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Mosaic and gradient single crystals for gamma ray Laue lenses

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Gamma Wave 2005

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Espace St. Jacques, Bonifacio, Corsica

CLAIRE and more

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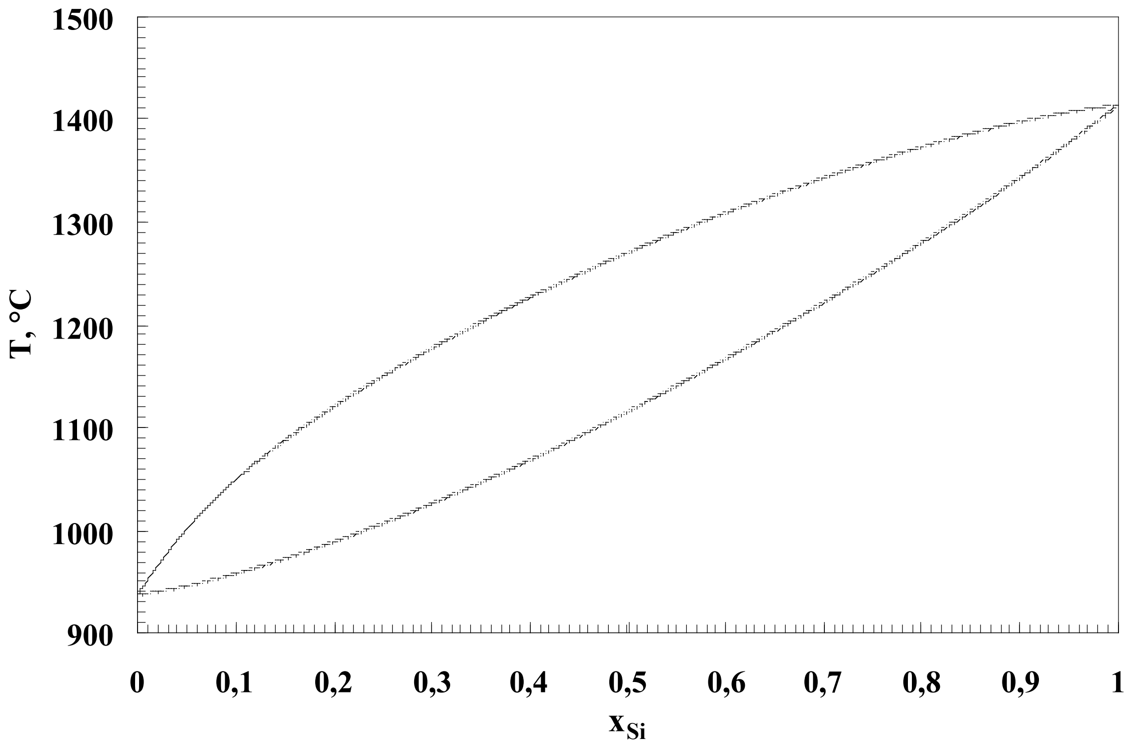
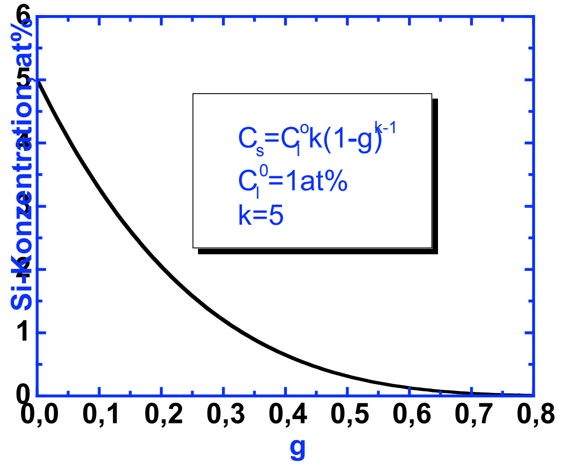
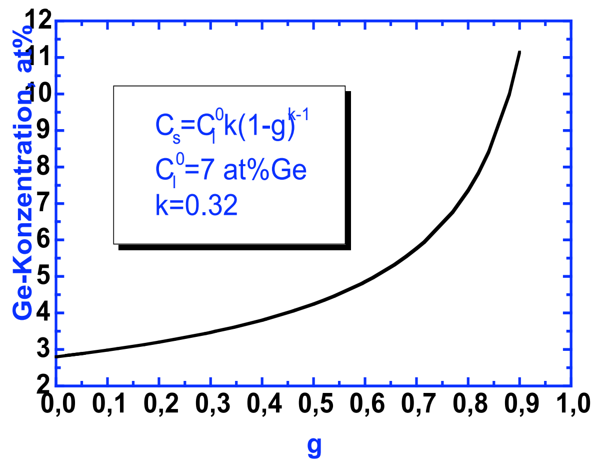
- A. Erko, A. Firsov – BESSY, Berlin, Germany
- O.V. Smirnova - Soft-Impact Ltd., St. Petersburg, Russia
- V.V. Kalaev, Yu.N. Makarov - STR GmbH, Erlangen, Germany

