MQW by light + LIC

Optimal light flux, λ=400 nm



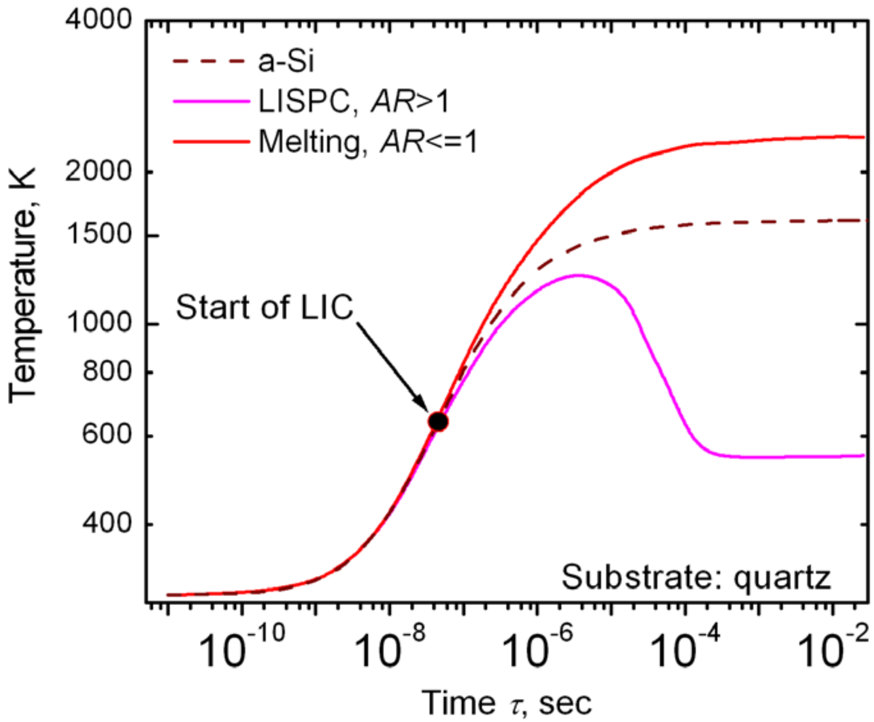
$$AR(\lambda) = \frac{Abs(a-Si)}{Abs(Si-nc)}$$



Wavelength dependence of LISPC was obtained experimentally

[T. Mchedlidze, et al., J. Appl. Phys. 107, 124302 (2010)]

Heating of MQW by light + LIC



$$AR(\lambda) = \frac{Abs(a-Si)}{Abs(Si-nc)}$$

- For *AR*>1, “negative feedback”, self-regulated LISPC possible.
- For *AR*≤1, “positive feedback”, LIC easily transfers to melting.
- Larger *AR* → more efficient LISPC, less changes in MQW after finish of crystallization.

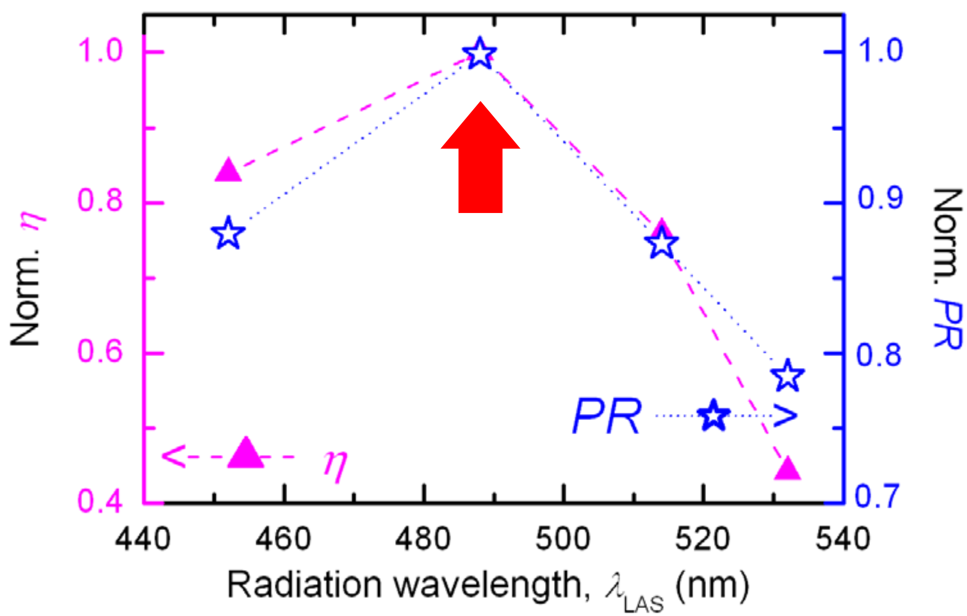
Wavelength dependence of LISPC was obtained experimentally

[T. Mchedlidze, et al., J. Appl. Phys. 107, 124302 (2010)]

