Спюрионы – паразитные пики в трехосной спектроскопии

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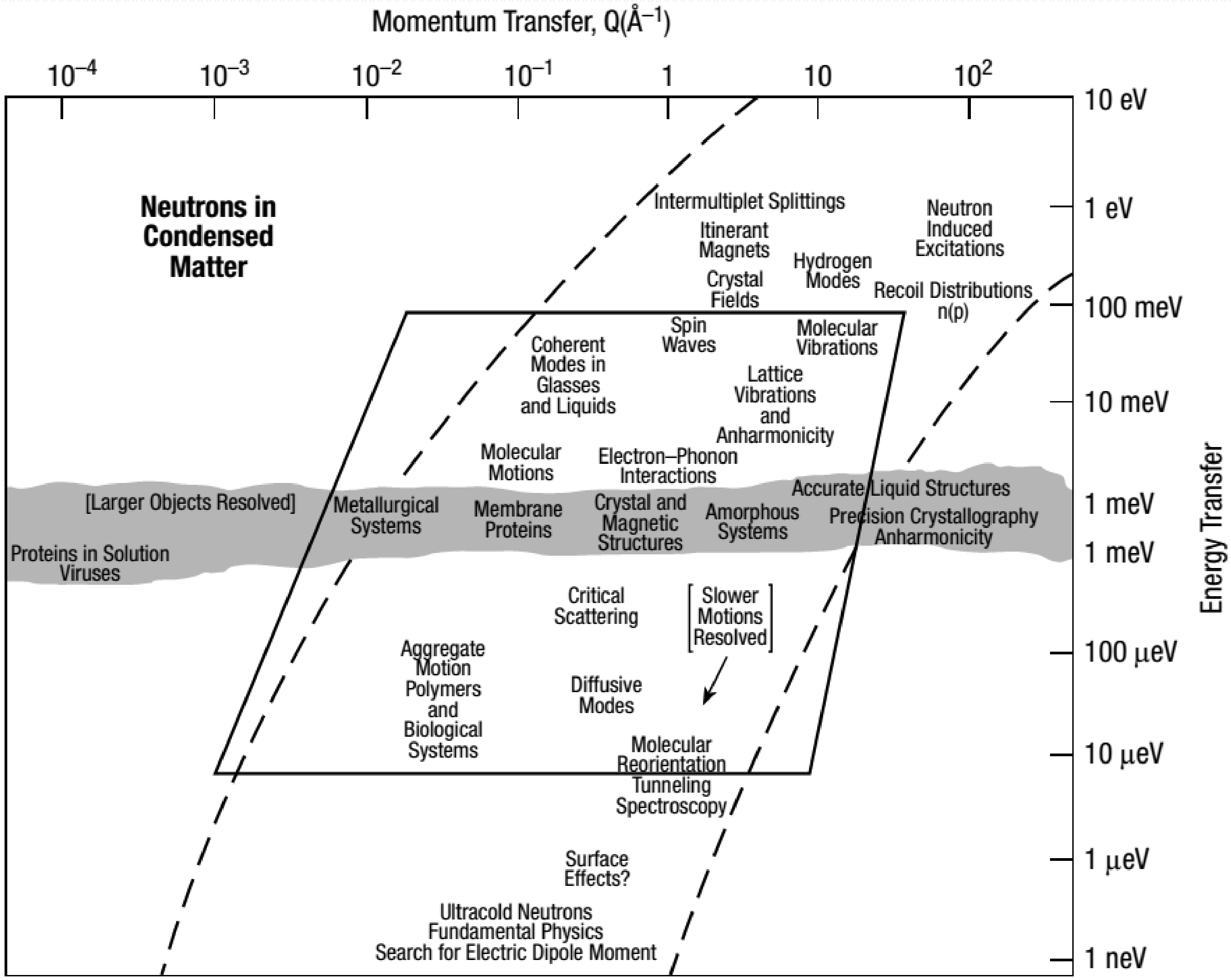
План:

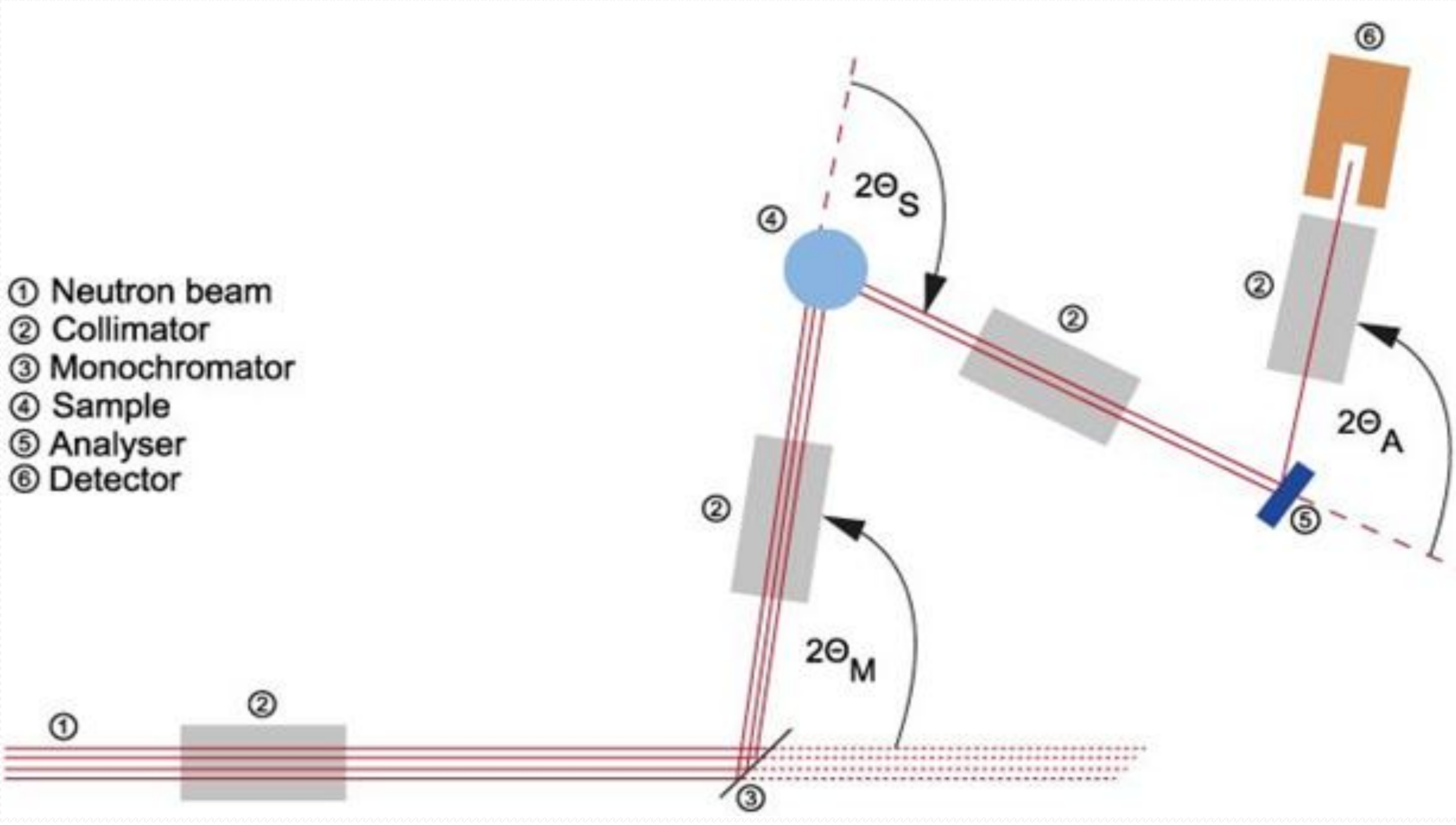
- Введение
  - Трехосный спектрометр
  - Функция разрешения
- Спюрионы
  - Более высокий порядок дифракции
  - Артефакты функции разрешения
  - Артефакты из-за окружения образца
- Алгоритм для обнаружения спюрионов