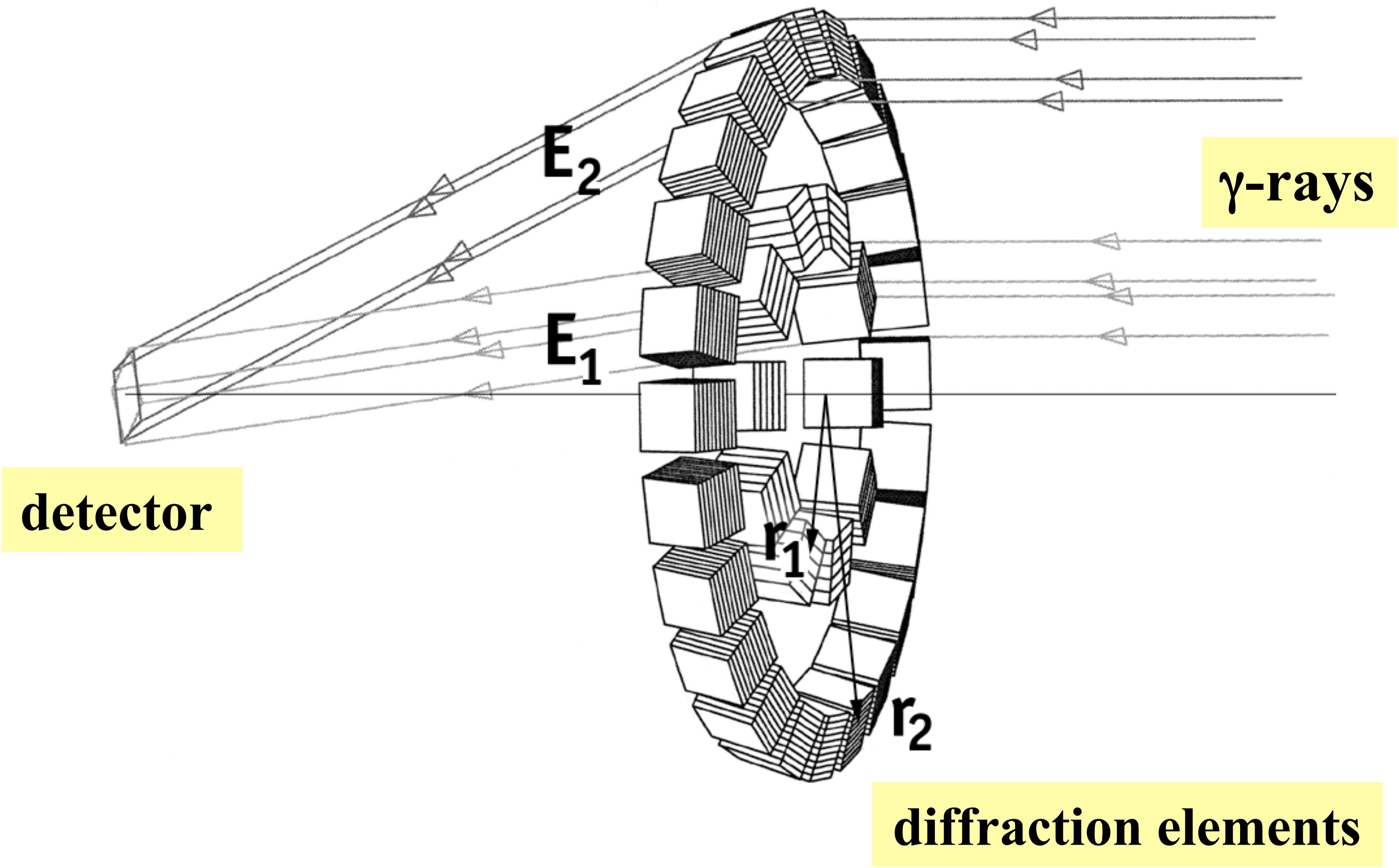
Phase diagram Si:Ge



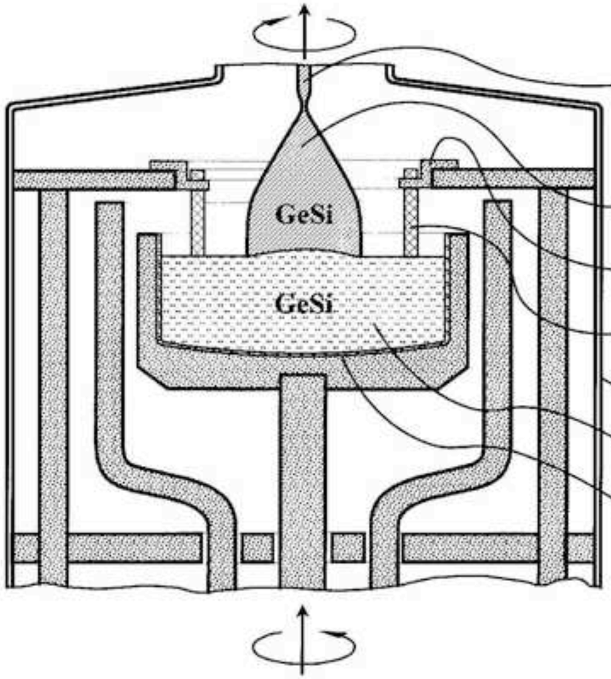




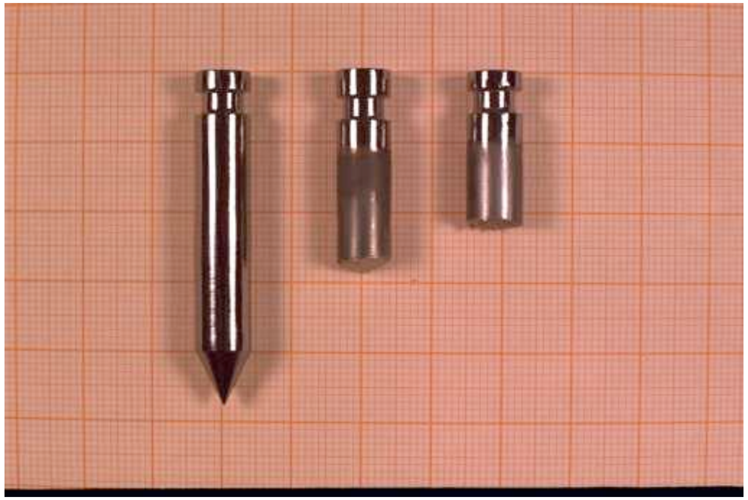
Focusing gamma-rays – the principles of Laue lenses

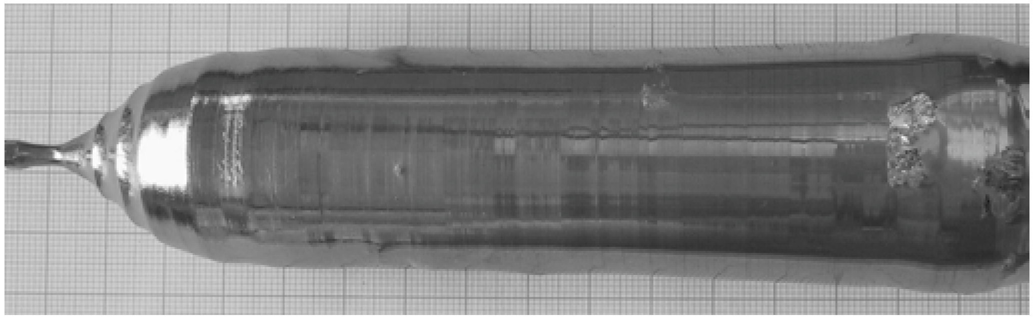


Czochralski growth of GeSi (mosaic) single crystals



feeding rods
before and after growth process





$Ge_{1-x}Si_x$
mosaic crystal
$x = 2.0 \pm 0.15$ at%

Visualisation of the cellular structure

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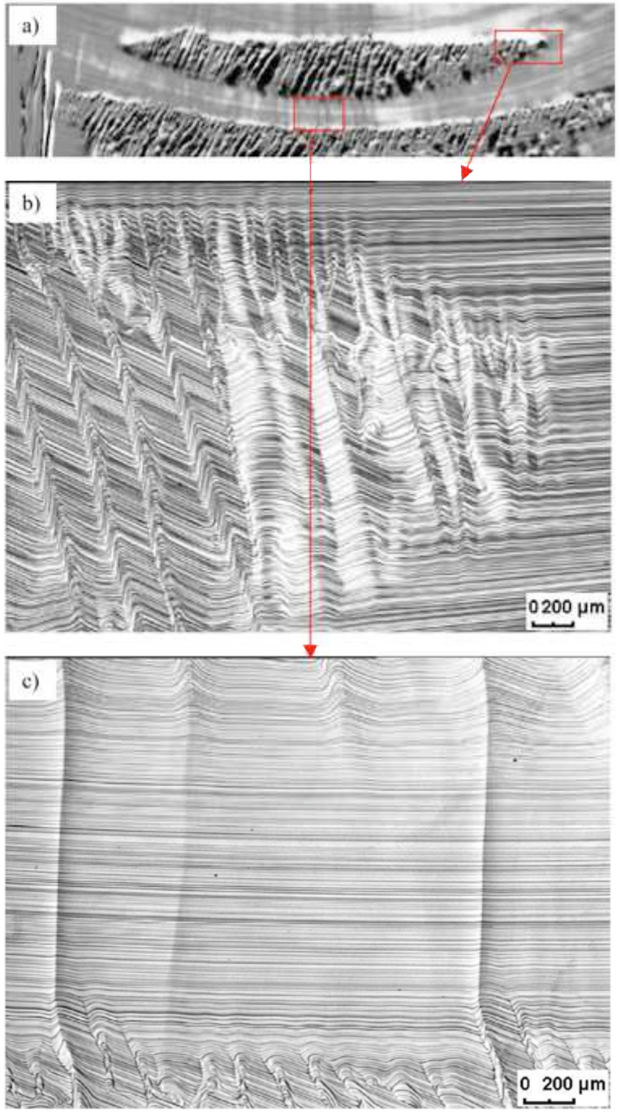
growth direction



LPS measurement
38 x10 mm

longitudinal section

sample surface (110)

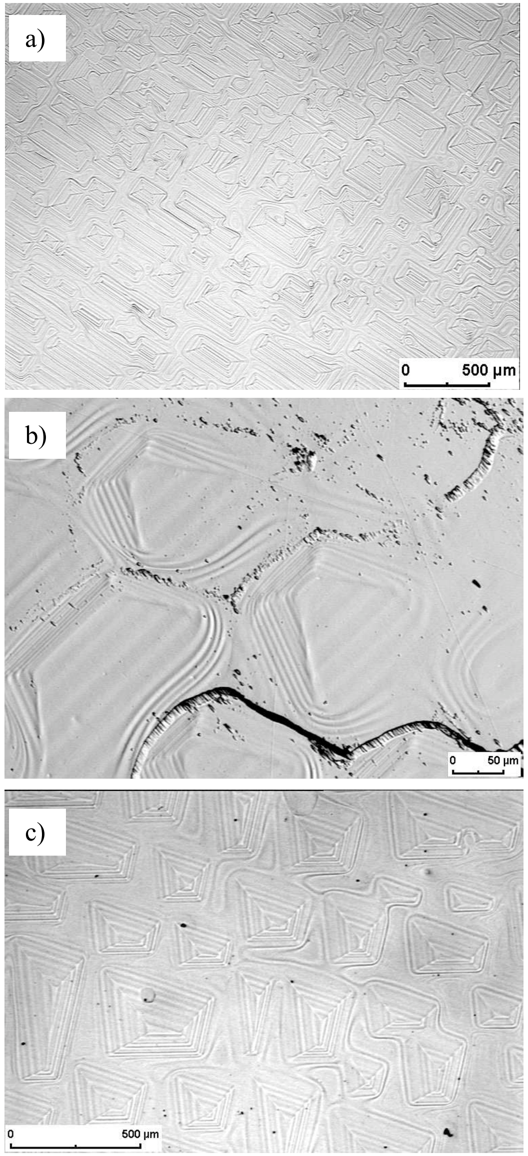
Etch pattern micrographs show the development of the cellular structure.

