



POWDER DIFFRACTION

Synchrotrons

Kenny Ståhl
DTU Chemistry



CONTENTS

- Why synchrotrons
- Resolution
- High angular resolution
- Time resolution
- Energy resolution
- High pressure



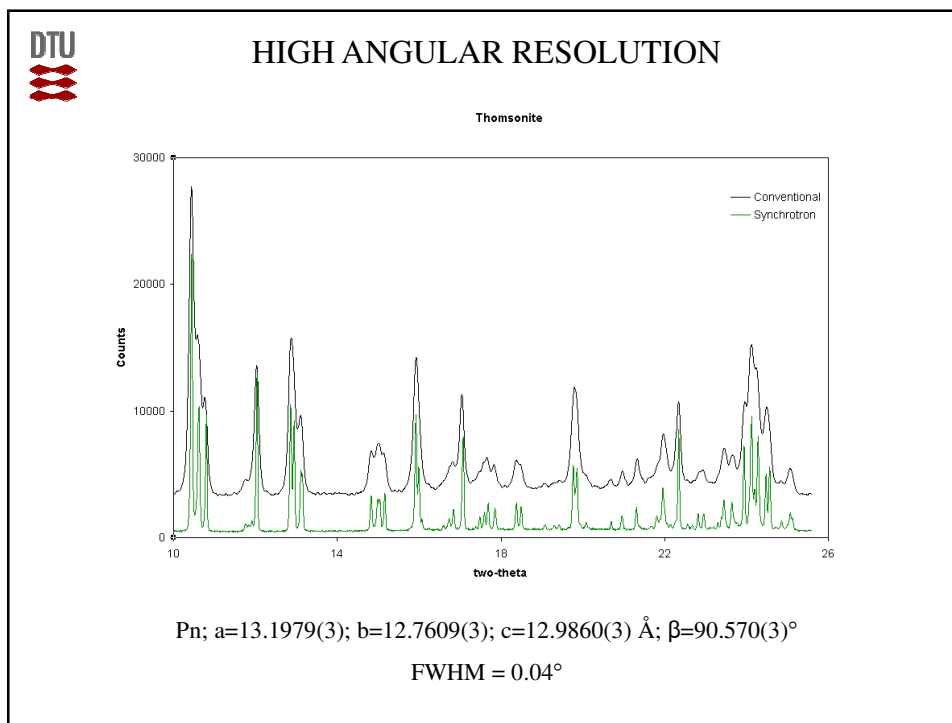
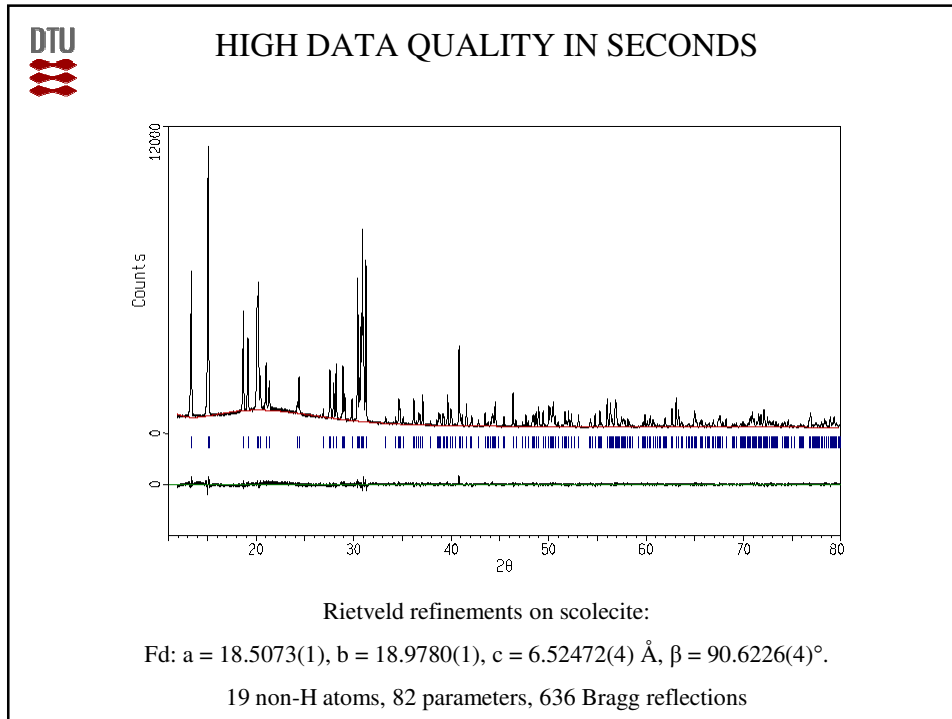
MATERIAL SCIENCES – WHY SYNCHROTRONS?