Использование трехосных спектрометров



Lander, G. H. and Emery, V. J. (1985). *Nucl. Instrum. Methods B* **12**, 525.

Схема трехосного спектрометра



TAS на холодных нейтронах

Rita-II **TASP**

Определение функции разрешения

$$Q_0 = \boldsymbol{k}_F - \boldsymbol{k}_I$$

$$\hbar\omega_0 = \frac{\hbar^2}{2m}({k_I}^2 - {k_F}^2)$$

Функция разрешения инструмента – вероятность детектирования нейтронов, как функция от $\Delta\omega$ и $\Delta\mathbf{Q}$, когда инструмент установлен на измерение рассеяния соответствующего точке ω_0,Q_0, в которой вероятность зарегистрировать нейтрон – наибольшая.

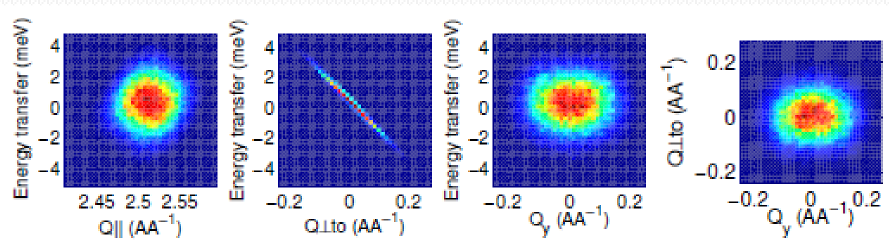
Эллипсы функции разрешения

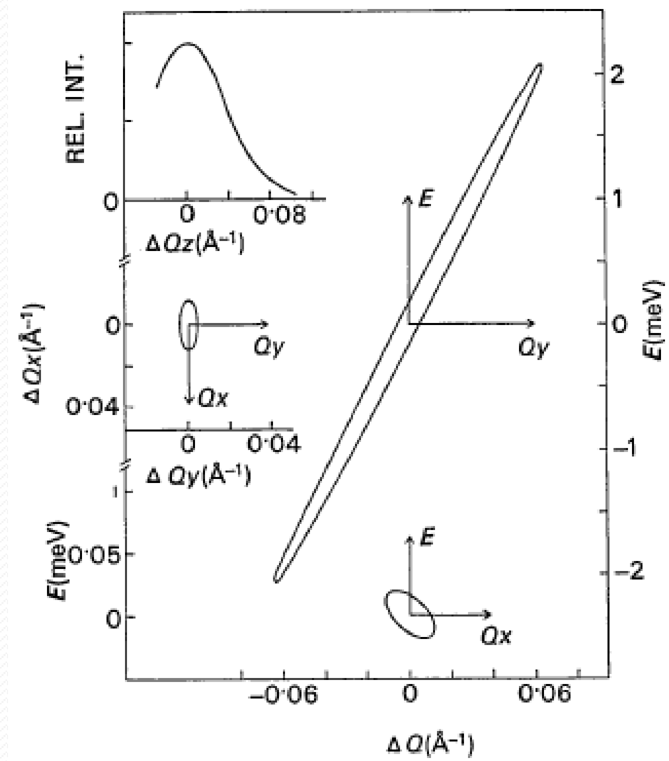
Функция разрешения
имеет следующий вид:

$$R(\omega_0 + \Delta\omega, \mathbf{Q}_0 + \mathbf{\Delta Q}) = R_0 \exp\{-\tfrac{1}{2} \sum_{k=1}^{4} \sum_{l=1}^{4} M_{kl} X_k X_l\}$$