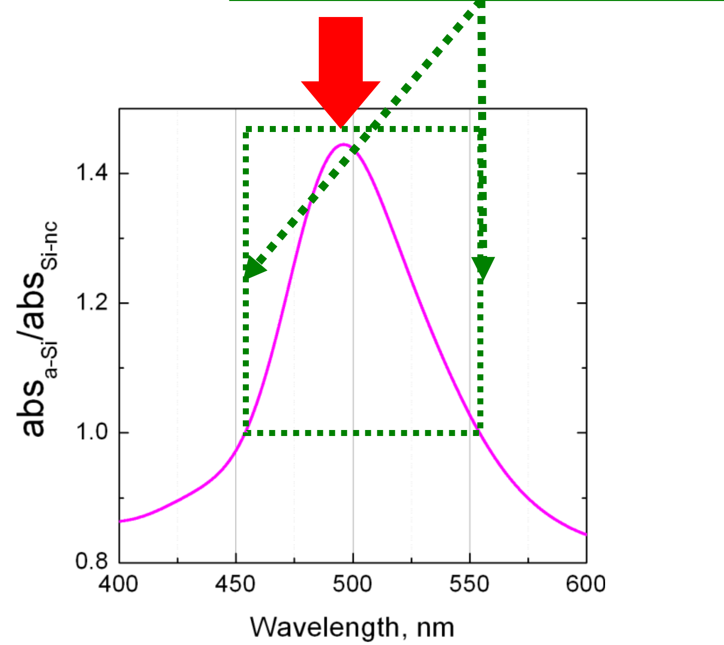
Efficiency of LIC at various λ_{LAS}

$$\eta = \left[\frac{I_{Si-nc}}{P_{LAS}}\right]_{OPT} \rightarrow \eta(\lambda_{LAS}) \propto \frac{I_{Si-nc}(\max)}{P_{OPT}\cdot[1-\exp(-\alpha n d)]}$$

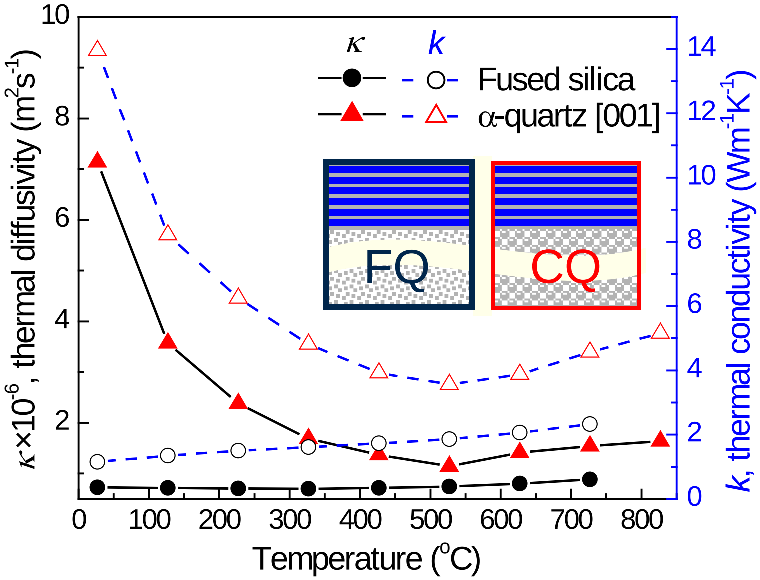
Optimal power ratio $\rightarrow$ $PR(\lambda_{LAS}) = \dfrac{P_{OPT}(I_{Si-nc})}{P_{OPT}(F_{CR})}$



λ_{LAS} Range for LISPC



Efficiency of LISPC for various substrates

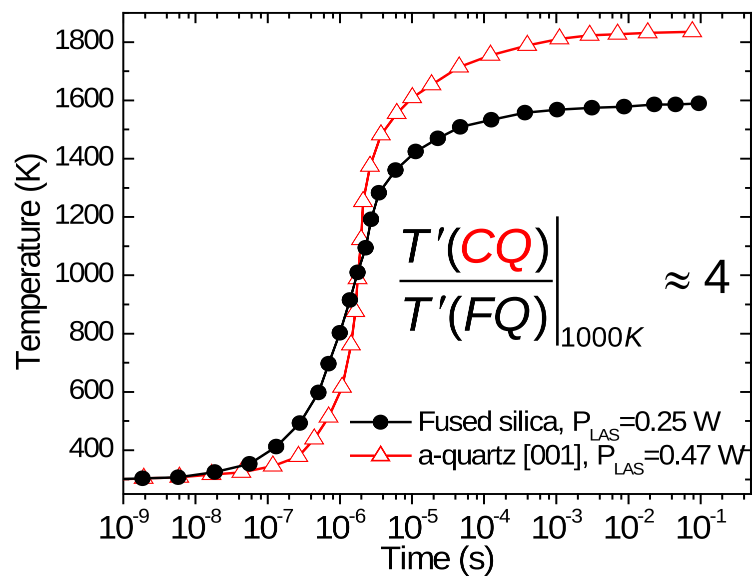


@ optimal LISPC conditions:

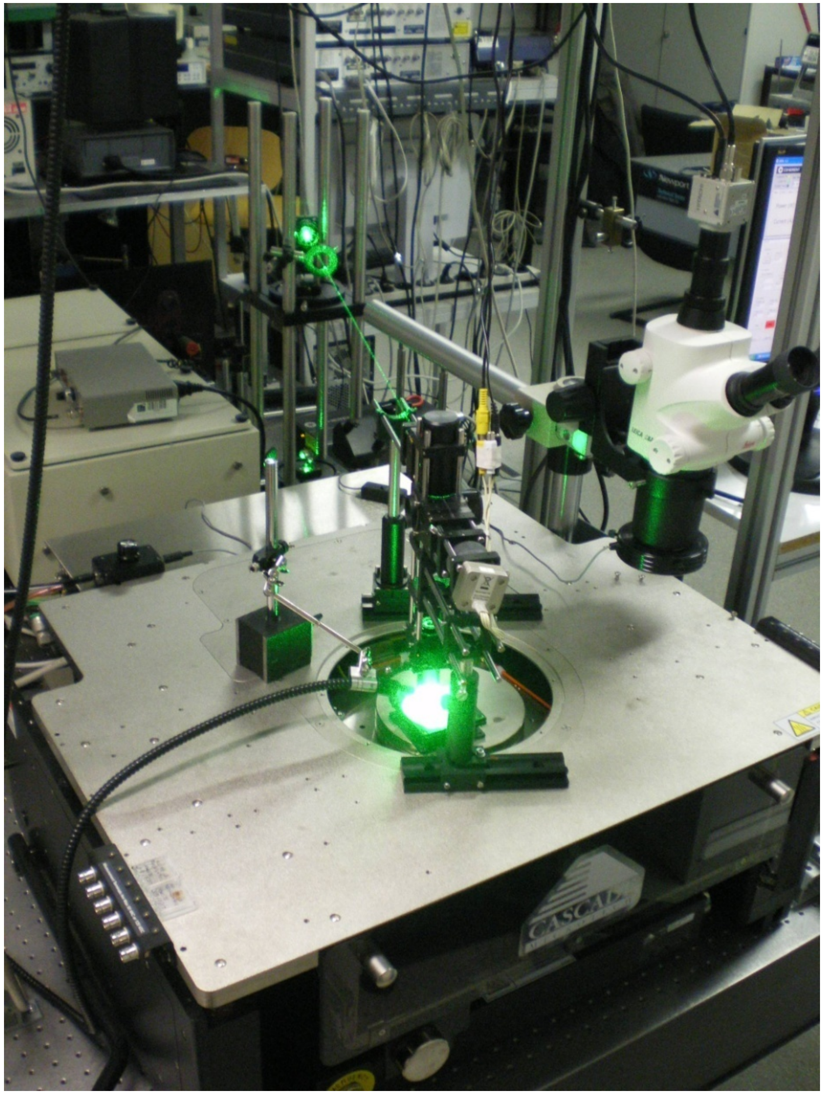
- $I_{Si\text{-}nc}$(FQ) ≈ 1.25 $I_{Si\text{-}nc}$(CQ)
- P_{OPT}(FQ) ≈ 0.5 P_{OPT}(CQ)
- Large compressive (CQ) vs. small tensile (FQ) residual stress.

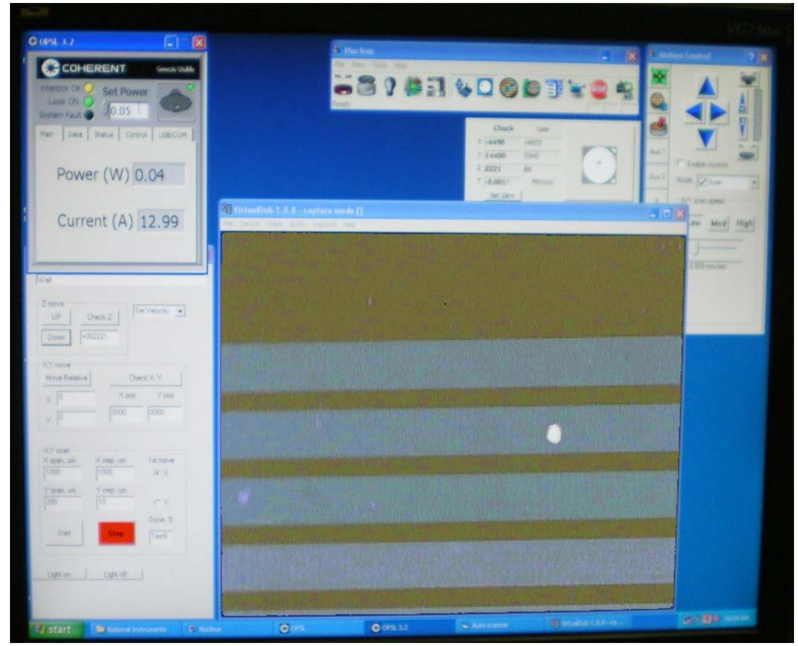
$$\frac{\eta(FQ)}{\eta(CQ)} \approx 2.5$$

- $T(t)$ dependencies could be roughly estimated using $\kappa(T)$ and $k(T)$.
- Larger $T'=(dT/dt)$ at the moment of crystallization for α-quartz substrate.