Features:

•the cell size increases during the growth

•the reversibility of the cellular structure (if only in some range

The cellular structure at the solid-liquid interface (etch patterns)

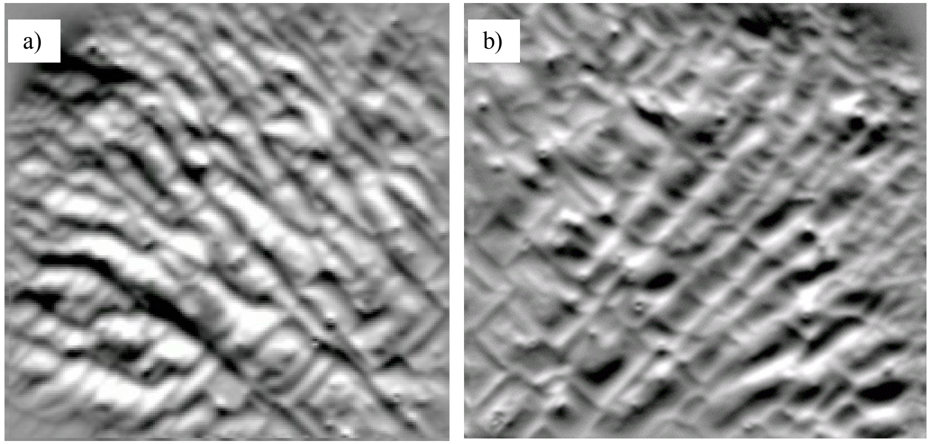


(100) growth direction
1.9 at% Si
mosaicity (not measured)

(112) growth direction
0.7 at% Si
mosaicity 20″

(130) growth direction
1.5 at% Si
mosaicity 42″

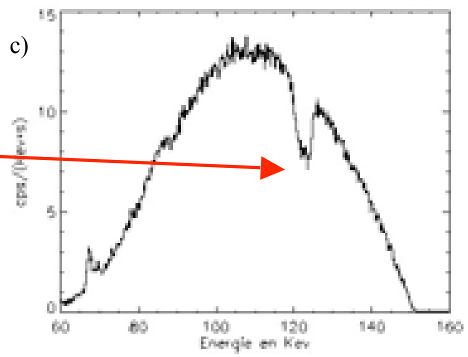
Cellular structure and diffraction properties

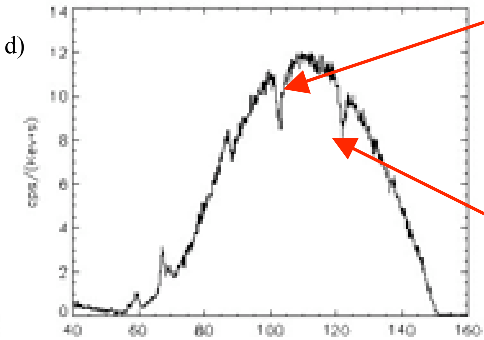


LPS measurement
10 mm x 10 mm
(100) surface orientation

transmitted beam

Centered at 122,4 keV
FWHM= 4,34 keV
Diffraction efficiency: 15%

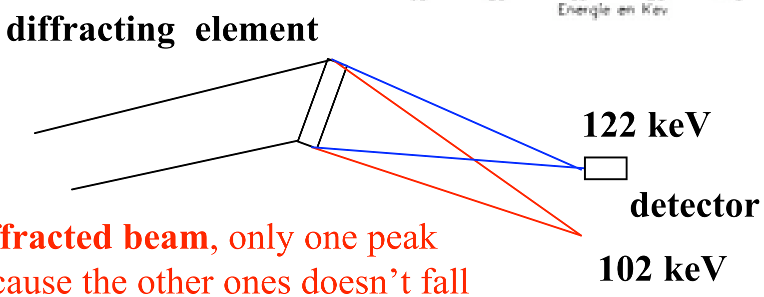




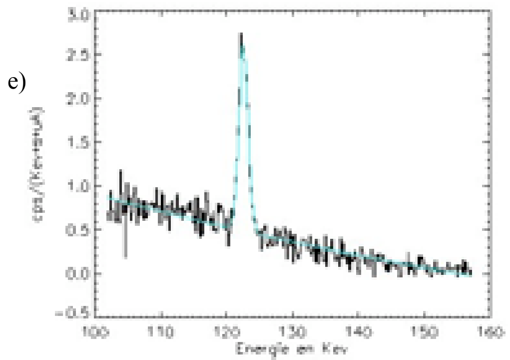
transmitted beam

Peak 1 :
Centered at 102,9 keV
FWHM= 2,31 keV
Diffraction efficiency : 10%

Peak 2 :
Centered at 122,0 keV
FWHM= 1,82 keV
Diffraction efficiency: 8,5%



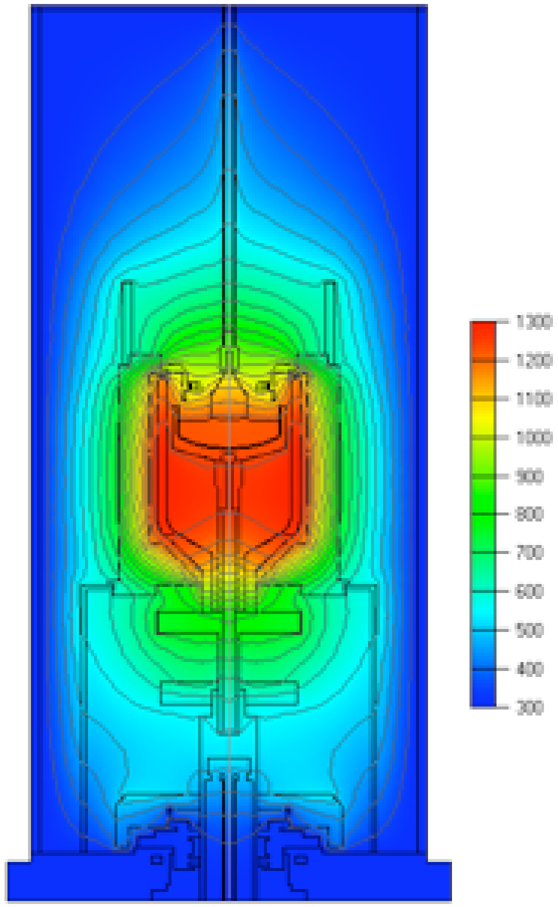
On the **diffracted beam**, only one peak targets because the other ones doesn't fall down on the detector for geometrical reasons