Где $X_1 = \Delta Q_x, X_2 = \Delta Q_y, X_3 = \Delta Q_z, X_4 = \Delta\omega$

$$\sum_{k=1}^{4} \sum_{l=1}^{4} M_{kl} X_k X_l = p$$

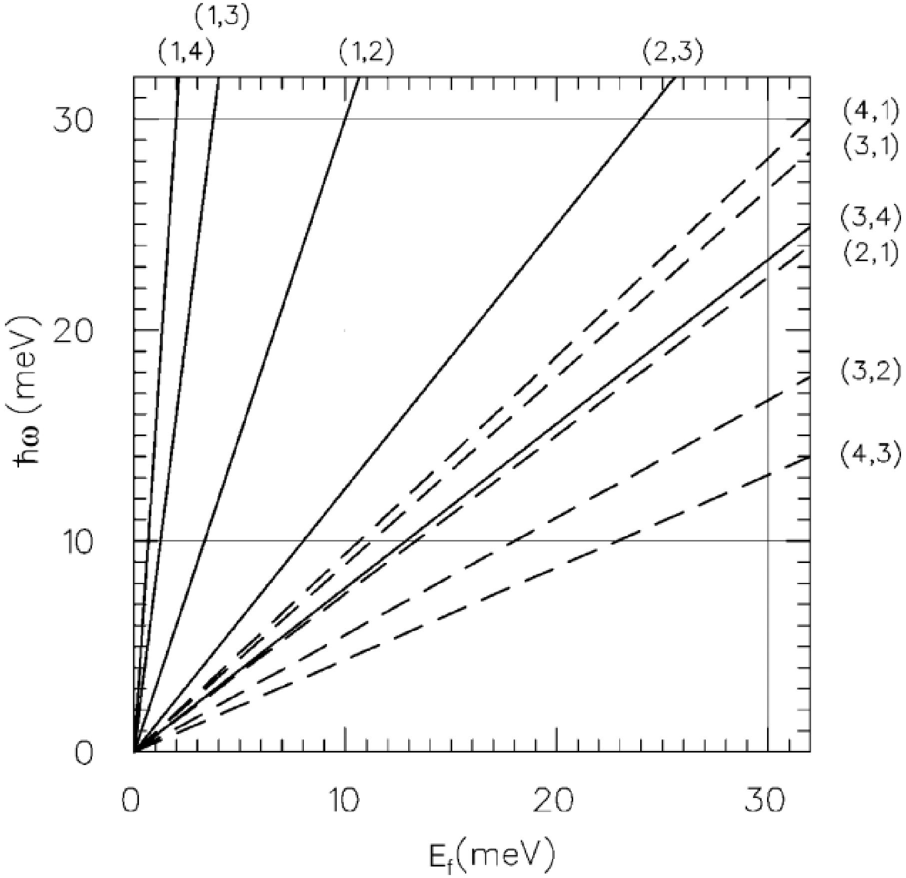




Спюрионы

- Более высокий порядок дифракции
- Артефакты функции разрешения
- Артефакты из-за окружения образца

Более высокий порядок дифракции



$$k_i(n_M) = n_M G_M / 2 \sin \theta_M$$

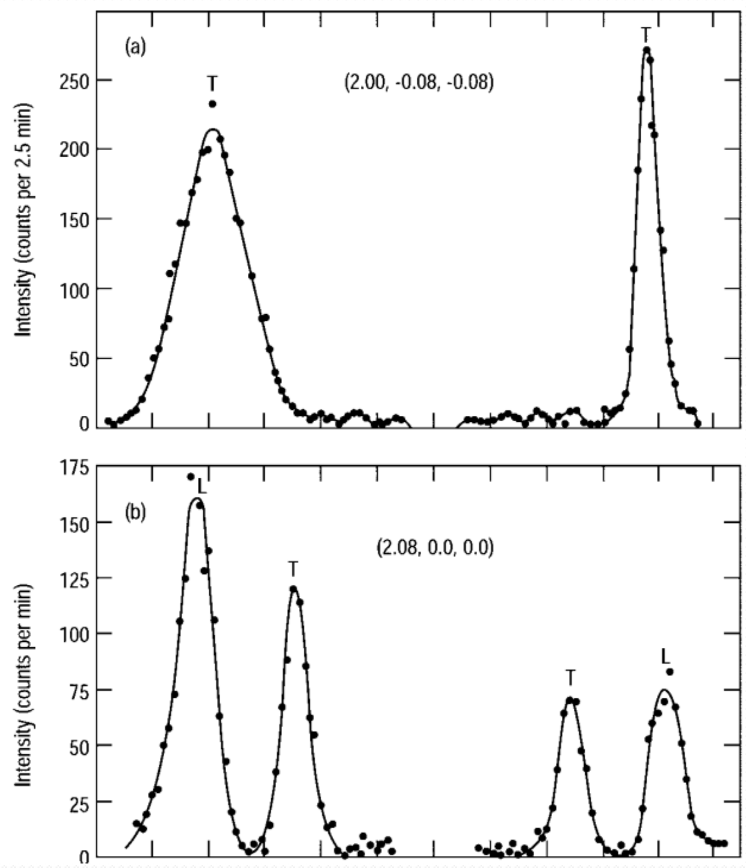
$$\hbar\omega = E_i - E_f = \left(\frac{n_A^2}{n_M^2} - 1 \right) E_f$$

n_M	$n_A =$ 1	2	3	4
1	0	3	8	15
2	$-\mathbf{\frac{3}{4}}$	0	$\frac{5}{4}$	3
3	$-\mathbf{\frac{8}{9}}$	$-\frac{5}{9}$	0	$\frac{7}{9}$
4	$-\mathbf{\frac{15}{16}}$	$-\frac{3}{4}$	$-\frac{7}{16}$	0

Артефакты функции разрешения

- Хвост функции разрешения
- Негауссовская форма функции разрешения
- «Запрещенные» моды