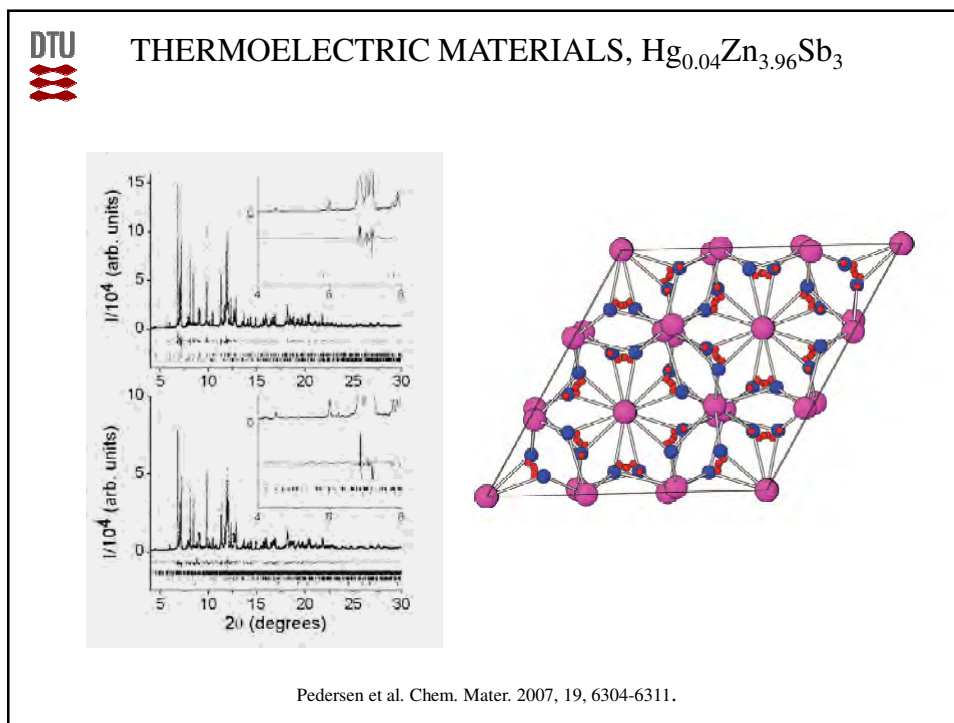
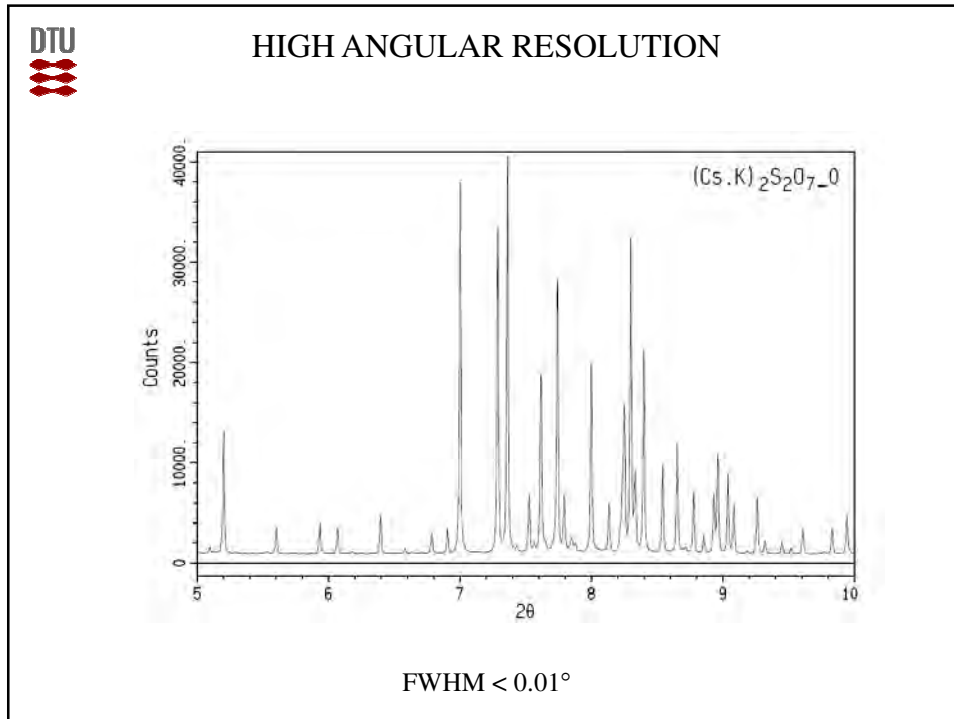
- | | |
|--------------------------|--|
| •High intensity | Good statistics
Short exposure - In situ measurements |
| •High angular resolution | Phase identification, structure refinements, structure solutions |
| •Short exposure | In situ measurements |
| •Variable wavelength | Anomalous dispersion contrast, short wavelengths for environmental cells |
| •High brilliance | Local probing |

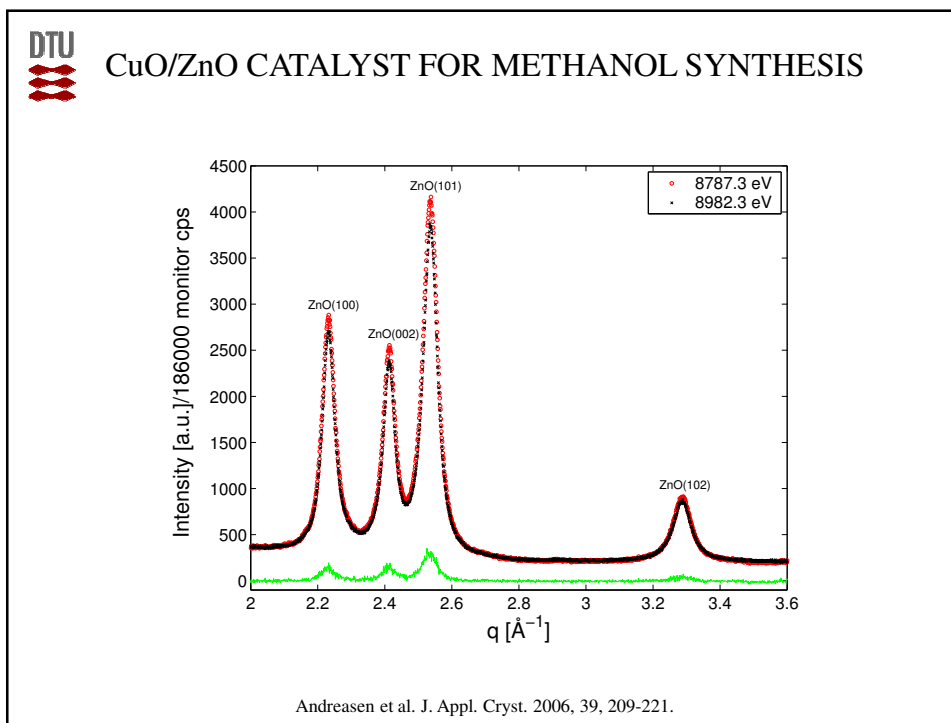
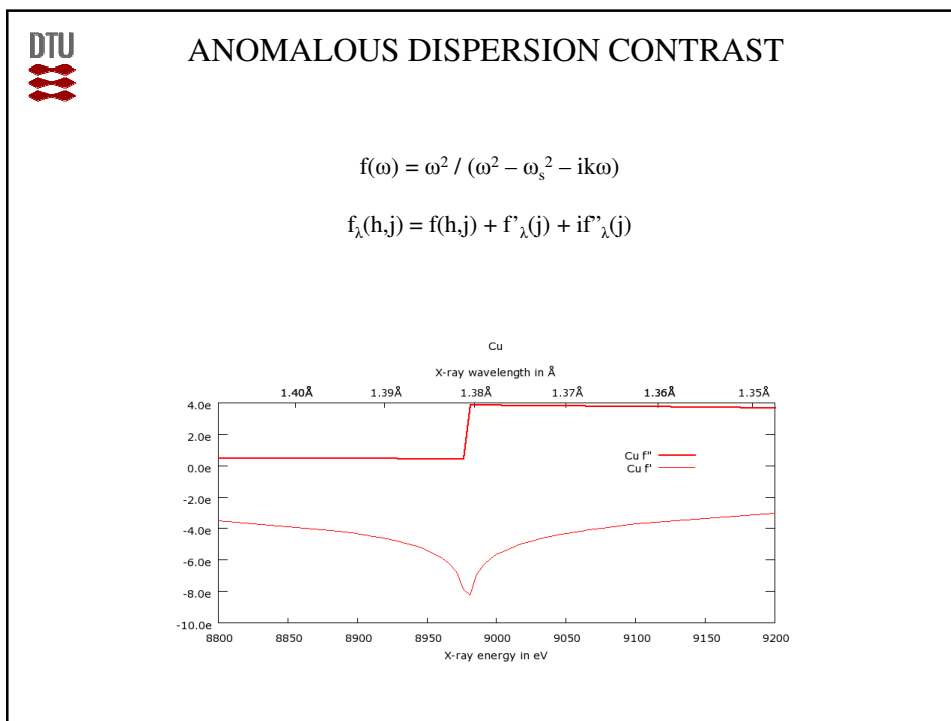