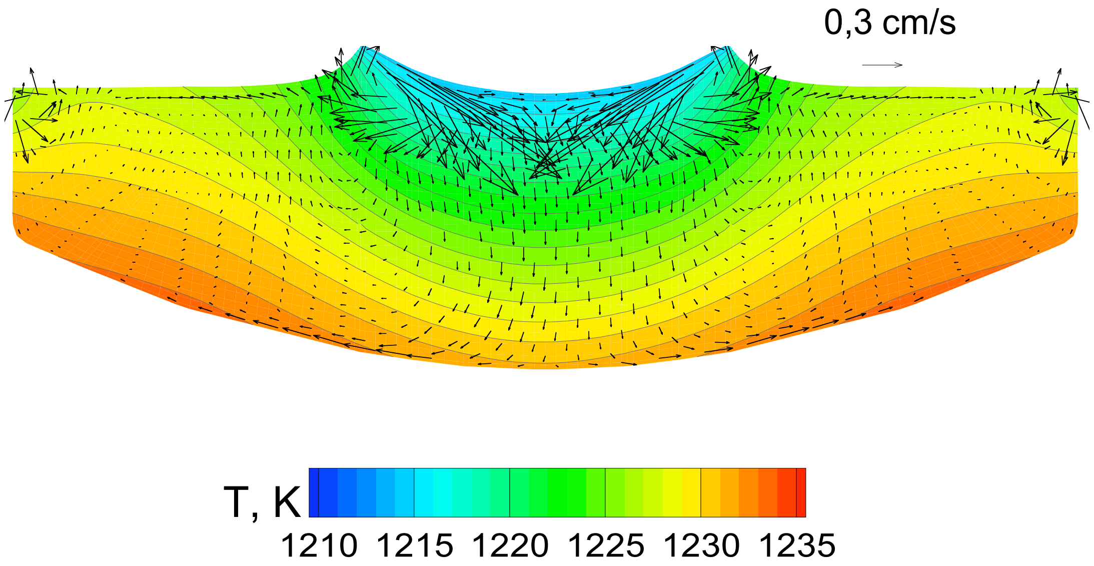
diffracted beam

Centered at 122,0 keV
FWHM= 1,62 keV

Global simulation of the growth process of GeSi crystal with mosaic structure

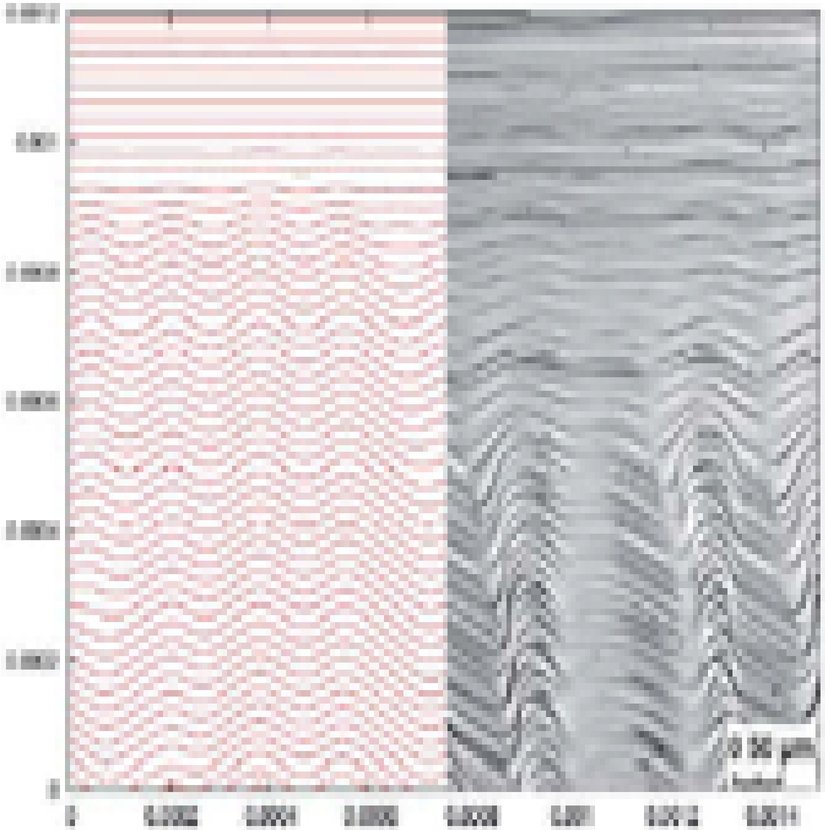


The temperature distribution in the whole growth setup obtained in 2D global heat computations



The averaged temperature distribution and the flow pattern in the melt obtained in the 3D computations during the growth of GeSi crystal

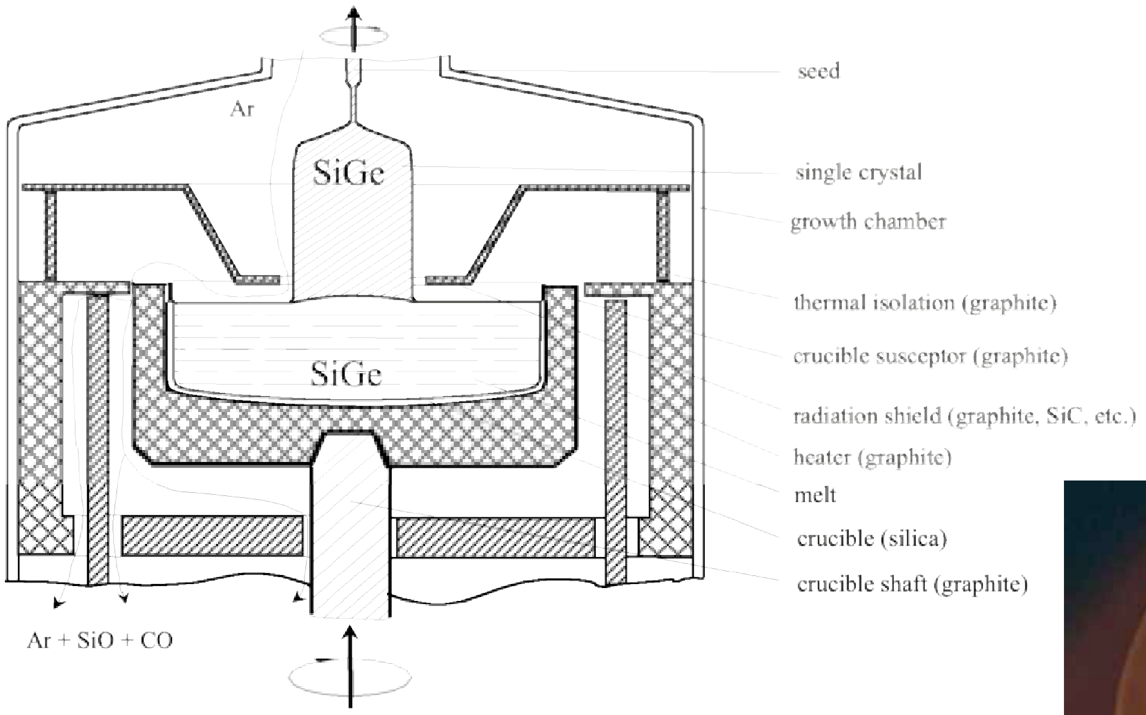
Simulation of growth interface of GeSi crystal with mosaic structure