Installation for fast LISPC





λ_{LAS}= 532 nm

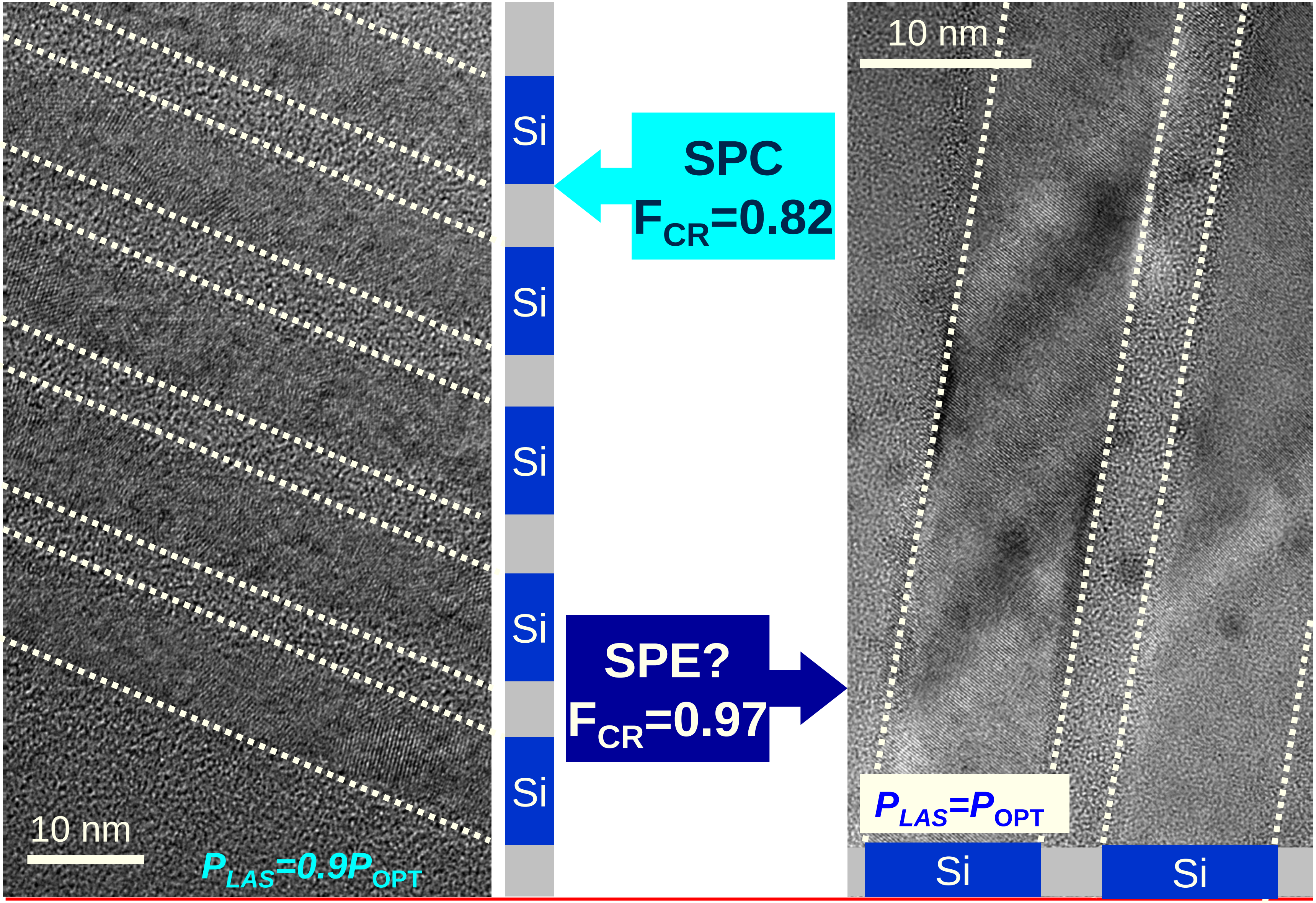
Laser power ~ 400 mW

Focal distance : 12-15 mm

Scanning speed: 0.3 mm/sec