«Запрещенные» моды

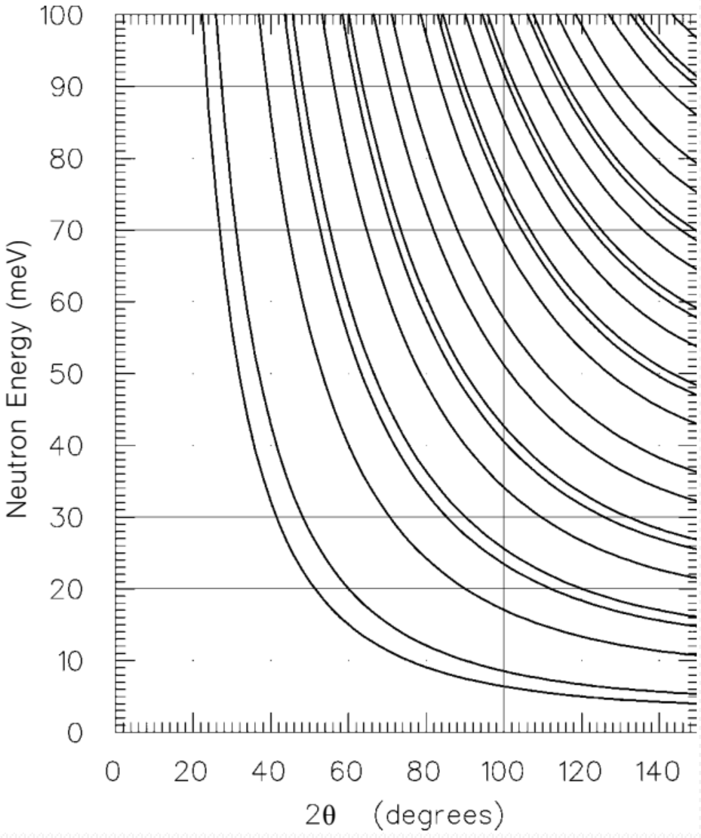


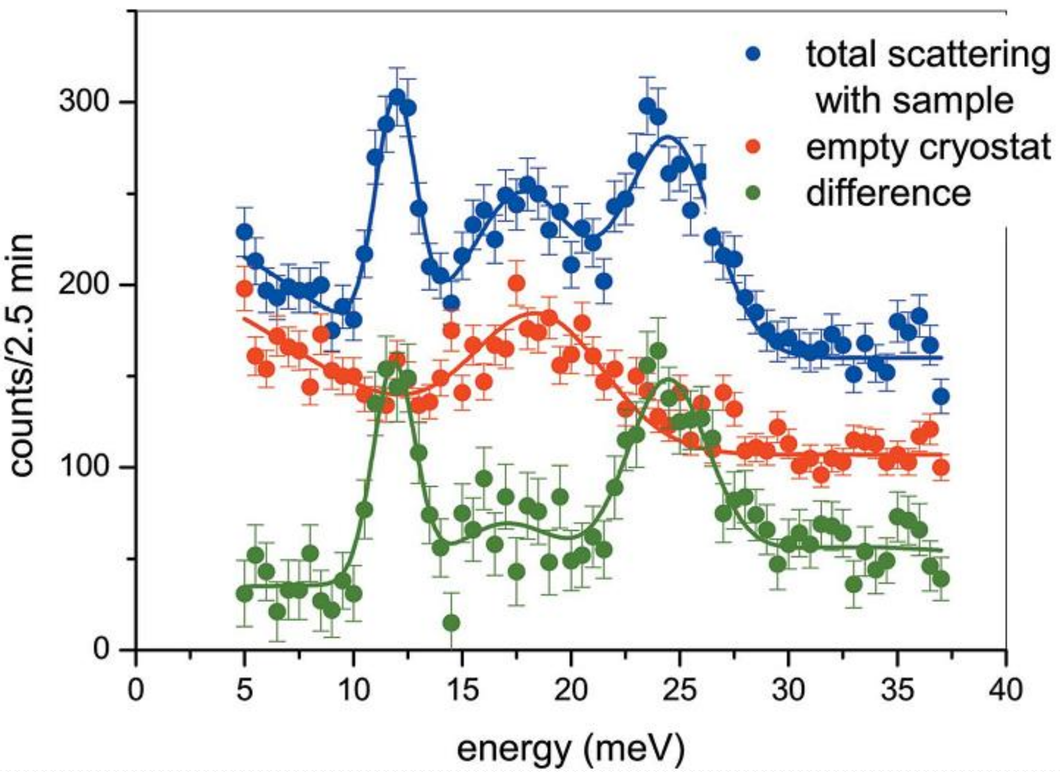
Skalyo, Jr., J. and Lurie, N. A. (1973). *Nucl. Instrum. Methods* **112**, 571.