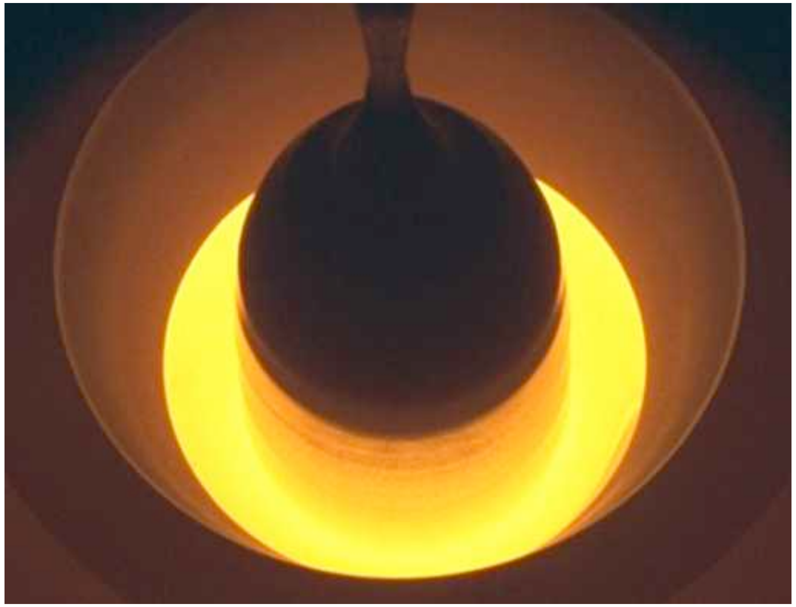


simulation

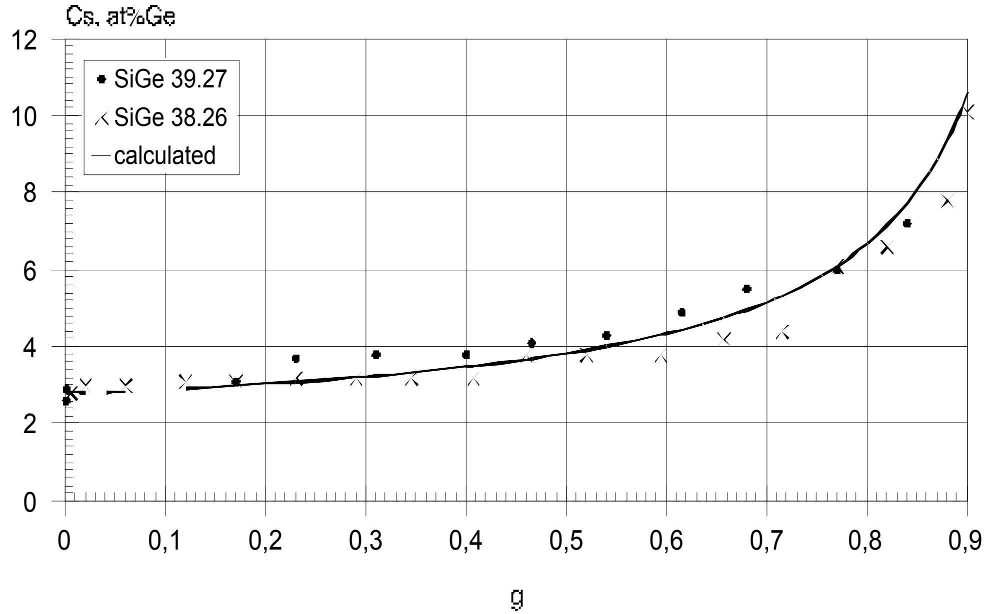
striations in GeSi crystal

Czochralski growth of SiGe (gradient) single crystals





Axial Ge distribution in $Si_{1-x}Ge_x$ grown by Czochralski technique



$$C_{Ge} = kC_{0,Ge}(1-g)^{k-1}$$

_Ge – Ge concentration in the crystal

_0,Ge – initial Ge concentration in the melt

k – distribution coefficient of Ge in Si

g – solidified fraction

$$g = M_{cr} / M_0 = \pi\rho_{cr}R^2L / M_0$$

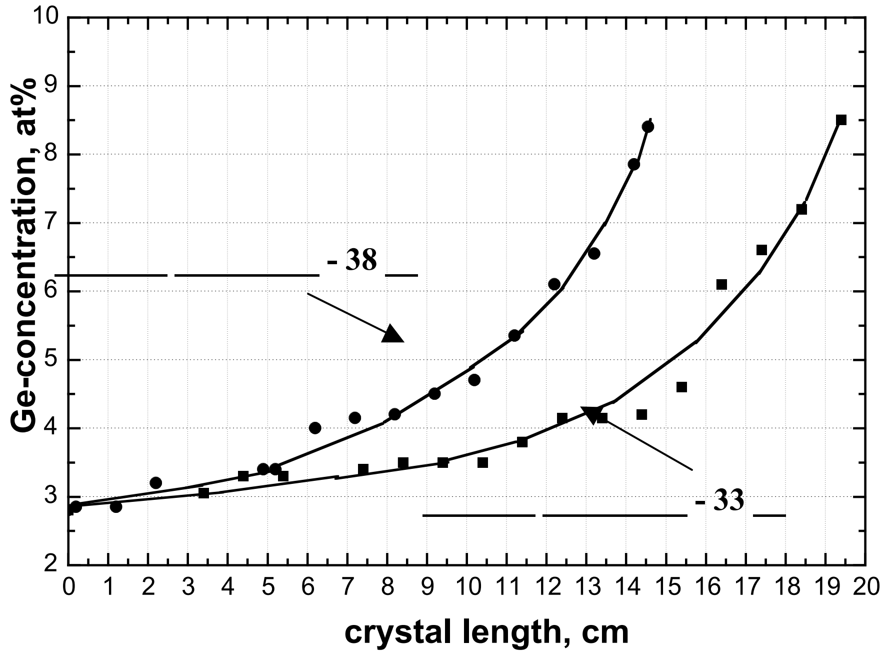
M_{cr} – current mass of the crystal

M_o – starting mass of the charge

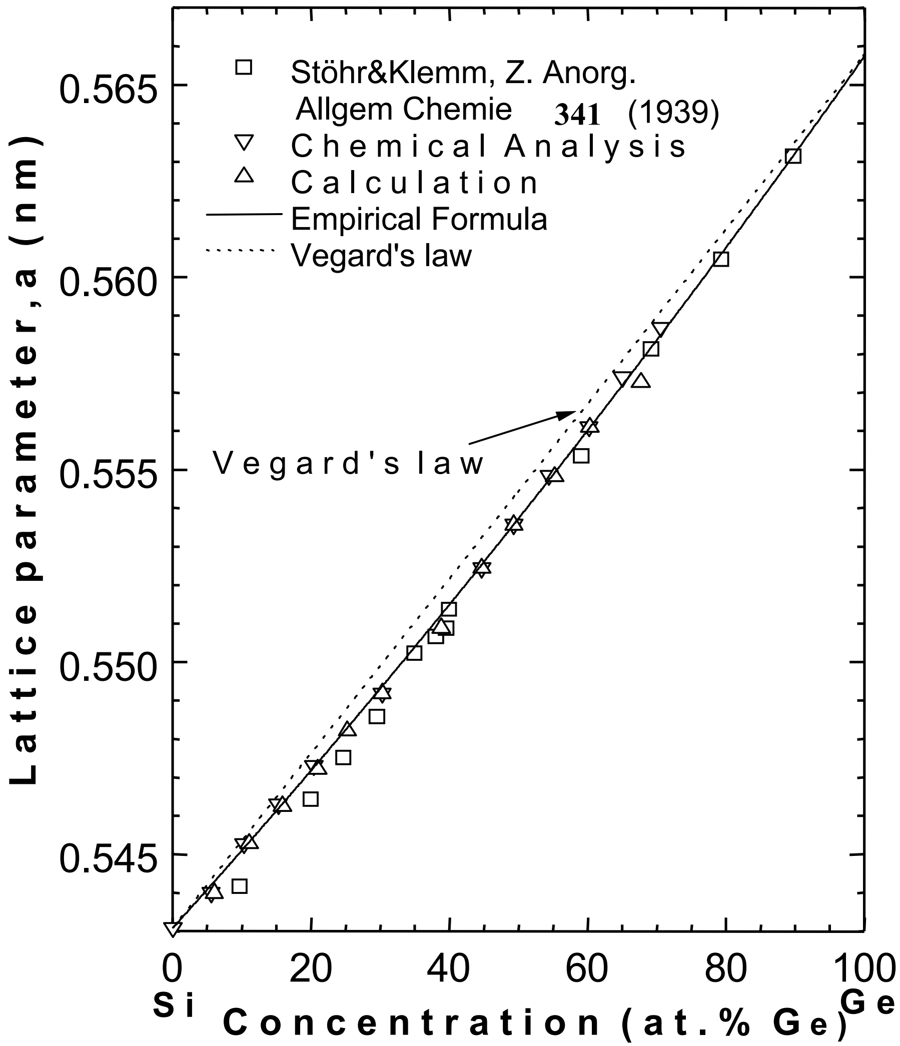
ρ_{cr} – crystal density

S – crystal cross-section

L – crystal length



Vegard’s law



Vegard’s law :

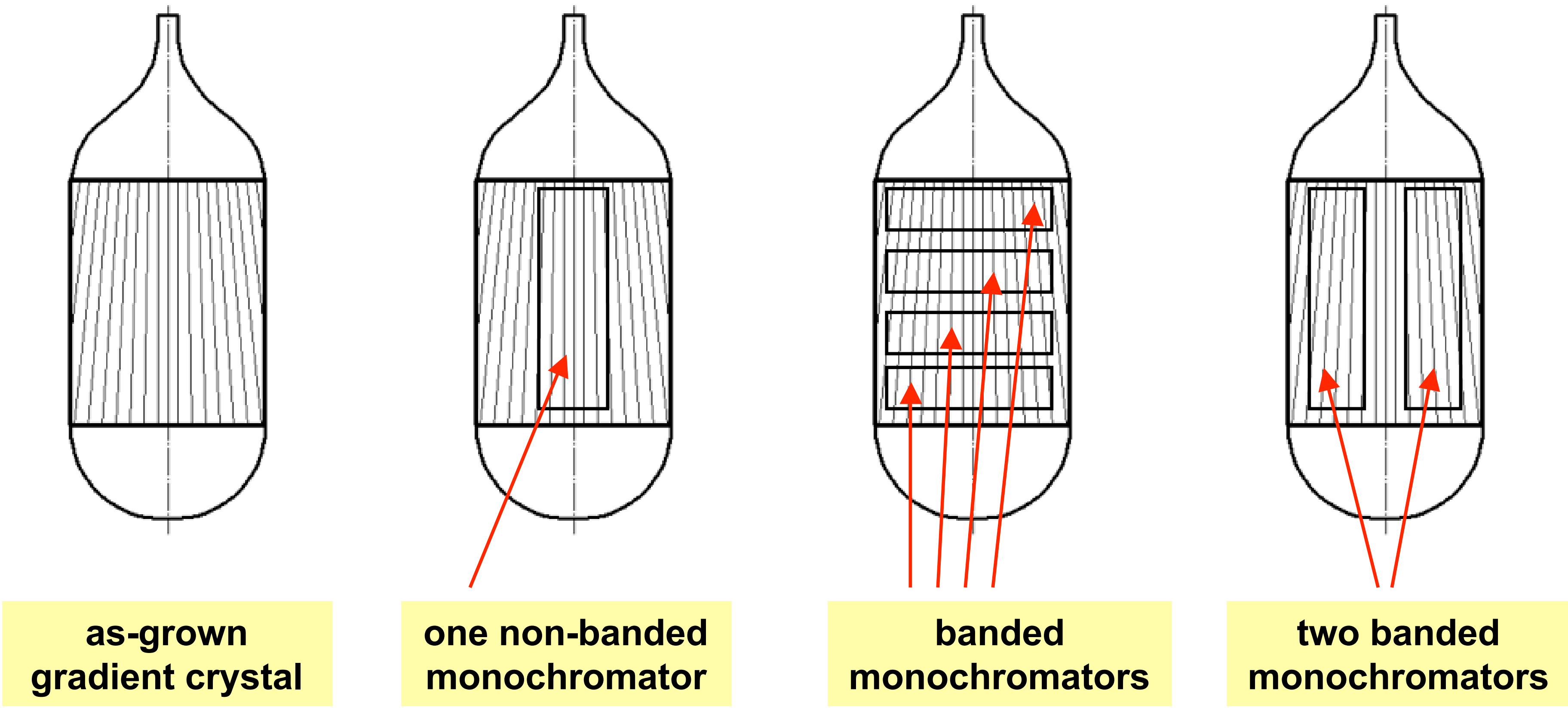
$$a_{SiGe} = x \cdot a_{Ge} + (1-x) \cdot a_{Si}$$