Process rate: 5×10^{-3} mm^2/sec

XHRTEM for MWQ with 10 nm thick Si layers



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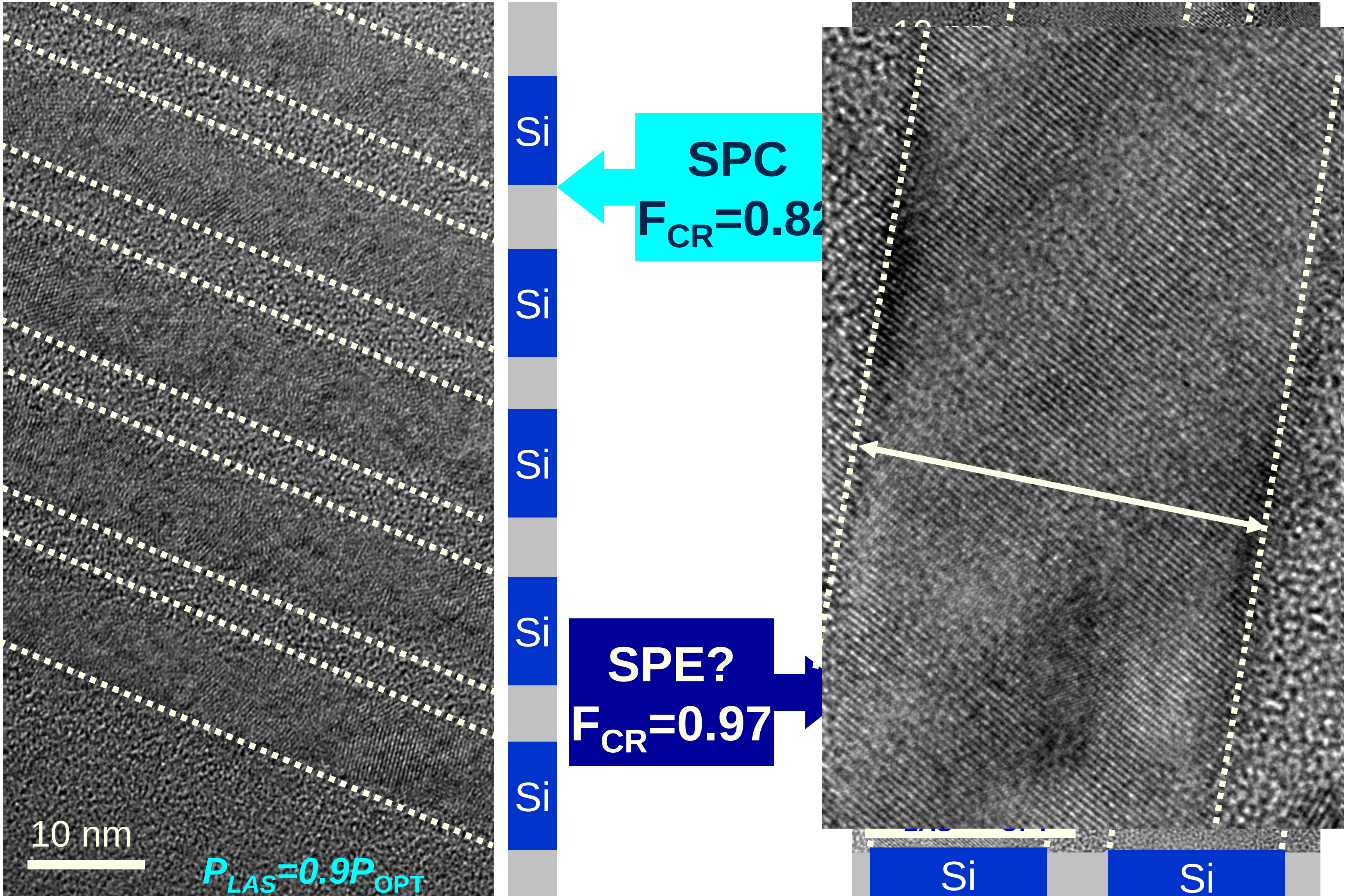
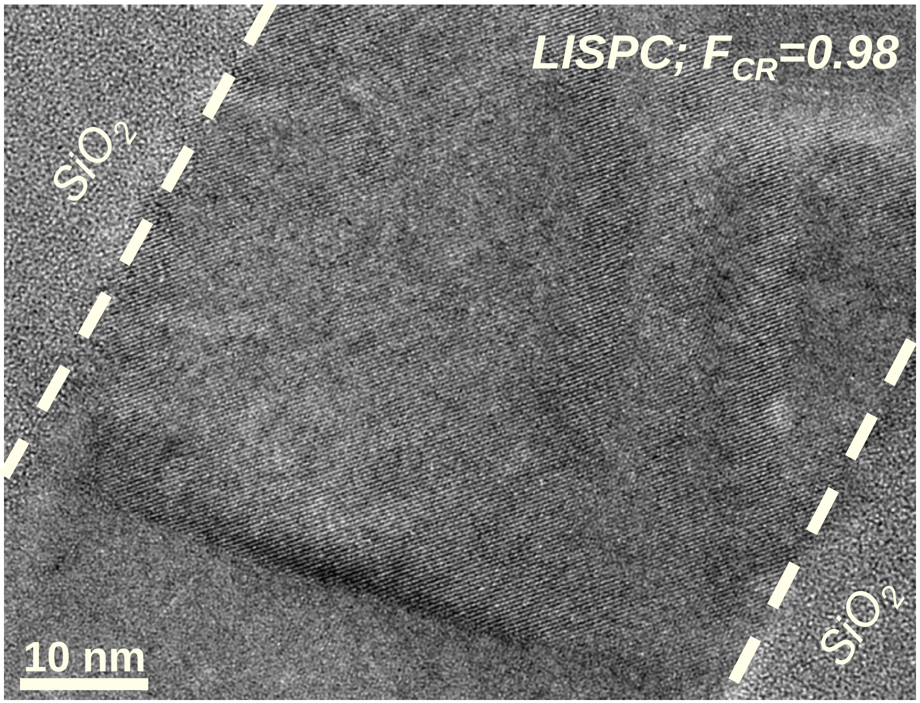
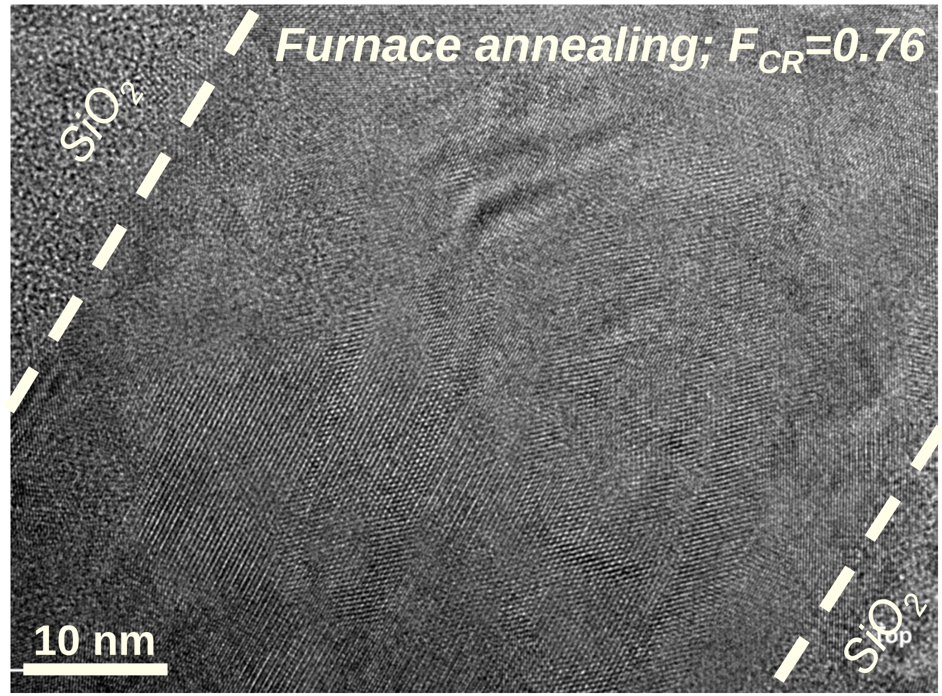
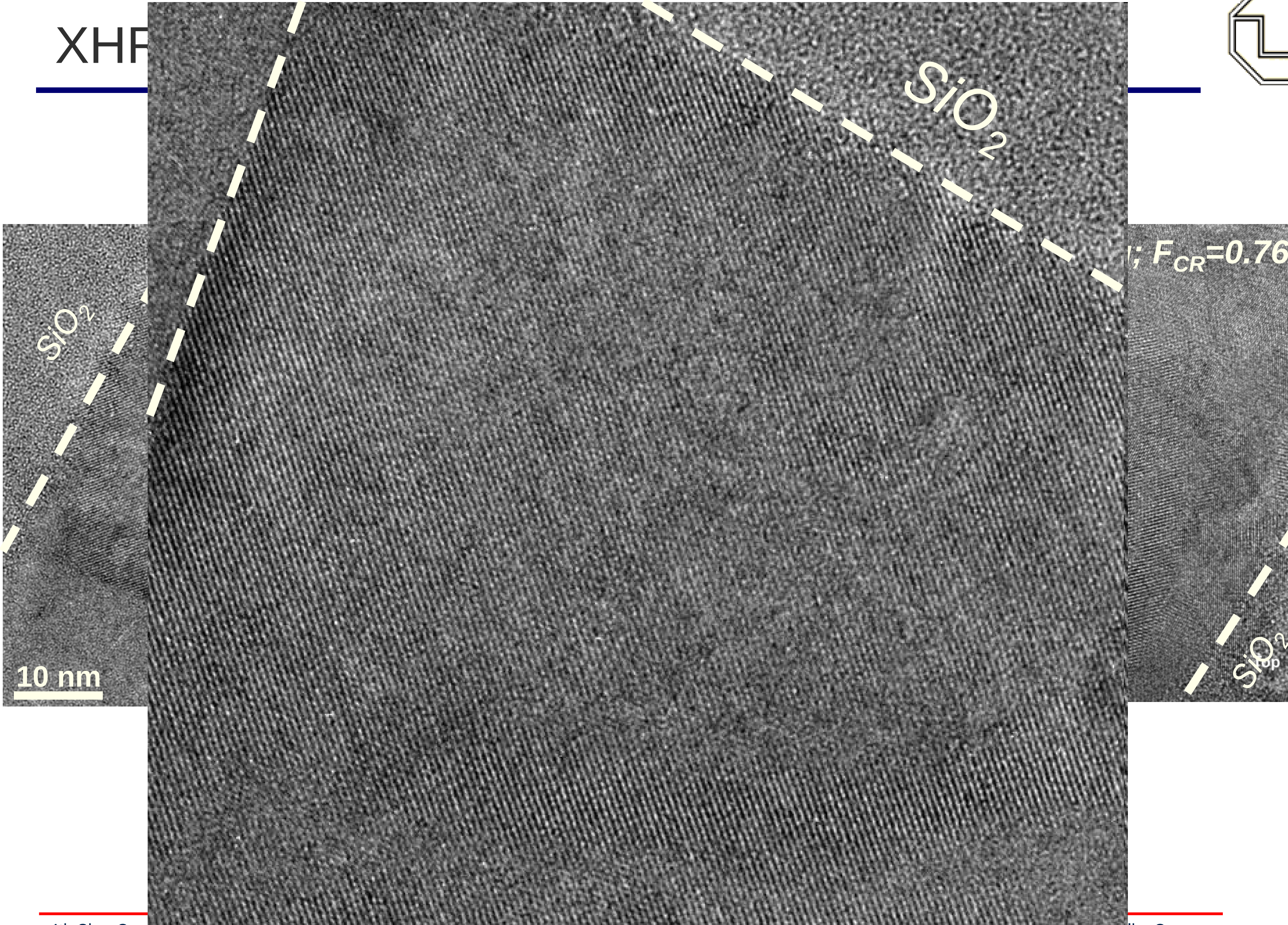