Окружение образца

- Алюминий
- Воздух, гелий

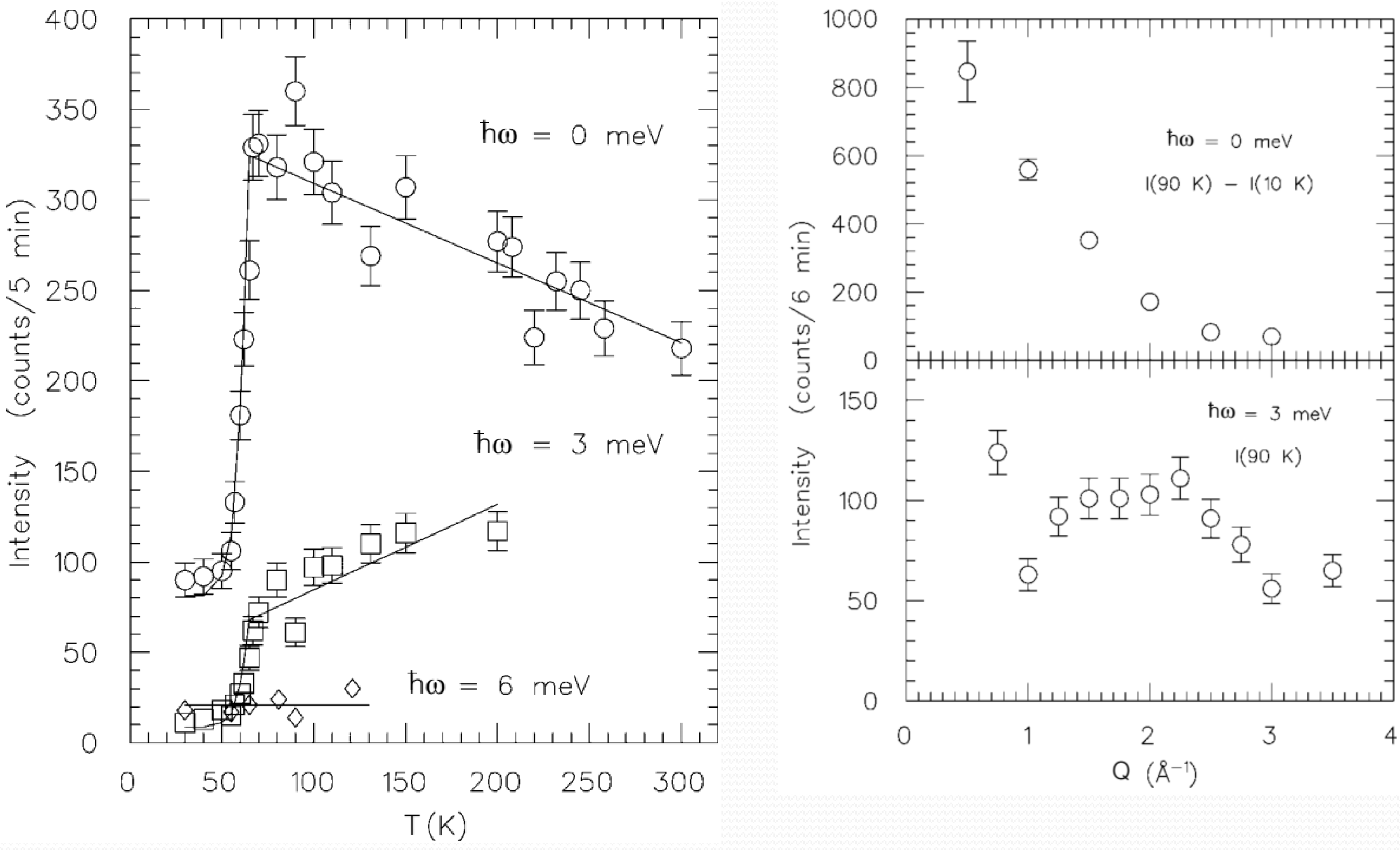
Алюминий





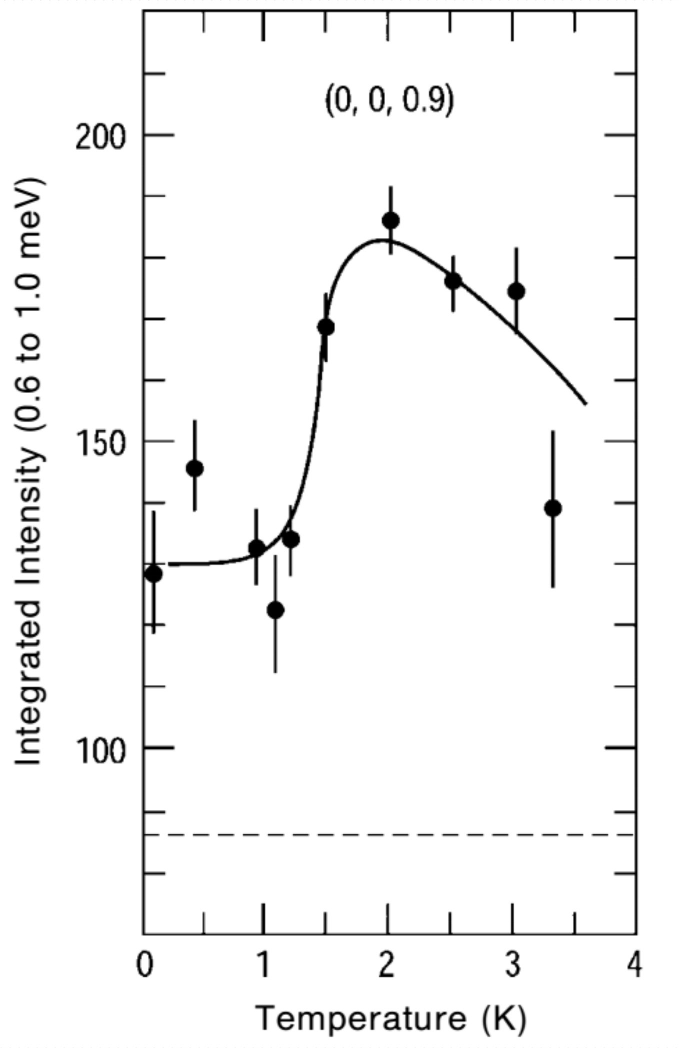
J. Appl. Cryst. (2014). **47**, 1472–1476

Воздух



ħω = 0 meV
ħω = 3 meV
ħω = 6 meV
Intensity (counts/5 min)
T (K)
ħω = 0 meV
I(90 K) − I(10 K)
ħω = 3 meV
I(90 K)
Intensity (counts/6 min)
Q (Å⁻¹)

Гелий

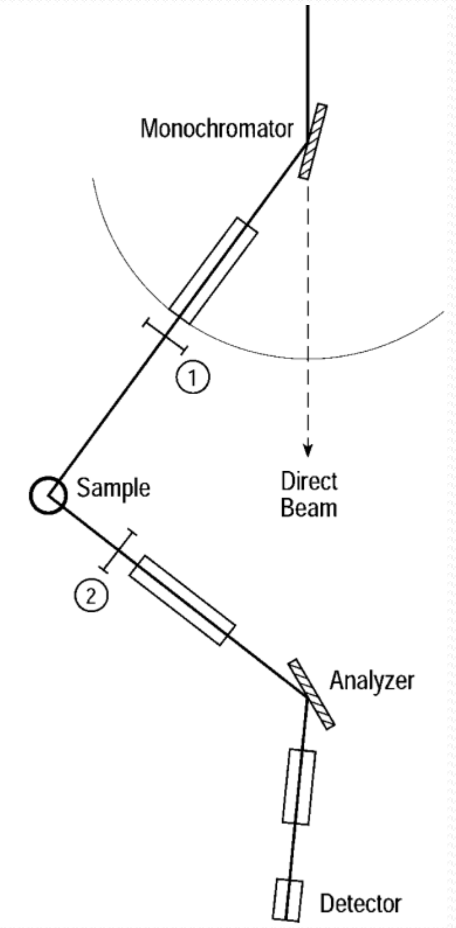


(0, 0, 0.9)
200
150
100
Integrated Intensity (0.6 to 1.0 meV)
0
1
2
3
4
Temperature (K)

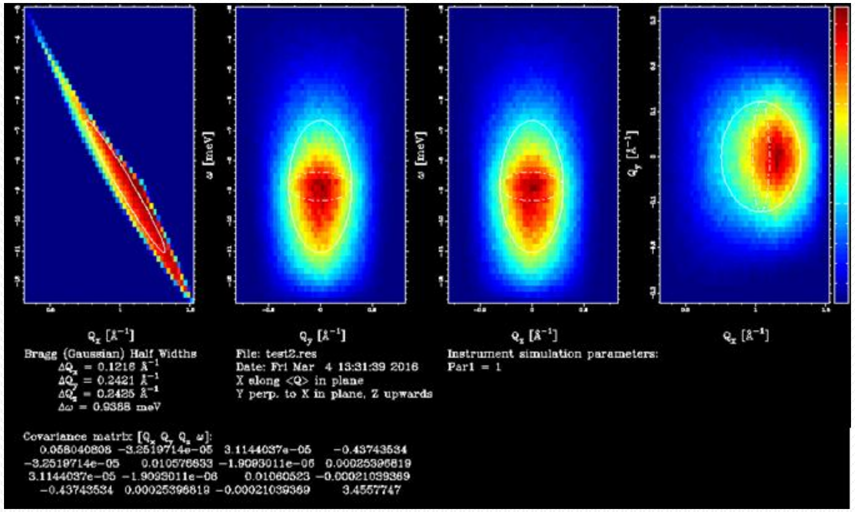
Определение спюрионов

Алгоритм:

1. Проверка нейтронного пути
2. Последовательное изменение углов монохроматора, образца, анализатора
3. Исследование подозрительной особенности, используя нейтроны другой энергии
4. Влияние окружения образца
5. Q-зависимость любой особенности должна соответствовать кристаллической симметрии образца



Спасибо за внимание!