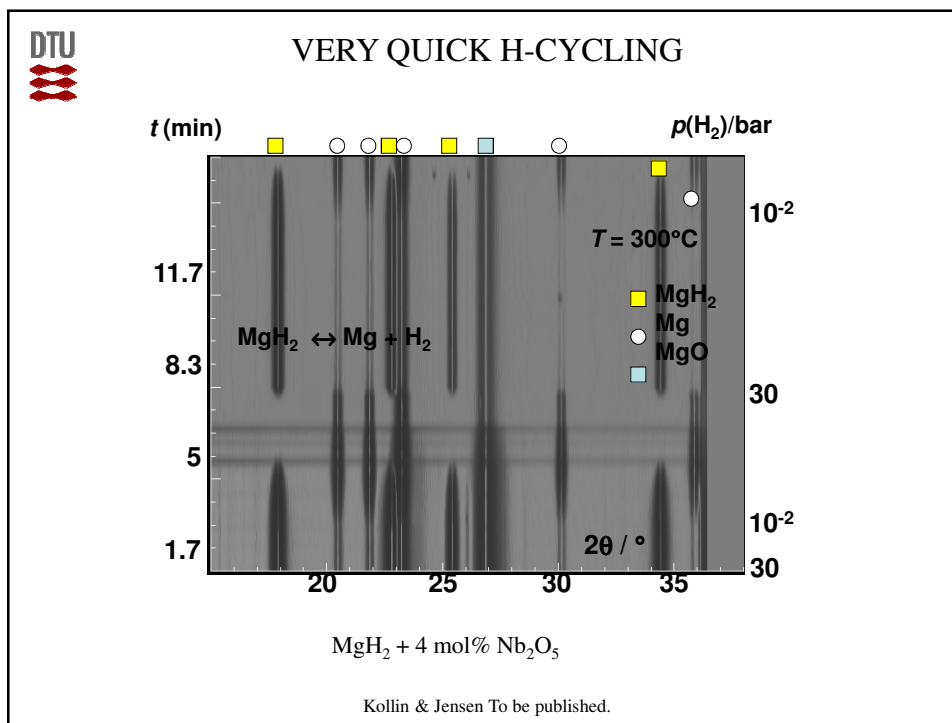
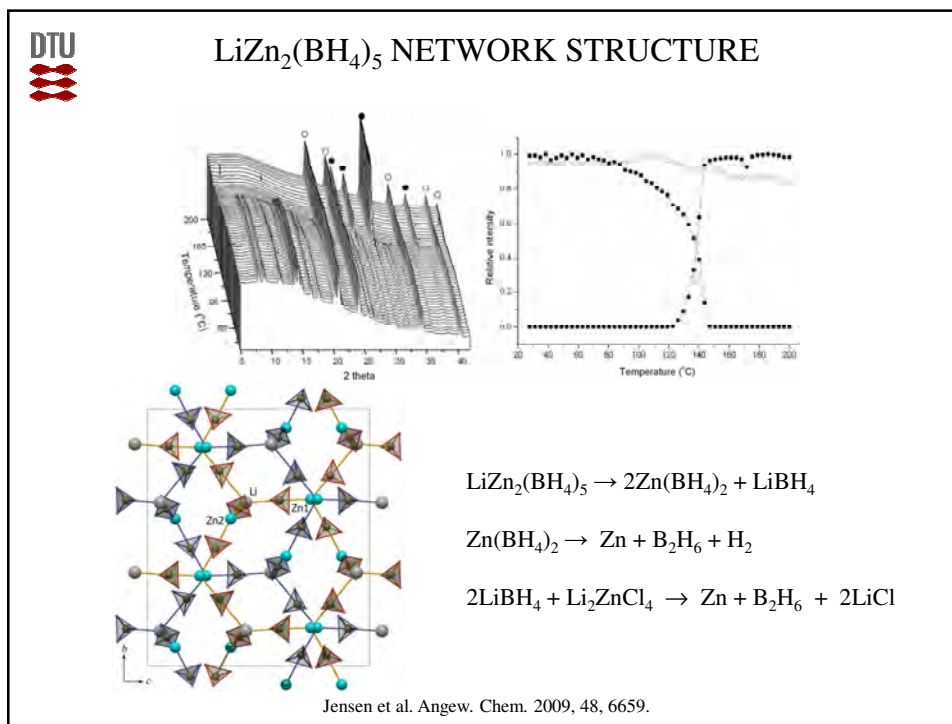
RESOLUTION