Empirical formula

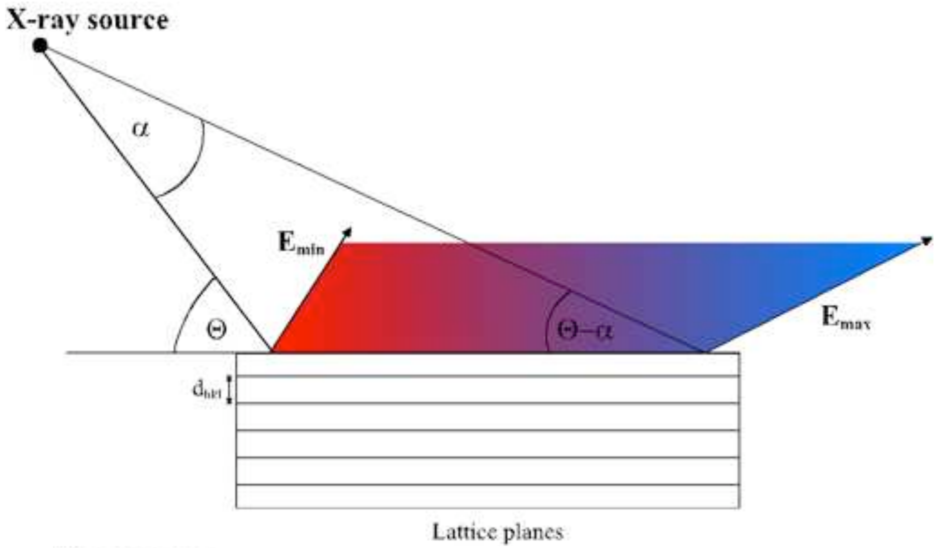
$$a_{SiGe} = (0.002733 \cdot x^2 + 0.01992 \cdot x + a_{Si})\ \mathrm{nm}$$

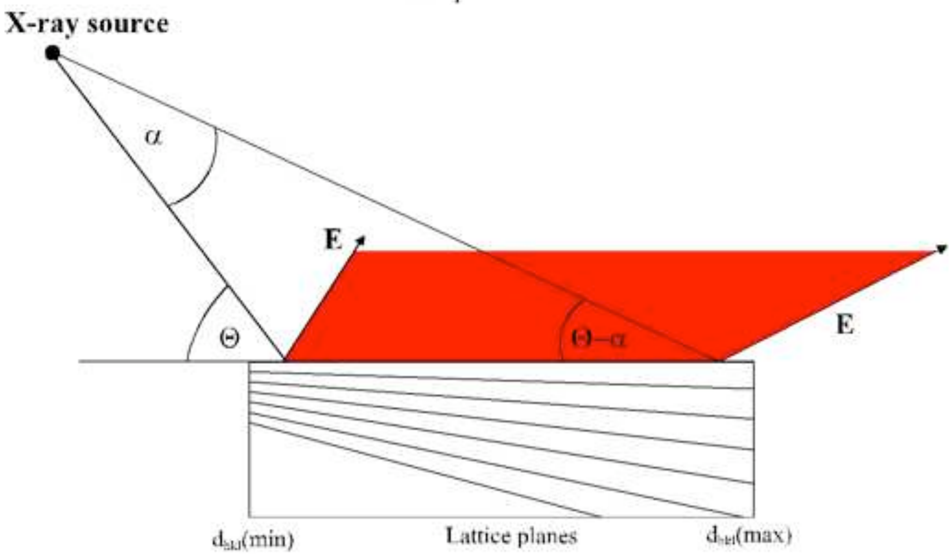
$$a_{Si} = 0.5431\ \mathrm{nm}$$

Some possibilities to cut monochromators from the gradient crystals



SiGe gradient crystal as monochromator for X-rays





Bragg's law :

$2\ d\ sin\ \Theta = \lambda$

for gradient crystals

$2\ d\ (1 + \Delta d/d)\ sin\ (\Theta\text{-}\alpha) = \lambda$

optimized gradient

$B{=}(\Delta d/d)/L{=}cos\Theta_0/R$

$Si_{1-x}Ge_x$ gradient crystals for high resolution synchrotron optics

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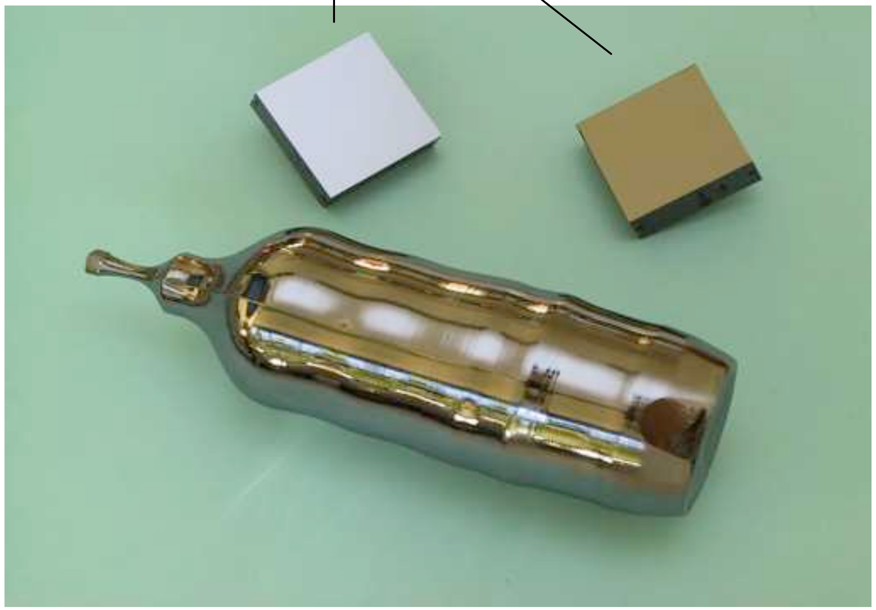
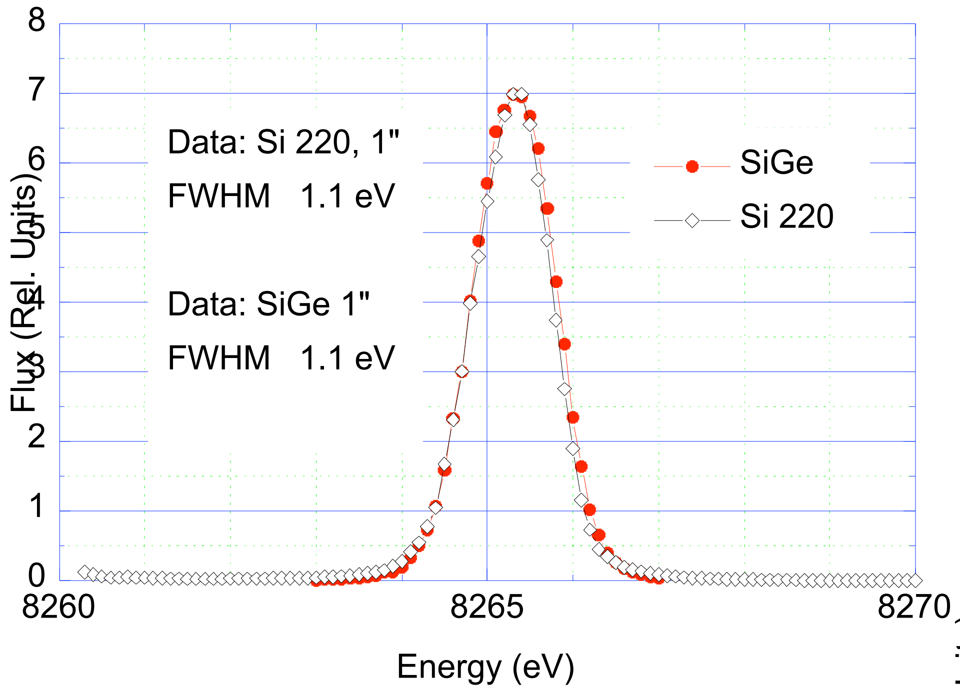
SiGe-monochromators
30 x 30 x 10 mm^3