ω [meV]
ω [meV]
Q_y [Å^{-1}]
Q_x [Å^{-1}]
Q_y [Å^{-1}]
Q_z [Å^{-1}]
Q_x [Å^{-1}]
Bragg (Gaussian) Half Widths
ΔQ_x = 0.1216 Å^{-1}
ΔQ_y = 0.2421 Å^{-1}
ΔQ_z = 0.2425 Å^{-1}
$\Delta\omega$ = 0.9388 meV
File: test2.res
Date: Fri Mar 4 13:31:39 2016
X along <Q> in plane
Y perp. to X in plane, Z upwards
Instrument simulation parameters:
Par1 = 1
Covariance matrix [Q_x Q_y Q_z ω]:
0.058040808 −3.2519714e−05 3.1144037e−05 −0.43743534
−3.2519714e−05 0.010576633 −1.9093011e−06 0.00025396819
3.1144037e−05 −1.9093011e−06 0.01060523 −0.00021039369
−0.43743534 0.00025396819 −0.00021039369 3.4557747

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- Спюрионы
  - Нейтроны более высокого порядка
  - Случайное Брэгговское рассеяние
  - Упругие полосы для малых q
  - Артефакты функции разрешения
  - Артефакты из-за среды образца
- Техники обнаружения спюрионов
- Заключение

2.ABS

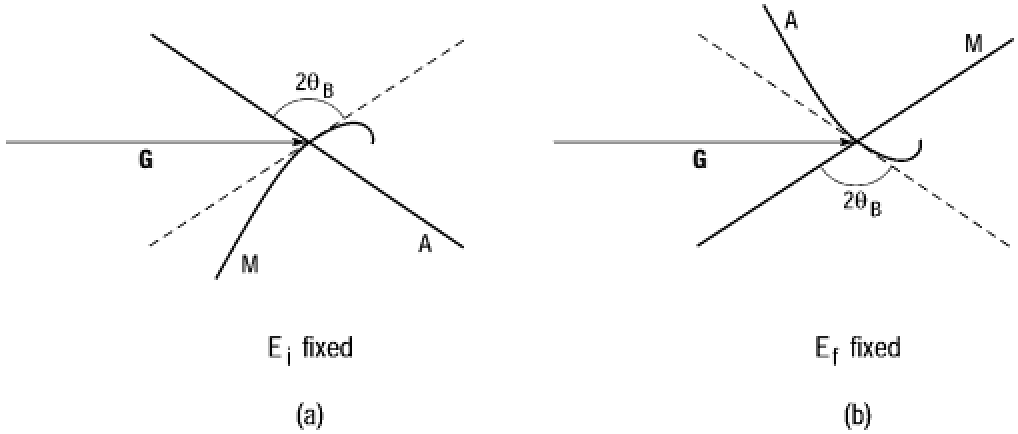


Fig. 6.3. Schematic diagrams of the lines in reciprocal space along which type-A and type-M accidental Bragg scattering can occur relative to a reciprocal-lattice vector **G**. (a) E_i-fixed mode. (b) E_f-fixed mode.

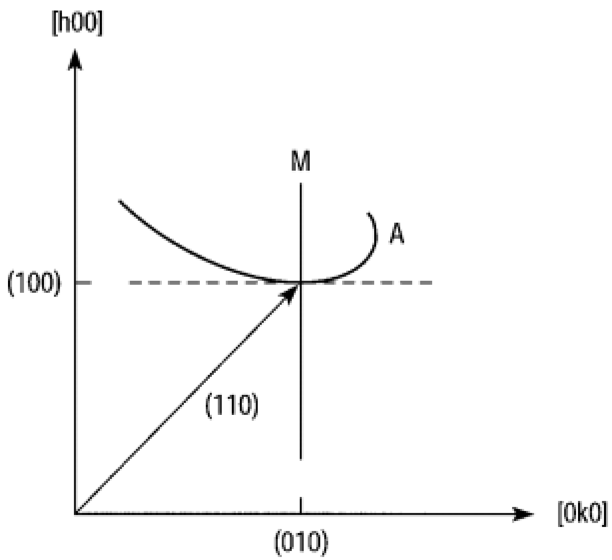


Fig. 6.4. Example of a situation in which the lines of accidental Bragg scattering could overlap with symmetry directions in a sample.

3.Small q

$$\hbar\omega = \frac{\hbar^2}{2m_n}\left(k_i^2 - k_f^2\right).$$

e keep terms of no higher t
)/k_i and q/G. The result is

$$\hbar\omega_A \approx -4E_i\left(\frac{\mathbf{q}\cdot\mathbf{G}}{G^2}\right).$$

ılation for type M modes yie

$$\hbar\omega_M \approx 4E_f\left(\frac{\mathbf{q}\cdot\mathbf{G}}{G^2}\right).$$