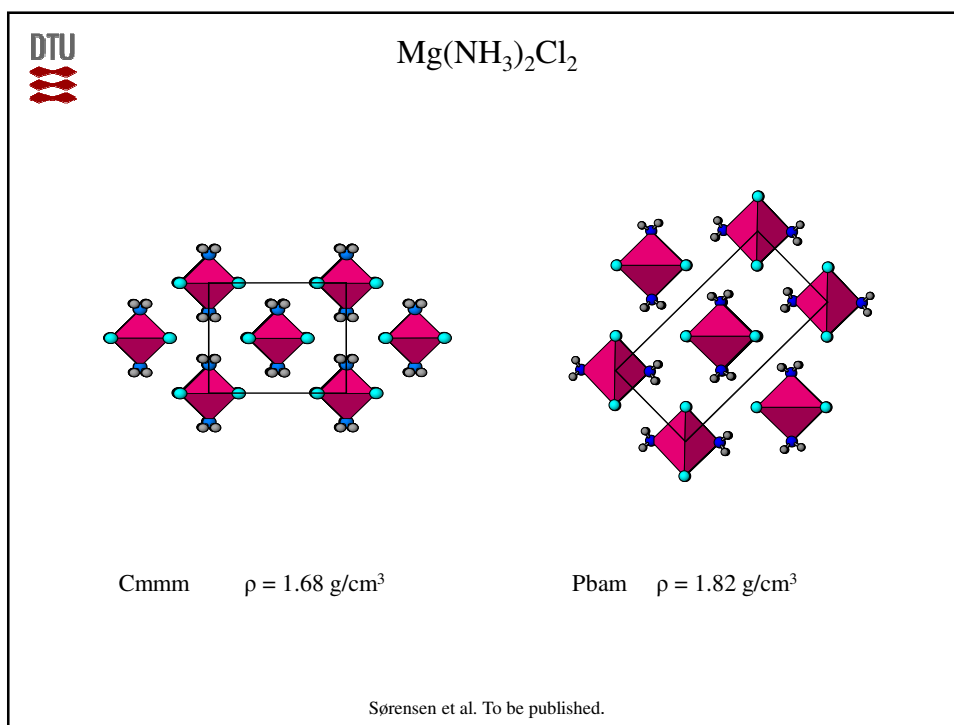
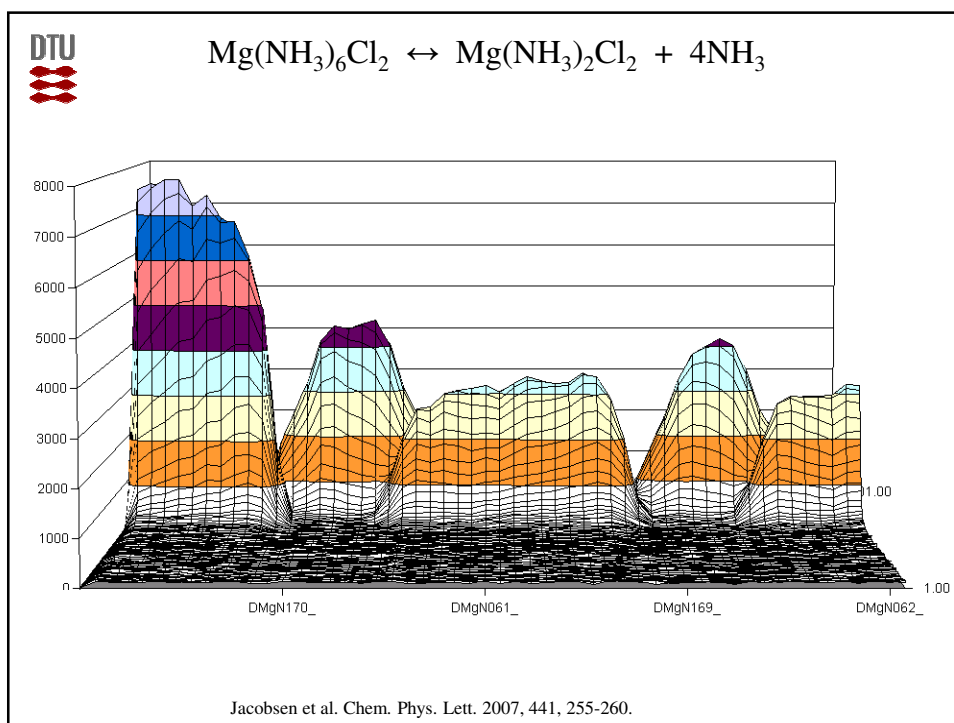
- | | |
|-----------------------|---|
| •Angular resolution | Peak resolution
$\sin\theta/\lambda$ -resolution |
| •Time resolution | Beam intensity vs. detectors |
| •Energy resolution | Peak resolution vs. time resolution |
| •Intensity resolution | Dynamic range |
| •Spatial resolution | Beam size
Room for experiments |







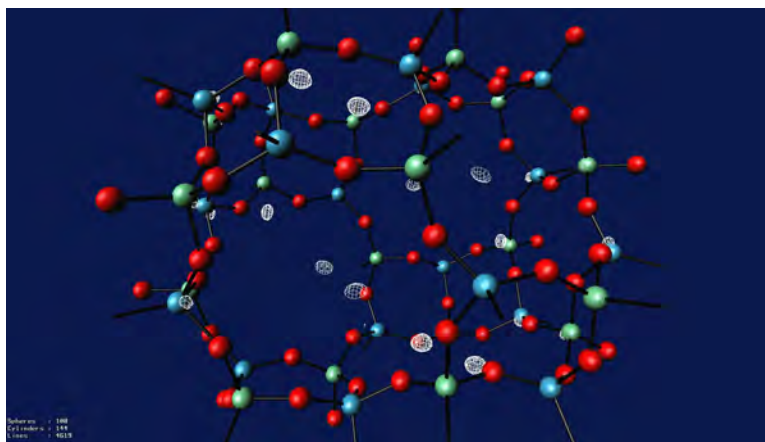






SAPO-34 METHANOL-TO-OLEFIN CONVERSION

t = 0 min

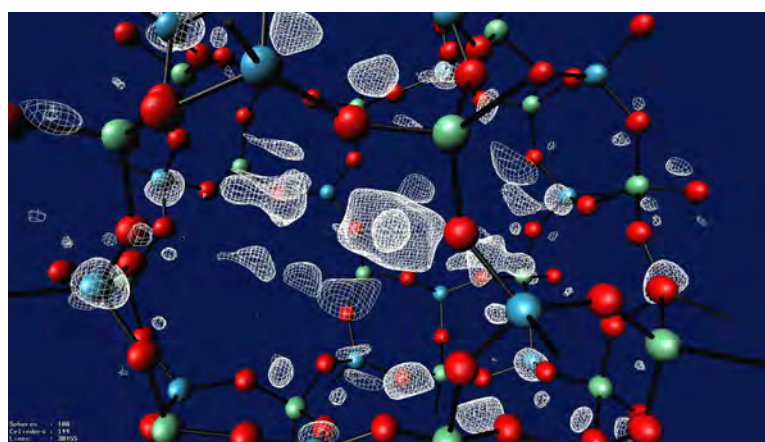


Wragg et al. J. Catal. 2009, 268, 290-296.