XHRTEM for 60 nm Si film inside SiO_2 layers

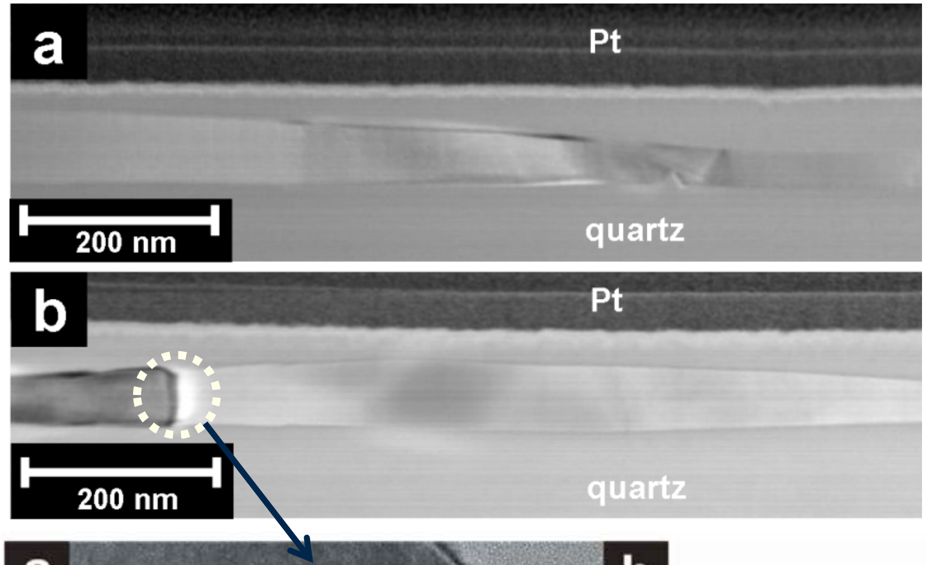




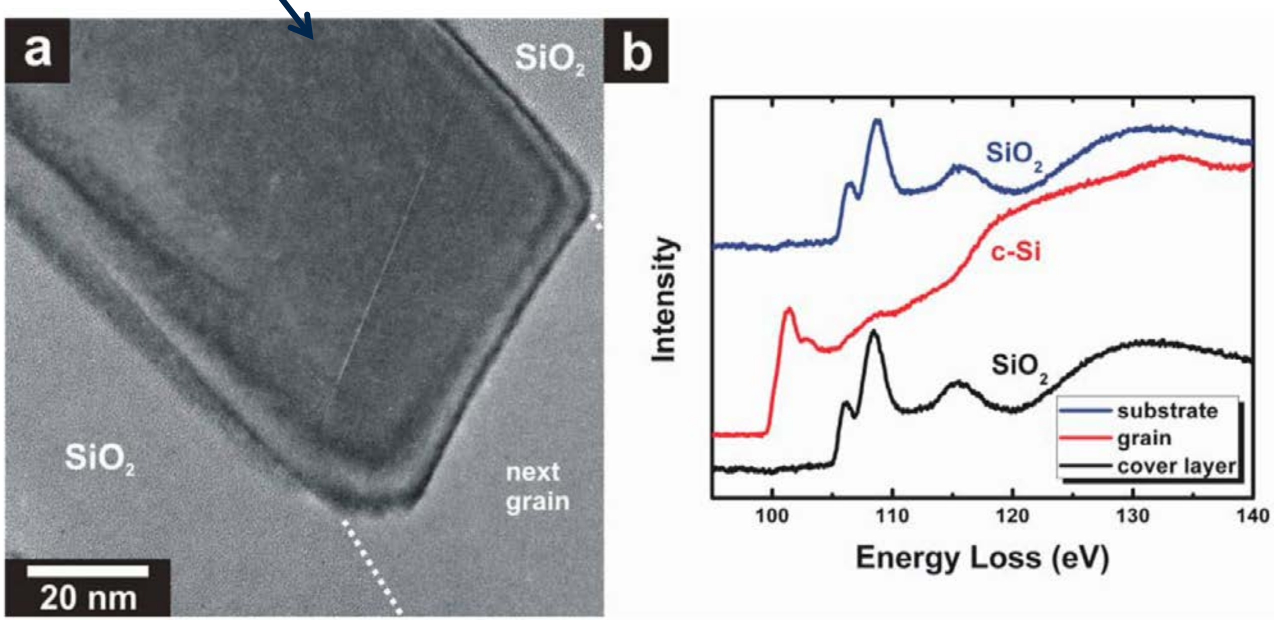
XHR



Quality for 60 nm Si film inside SiO_2 layers



Long-range "panoramic" images show high quality crystalline layers for the distances comparable with the diameter of light beam.