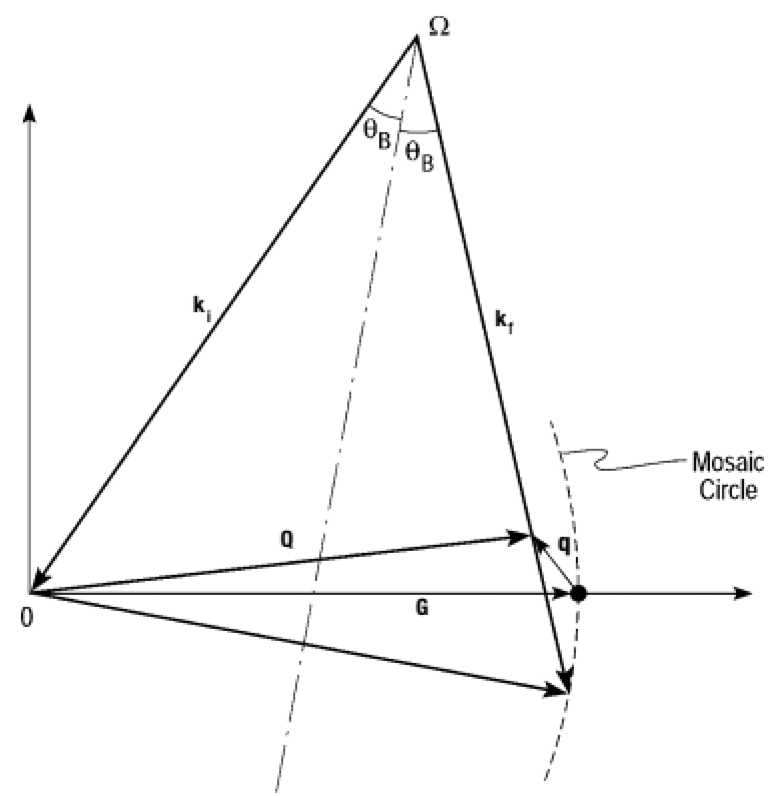


Fig. 6.7. Scattering diagram for accidental type-A Bragg scattering when q/G is comparable to the mosaic width η.

4.ASQ

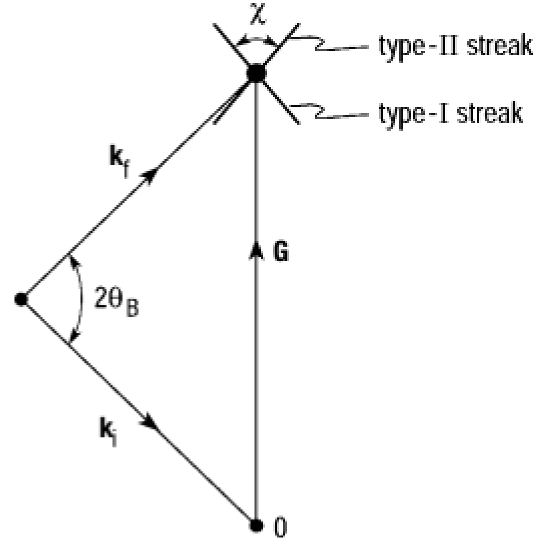
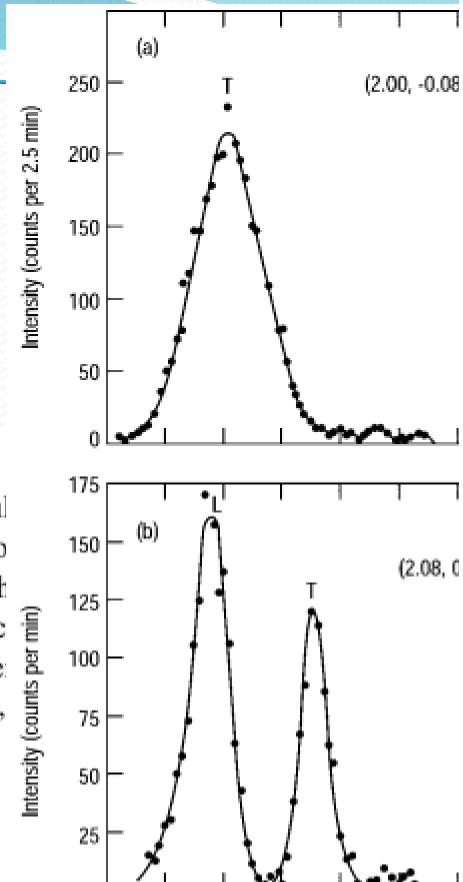


Fig. 6.8. Orientation in reciprocal space of elastic streaks due to non-ideal collimator performance and small-angle scattering.

5.RFA



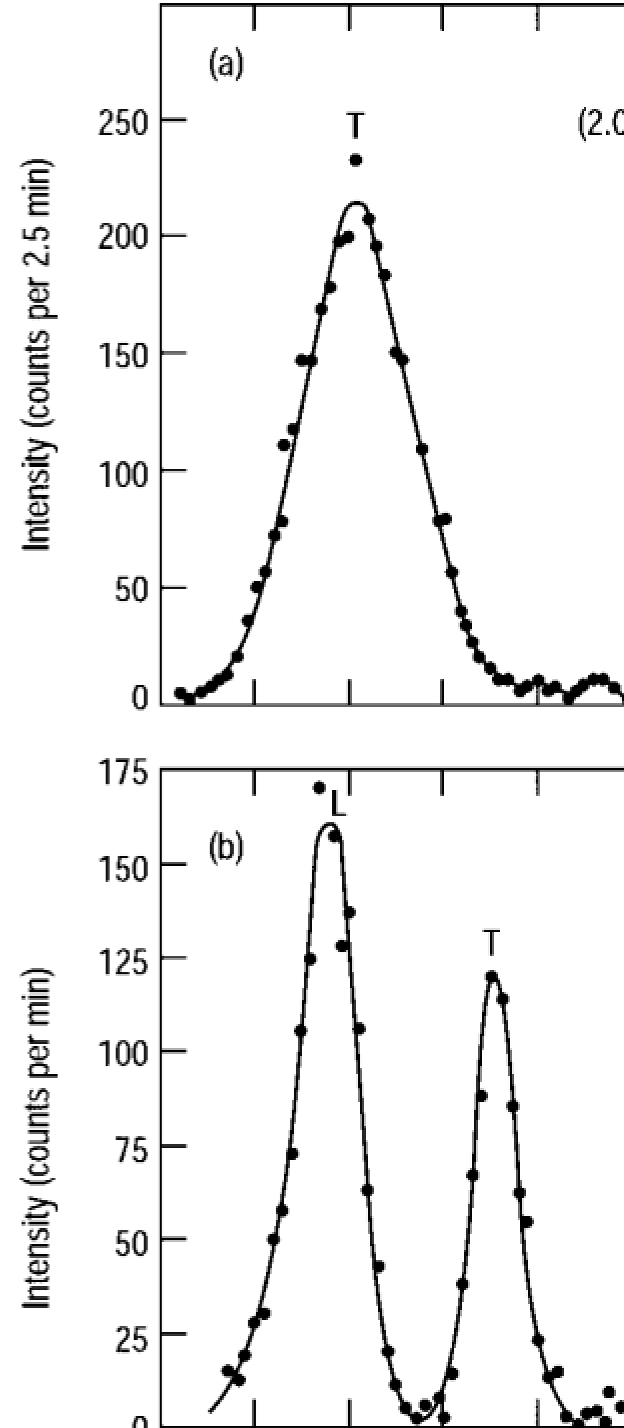
6.4 Resolution function artifacts

Artifacts associated with the resolution function shoul
spurious, since they involve the intrinsic cross section o
non-isotropic shape of the resolution function. Neverth
of Bragg-tail peaks and "forbidden" modes in inelastic
significant consternation the first time one confronts the
already discussed these features in the previous chapter,
for the sake of completeness.