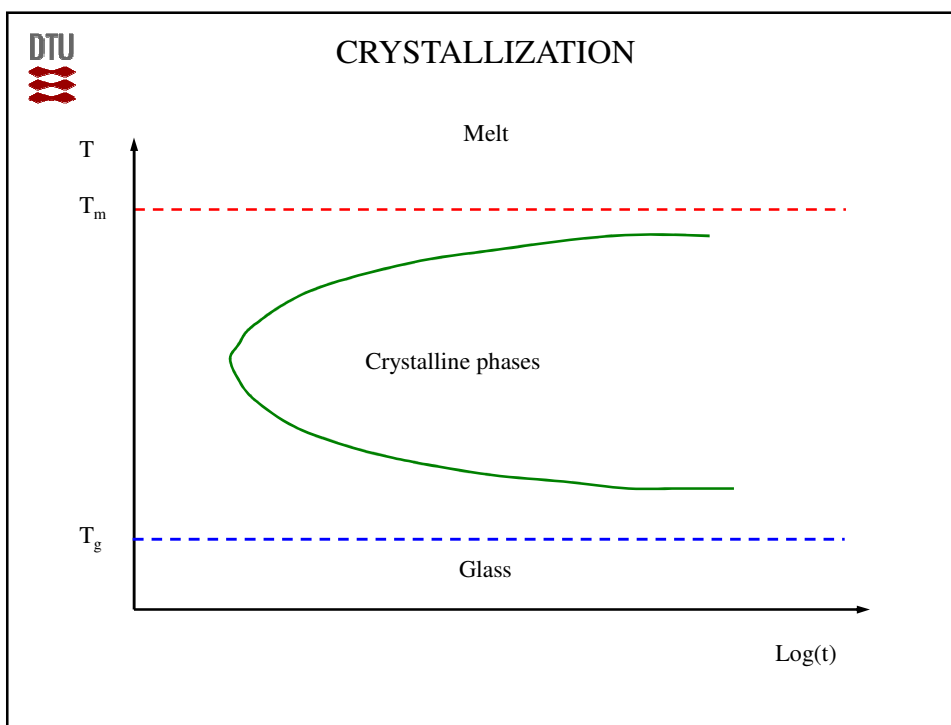
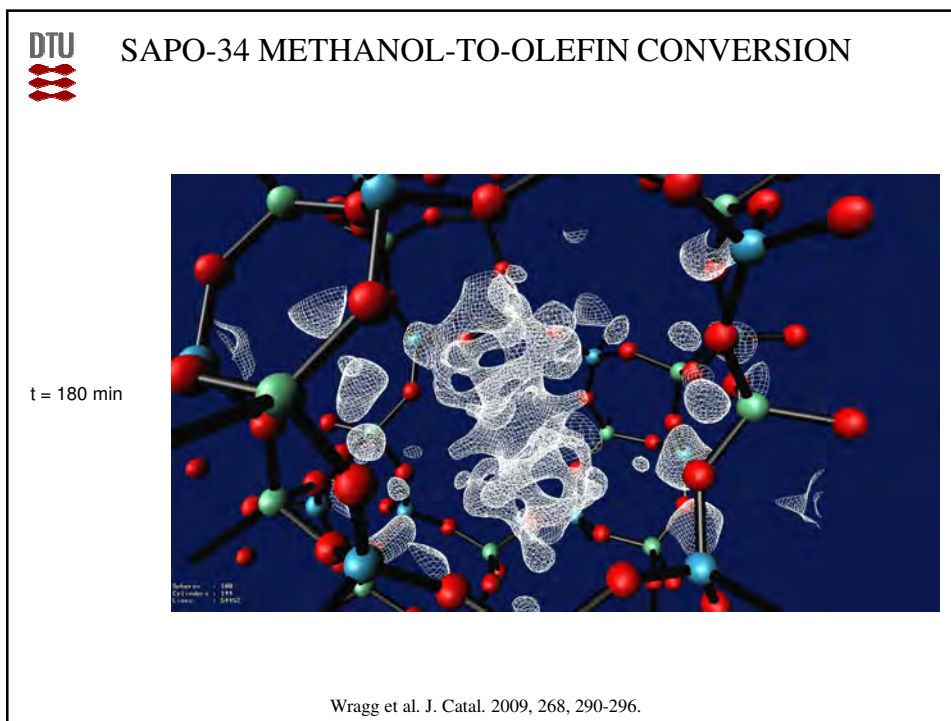


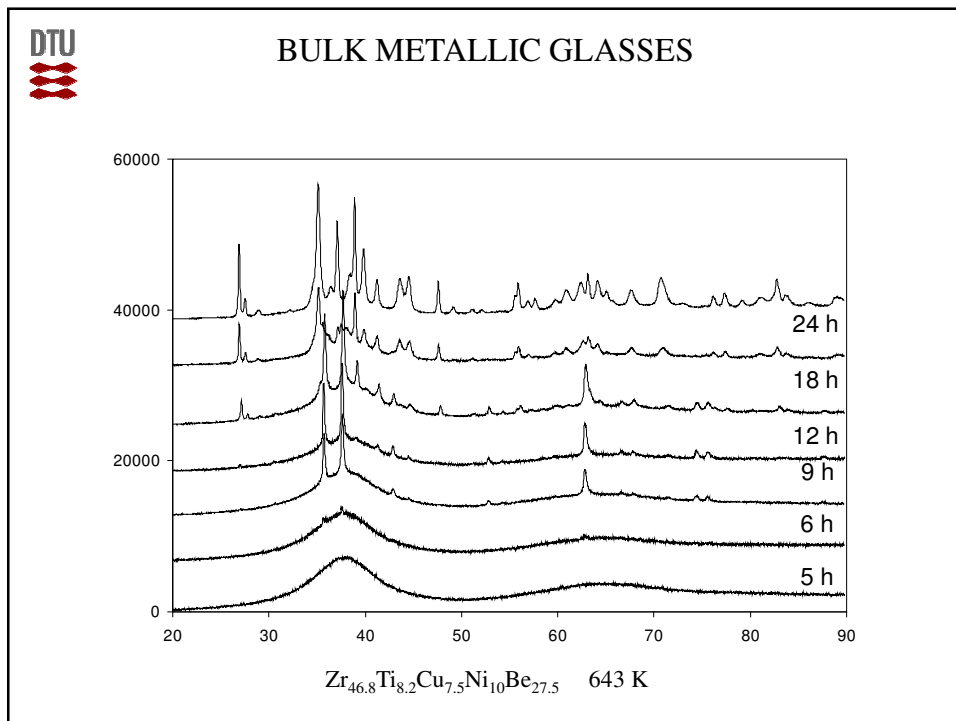
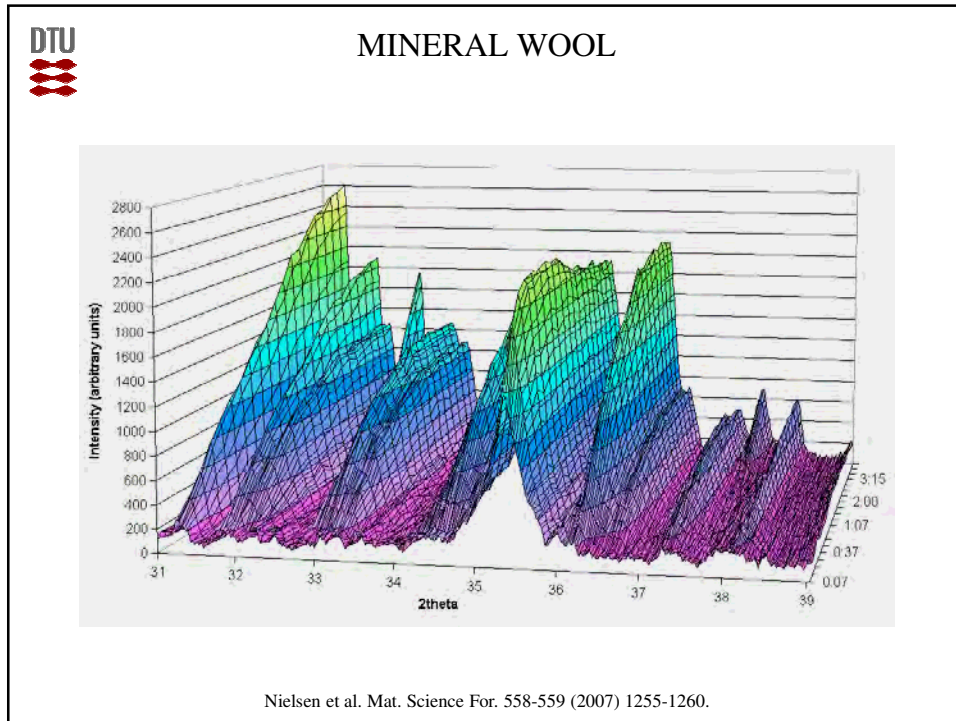
SAPO-34 METHANOL-TO-OLEFIN CONVERSION