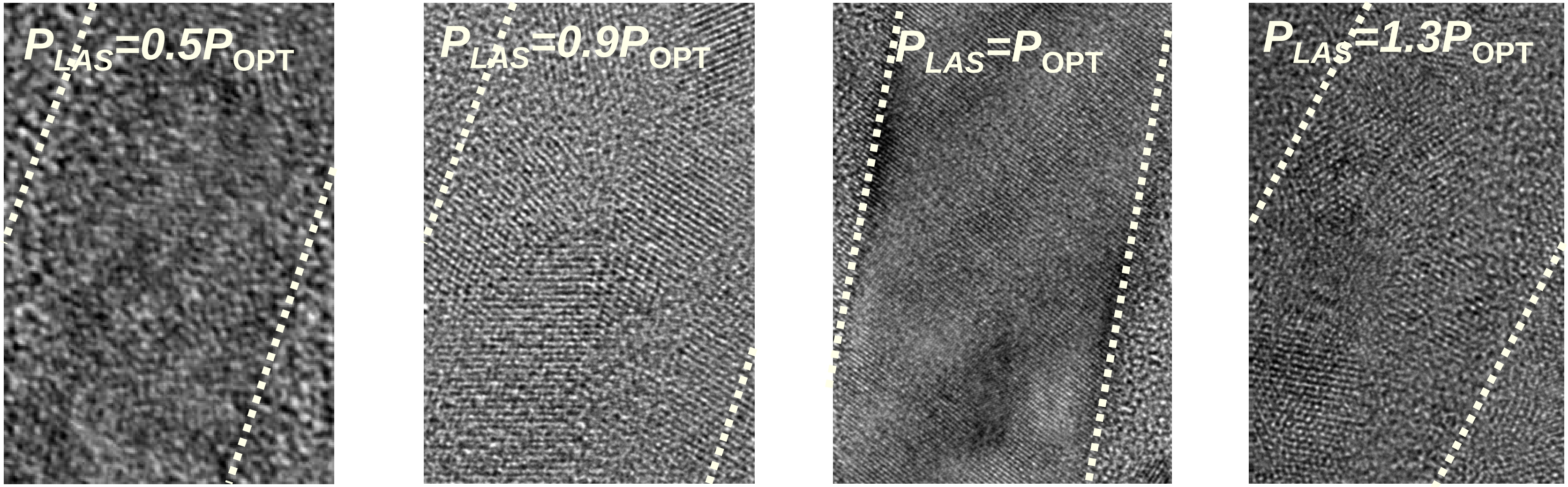


The EEL spectrum of the grain is typical for single crystalline silicon with a low content of lattice defects and reflects the high grade of crystallinity.

Influence of hydrogen and external conditions

- ***Hydrogen*** contained in a-Si layers enhances possibilities of successful LIC. For Si layers with outdiffused hydrogen "window" of optimal illumination conditions shrinks. However, too much hydrogen is also not good!
- Presence of ***oxygen*** in the ambient has small influence on the process – "internal" oxidation plays the major role.
- ***Thermal properties of ambient*** can change thermal exchange in the system during crystallization. Namely, LISPC in water ambient although possible requires much larger light fluxes.
- ***Gas pressure*** has small influence on the crystallization process itself but at low ambient pressure outgassing of hydrogen may cause damage of the MQW structure (formation of craters).
- The results on controlling of ***substrate temperature*** can be applied for optimization of LISPC process for various substrate materials.

Summary: Light power dependence



$(0.95\div1.05)P_{OPT}$
$F_{CR}=0.95\div1$
SPE

$(0.8\div0.95)P_{OPT}$
$F_{CR}=0.8\div0.95$
SPC

$(1.1\div1.5)P_{OPT}$
$F_{CR}=0.9\div0.5$
Melting

$(0.3\div0.8)P_{OPT}$
$F_{CR}=0.1\div0.8$
Nucleation

Flux=n×10^5 W/cm^2

$(1.5\div2)P_{OPT}$
$F_{CR}=0.5\div0.1$
Intermixing

$<0.3P_{OPT}$
$F_{CR}<0.1$
Heating

n depends on: λ, H content, substrate, layer thickness…

$>2P_{OPT}$
$F_{CR}<0.1$
Dissolution

Summary

- LISPC is fast, self-regulated, a-Si→Si-nc solid-to-solid transition process at *λ* when $\alpha_{a\text{-}Si}(\lambda) > \alpha_{Si\text{-}nc}(\lambda)$;
- The maximal efficiency for LISPC:
    - $\alpha_{a\text{-}Si}(\lambda)/\alpha_{Si\text{-}nc}(\lambda)$ @ max;
    - Light flux should be maximally accommodated by the crystallization process;
    - Optimal substrate should be used.
- Crystalline quality after LISPC is much better then after RTA or LA.
- The process should be applicable also for crystallization of a-Si films on a substrate.

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  B. Berghoff and N. Wilck (RWTH, Aachen, Germany).

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  M. Schade and H. S. Leipner (Interdisziplinäres Zentrum für Material-wissenschaften, Halle, Germany).

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Thank You for attention!