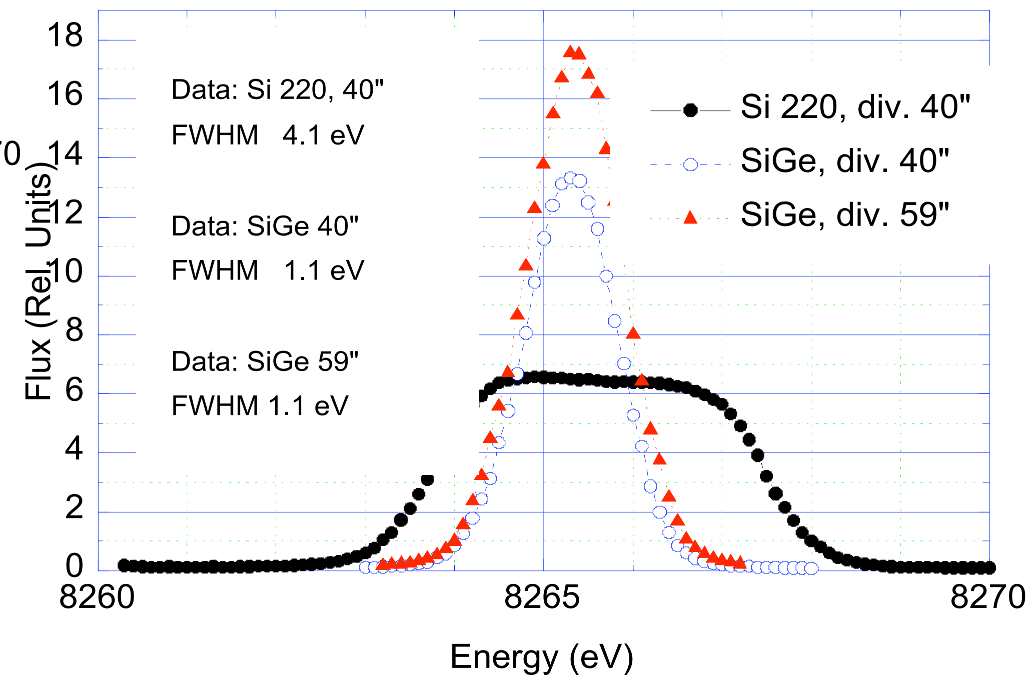
Energy spectrum from the SiGe (220) und Si (220) monochromators



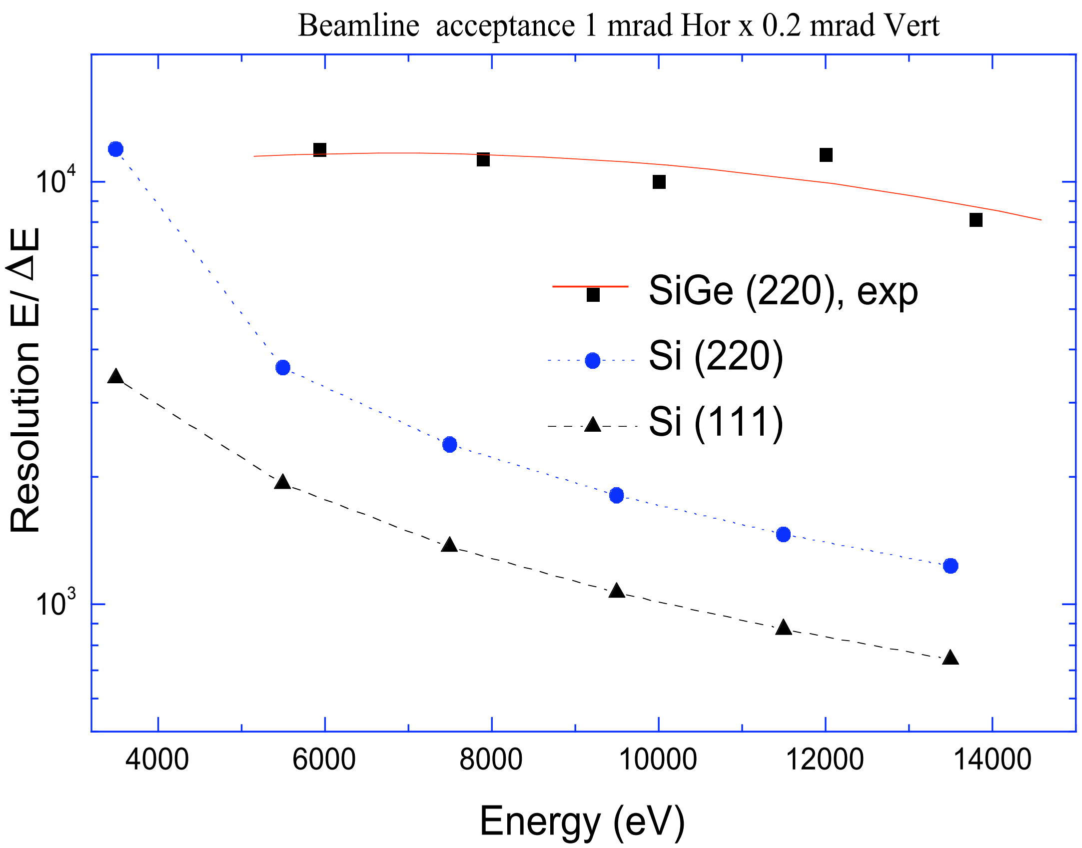
beam divergence 1 arc sec

Reflection curves with a fixed Bragg angle

beam divergence 40 or 59 arc sec



Energy resolution of the graded double SiGe (220) monochromator (in comparison with double Si (220) and Si (111) monochromators)



KMC-2 beamline (BESSY II)

Double crystal monochromator

2 SiGe (111) graded crystals

Energy range - 4 keV – 15 keV

Resolution - E/ΔE ~ 4000

Exit flux - 10^7-10^{10} phot/sec/100mA

Spot size at experiment :

- **250 µm, horizontal**
- **600 µm, vertical**
- **5µm x 5 µm (with capillary optics)**

Instrumentation:

- **EXAFS**
- **XANES**
- **X-ray diffractometry**
- **X-ray reflelectometry**

Calculation of crystal form to get constant gradient of Ge in $Si_{1-x}Ge_x$

$$C_{Ge} = kC_{0,Ge}(1-g)^{k-1}$$

$$g = M_{cr}/M_0 = \pi\rho_{cr}R^2L/M_0$$

$$R = R(L)$$

$$\frac{\partial C_{Ge}}{\partial L} = B \Rightarrow \tilde{N}_{Ge} = BL + kC_{0,Ge}$$

B – ________ ________

$$g = 1 - \left(\frac{B}{kC_{0,Ge}}L + 1\right)^{\frac{1}{1-k}}$$

$$\frac{\partial g}{\partial L} = \frac{\pi\rho_{cr}}{M_0}R^2(L)$$

$$R(L) = \sqrt{\frac{M_0B}{\pi\rho_{cr}(1-k)C_{0,Ge}}\left(\frac{B}{kC_{0,Ge}}L + 1\right)^{\frac{2-k}{k-1}}}$$