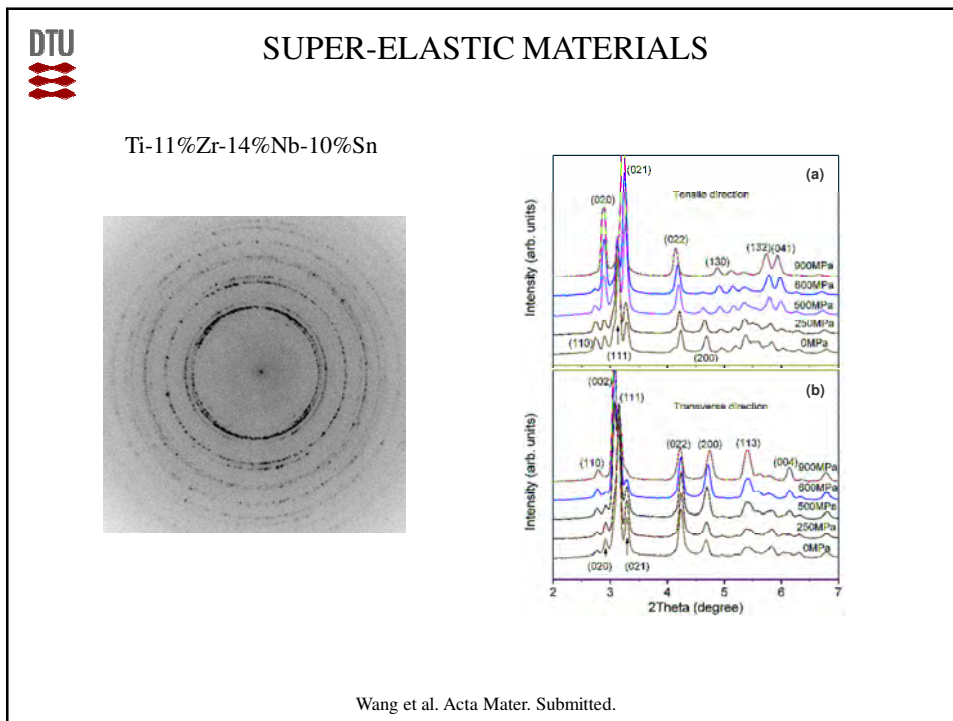
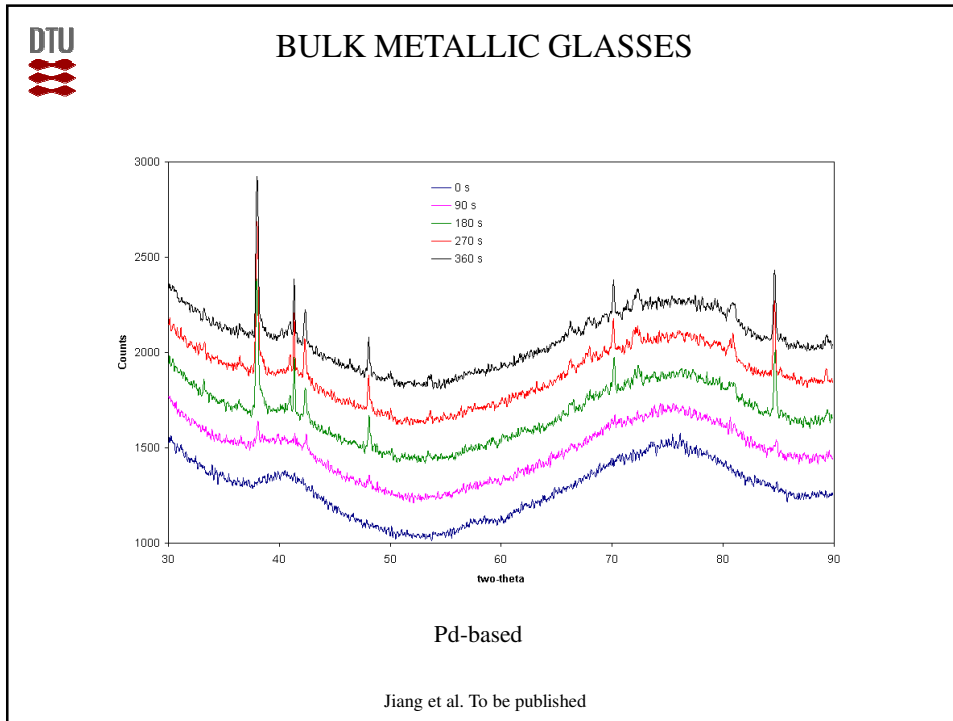
t = 3 min