6.4.1 Bragg tail

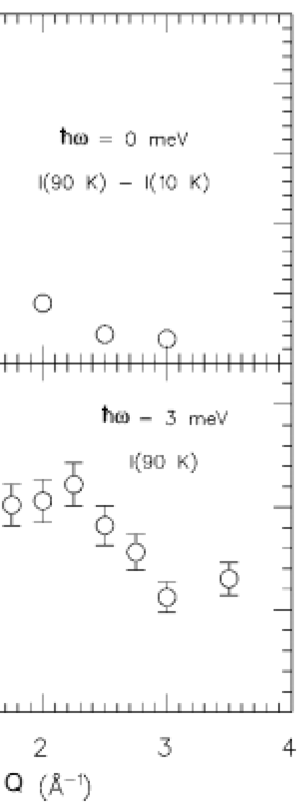
of this pl

When performing an inelastic scan close to a Bragg reflection, a Bragg-tail peak will be observed if the tail of the resolution function sweeps through the corresponding reciprocal-lattice point. Because of the shape and typical orientation of the resolution function, the Bragg-tail scattering appears to disperse like a transverse acoustic phonon. The intensity of the scattering drops off rapidly as **q** and ω are increased. It is good practice to locate and quickly map out the Bragg-tail signal before starting inelastic measurements near a Bragg peak.



6.SA

peaks



attering at two different energy transfers.

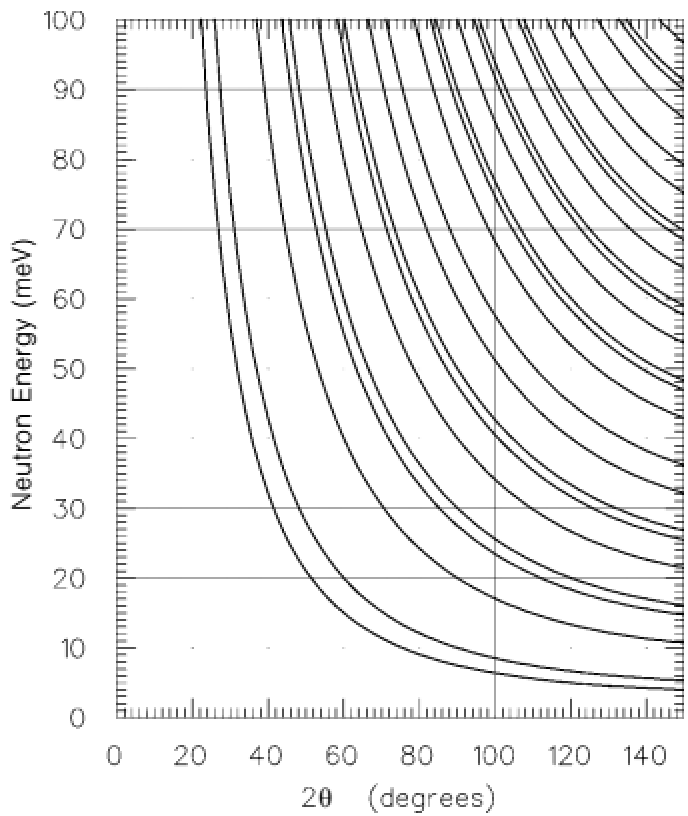


Fig. 6.9. Scattering angles of room-temperature aluminum Bragg peaks vs. neutron energy.

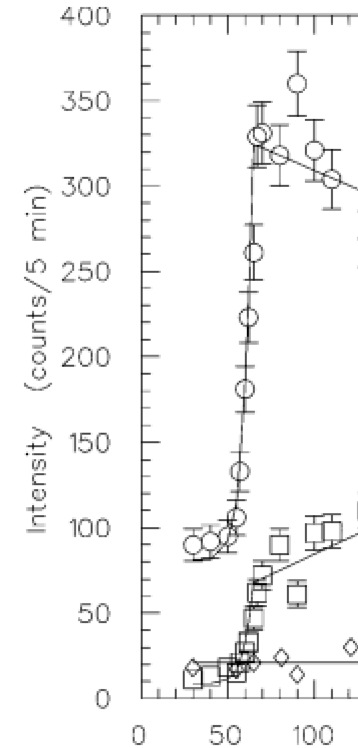


Fig. 6.10. Temperature dependence of a
Measurements were performed at $Q = 1.5$

7.Spoting

(i) Begin with a quick check of the spuri
the neutron beam before the sample,
(see Fig. 6.13), one can determine wheth
following the intended scattering path
whether they reach the detector because o
through gaps in the monochromator shie
of spurious signal. Another is neutrons in
intercepted by the sample; when there i
the sample, the direct-beam neutrons ca
(relative to the background level) if they

other unexpected scattering paths are po
seems unlikely, this simple test should be
possibility.

(ii) Set the spectrometer to the suspect peak
ually scan each of the six motors (ϕ ar
sample, and analyzer) through the nomi
genuine, then moving any given motor a
tion should detune the spectrometer, rap
background level. However, if, for examp
an accidental Bragg scattering feature of

(iii) Measure the suspect feature using neutrons
is a crucial and quite effective test. For ex
peak has been observed with a fixed final
repeat the measurement with $E_f = 13.7$ r
working at $E_f = 41$ meV, try again at 3
should be small enough that the resolution
do not change significantly, but large enou
of the peak position on neutron energy is
feature disappears or shifts in energy, then
double scattering or higher-order neutrons

(iv) If the suspect feature passes the test abov
from the sample or sample environment. C
it is coming from the sample holder (e.g., A
N_2). If the signal is from the sample enviro
depend on the precise nature of the sampl