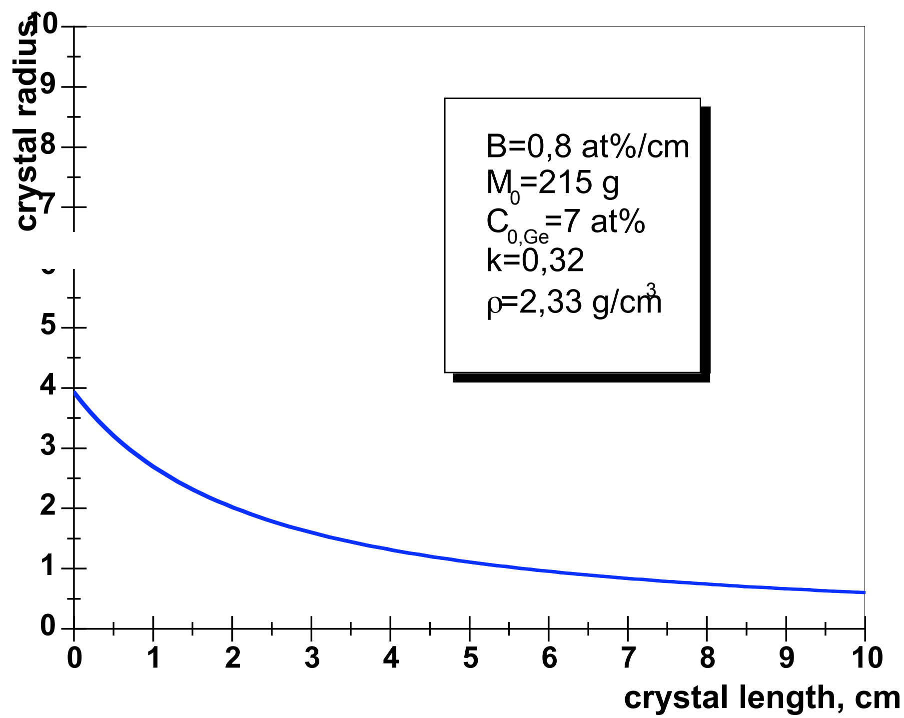
Axial distribution of impurities (Ge) in crystals grown by Czochralski technique

–0,Ge – initial Ge concentration it the melt

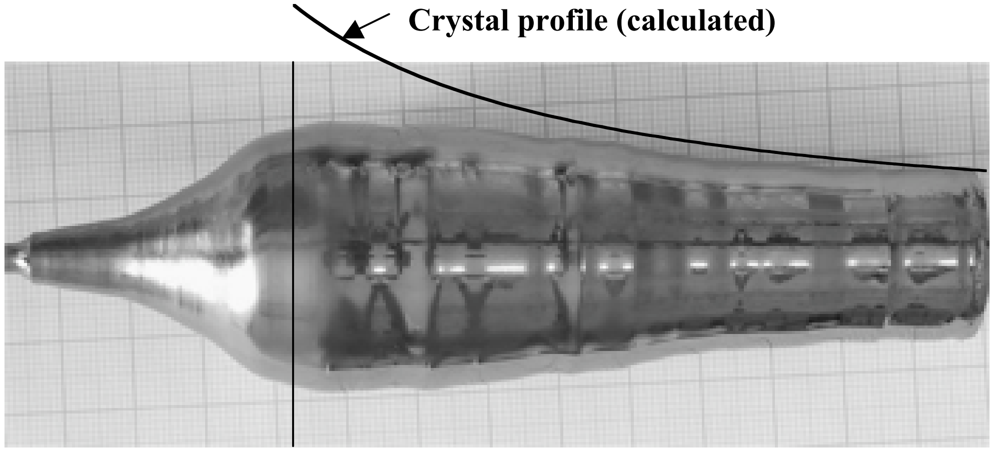
k – distribution coefficient

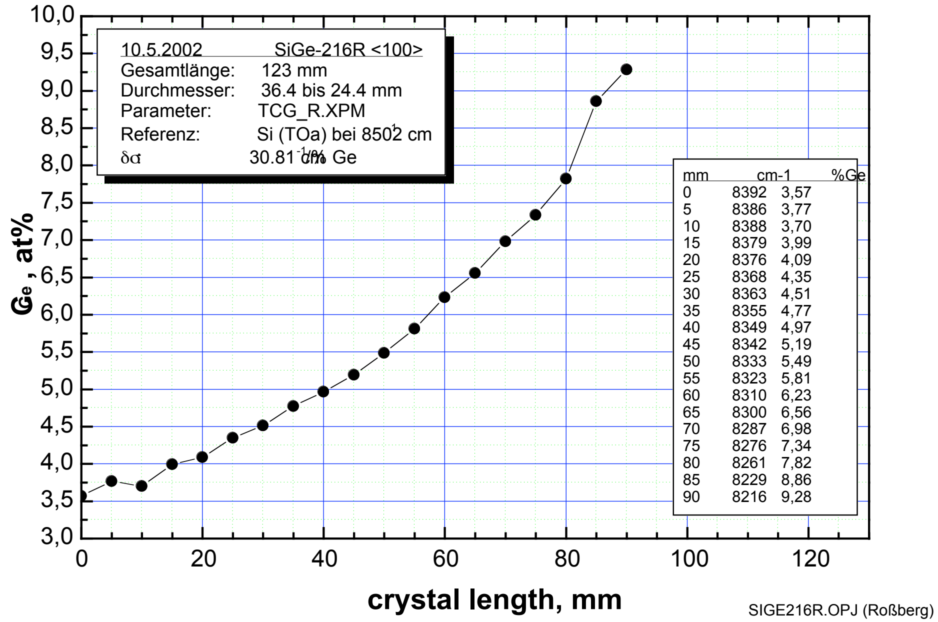
M_0 – starting mass (charge)

M_{cr}, ρ_{cr}, R, L – mass, density, radius and length of the crystal



$Si_{1-x}Ge_x$ crystal with near constant gradient of Ge





Conclusions

- A modified Czochralski technique could be used for the growth of $Ge_{1-x}Si_x$ mosaic crystals and $Si_{1-x}Ge_x$ gradient crystals. SiGe can be used for production of diffracting elements for gamma telescope lens.

- $Ge_{1-x}Si_x$ mosaic crystals were used to produce the diffracting elements for the CLAIRE gamma ray telescope. Although many of 556 diffracting elements had a diffraction efficiency up to 20 %, the overall efficiency of the lens is about 8.1±0.7 % due to different diffraction properties of the elements

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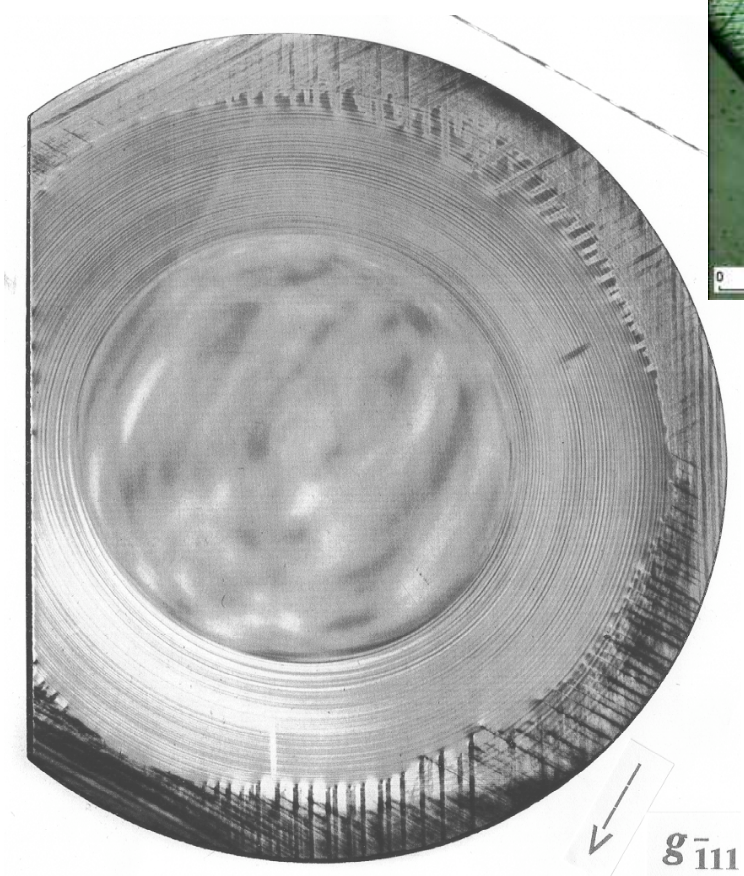
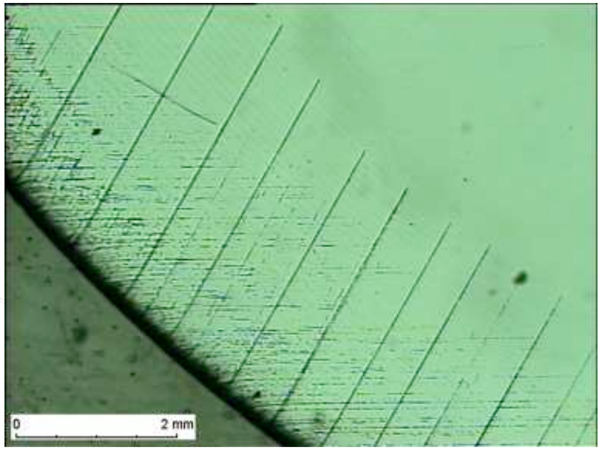
(111) SiGe-wafer with 4 at%Ge



X-ray topograph



Nomarski-contrast