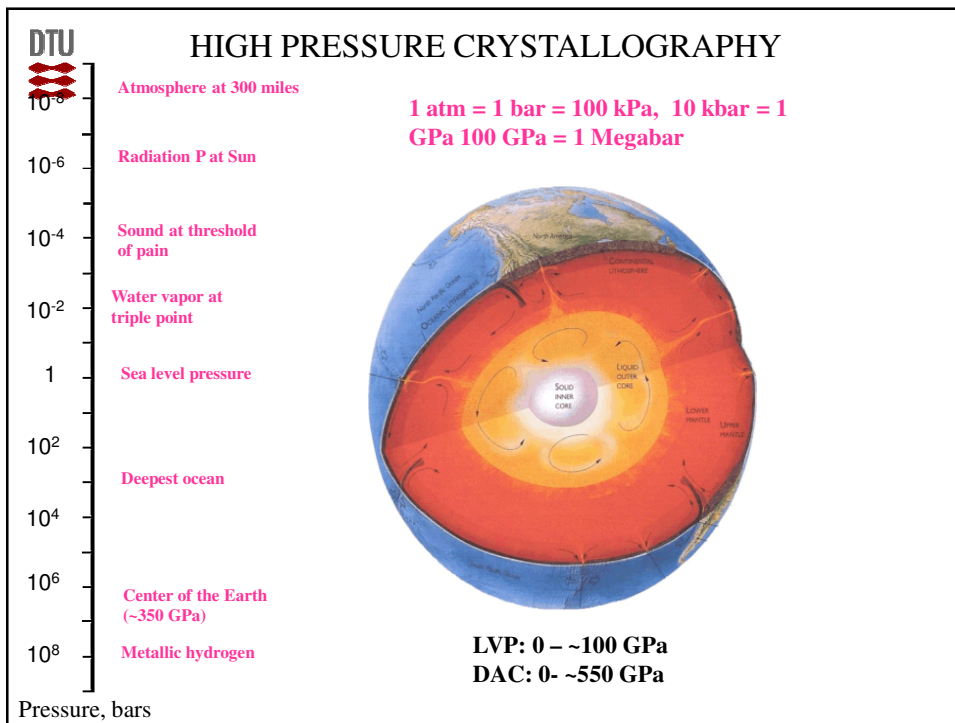
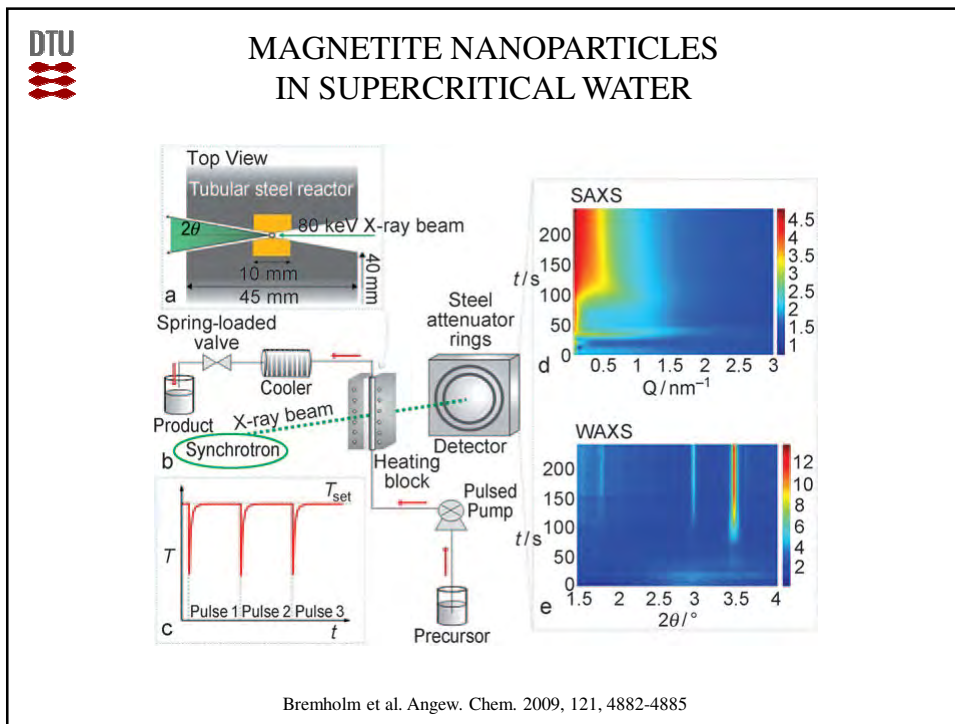


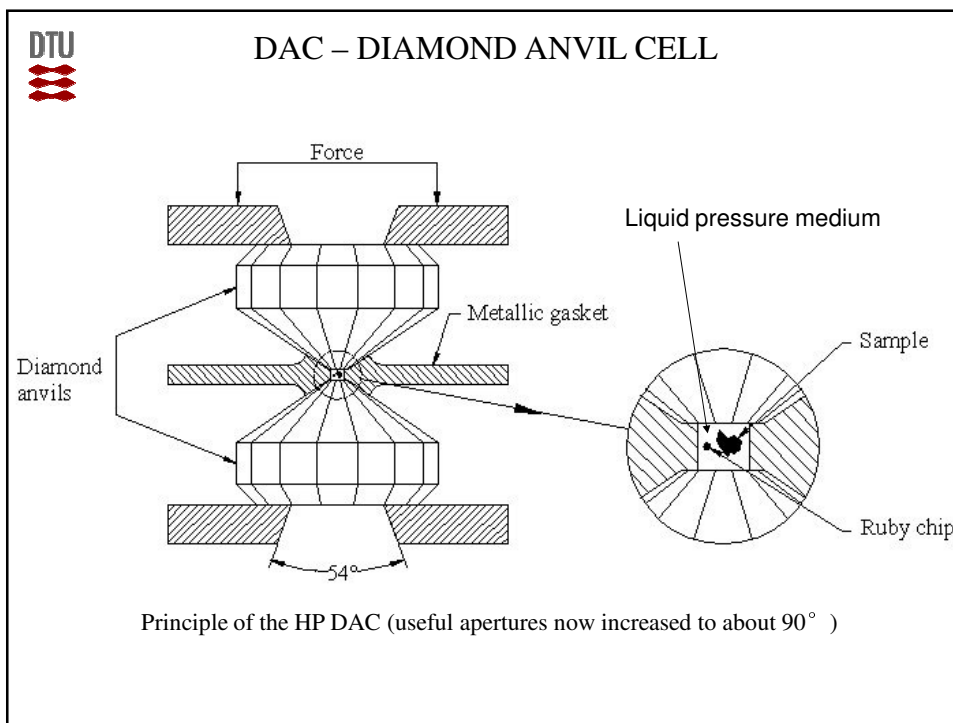
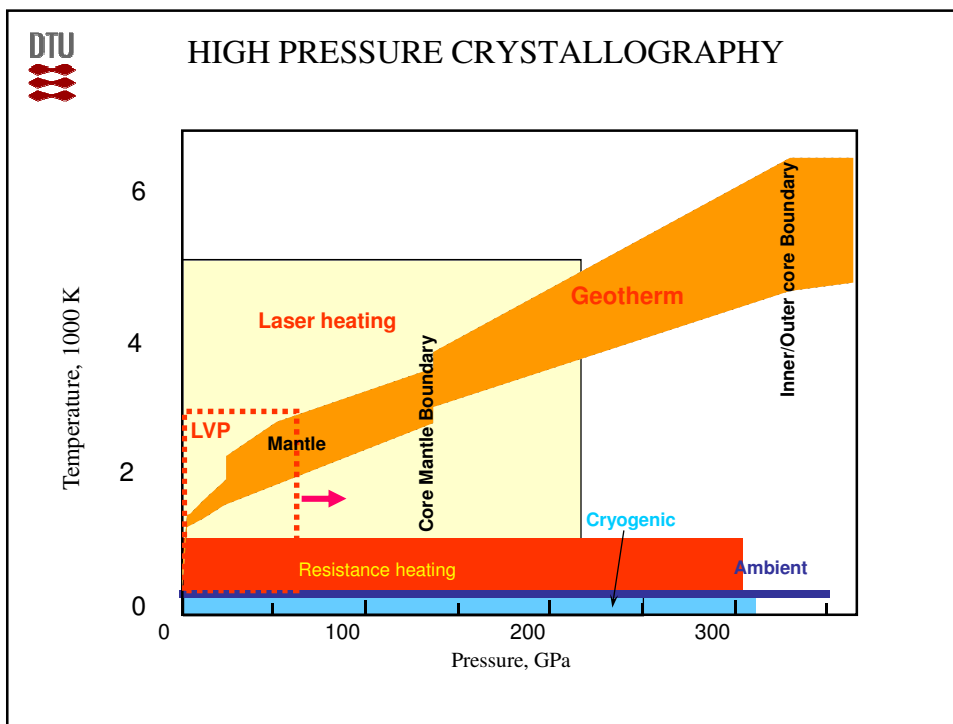
Wragg et al. J. Catal. 2009, 268, 290-296.

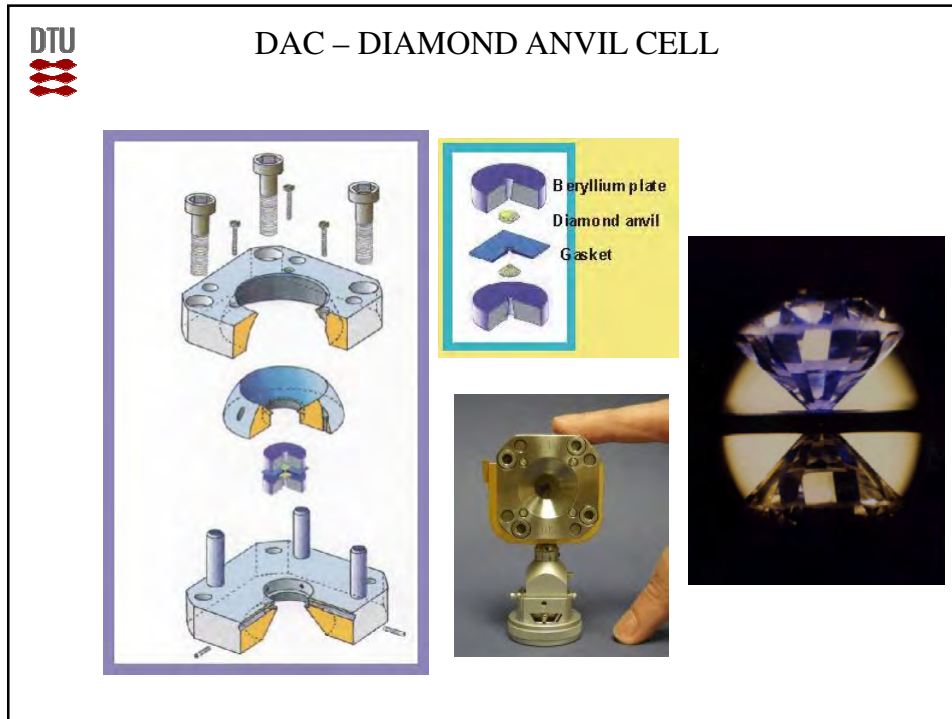












DTU

PRESSURE MEASUREMENT

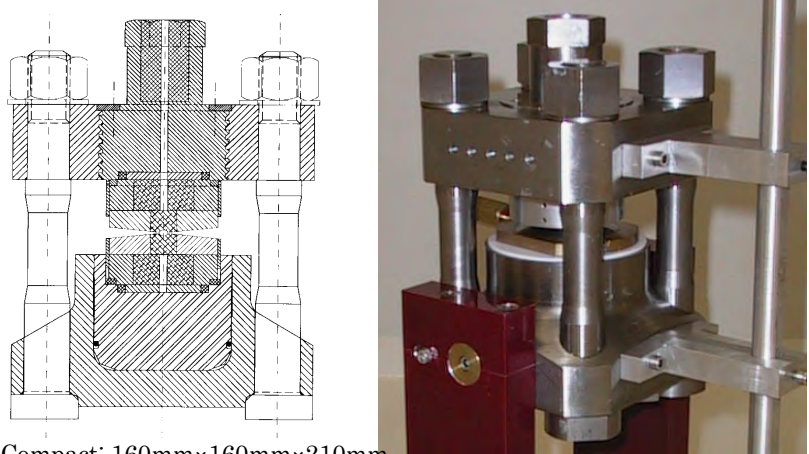
- Ruby is an optical pressure marker
- Ruby at zero pressure wavelength = 694.041nm

$$P = 380.8 \left[\left(\frac{\lambda}{\lambda_0} \right)^5 - 1 \right] \text{ GPa}$$

HK Mao, J Xu, and PM Bell, J. Geophys. Res. 91, 4673 (1986)

DTU

PARIS EDINBURG CELL

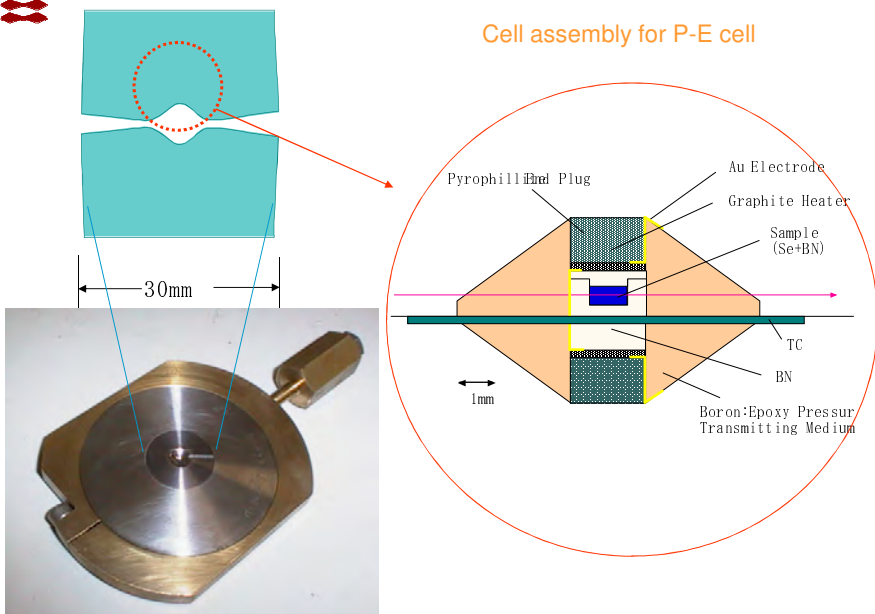


Compact: 160mm×160mm×210mm
Lightweight: 30 kg

DTU

PARIS EDINBURG CELL

Cell assembly for P-E cell



Pyrophyllite Plug

Au Electrode

Graphite Heater

Sample (Se+BN)

TC

BN

Boron-Epoxy Pressure Transmitting Medium

30mm

1mm

