帕纳科粉末衍射仪培训汇报

2018年3月19日~3月23日

上海

冯 蕊

2018年6月7日

培训通知函

马尔文-帕纳科公司

Malvern Panalytical

上海帕纳科亚太区实验室培训中心

各位尊敬的用户：

首先非常欢迎各位来到上海帕纳科亚太区实验室参加培训。

为了方便各位在此的培训生活， 敬请注意以下信息：

一、若贵司人员在应用方面有什么问题，可趁此机会将仪器的 user data （C:/Programefiles / Panalytical / SuperQ / User data） 刻成光盘，便于应用专家根据贵方的数据讨论解决。

二、培训结束后会进行考核，并颁发培训证书。

三、此次培训食宿费自理，酒店入住信息和公司地址请看后所附文件。

四、请3月19日早上9点30准时到上海实验室参加培训。

五、此次培训为期5天，培训时间为：2018年3月19日至3月23日。

最后，祝愿大家在上海帕纳科培训中心学有所获，度过愉快的学习生活。

X 射线分析仪器公司

培训地址：

上海思百吉仪器系统有限公司

帕纳科业务部

PANalytical Division,

Spectris Instrumentation and Systems Shanghai Ltd.

上海市徐汇区田州路99号楼新安大楼

13号楼102室（近古美路），200233

Unit 102,XinAn Plaza,Building 13,No.99 Tianzhou Road, Xuhui

District,Shanghai, China (near Gu Mei Road) 200233

X`Pert 3 Powder

Empyrean

Basic XRD Course培训内容

- **Introduction to Crystallography**
- **Additional Background Information**
- **Powder Diffractometers**
- **How are XRD Data Collected?**
- **X'Pert HighScore (Plus) 软件应用**

Introduction to Crystallography

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Outline（主要内容）

- Description of crystals(晶体的定义）
- Some simple crystal structures（晶体结构）
- Principles of diffraction（衍射原理）
- Calculation of diffraction pattern（衍射谱的计算）

Additional Background Information

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Origin and Characteristics of X-rays

- What are X-rays?
- Generation of X-rays
  - *Characteristic radiation（特征辐射）*
  - *Continuous radiation（连续辐射）*
- X-ray operation conditions
  - *Tube efficiency*
  - *Anode material: choice of wavelength*
  - *Power rating: mA & kV*
  - *Focus type and orientation*

Powder Diffractometers

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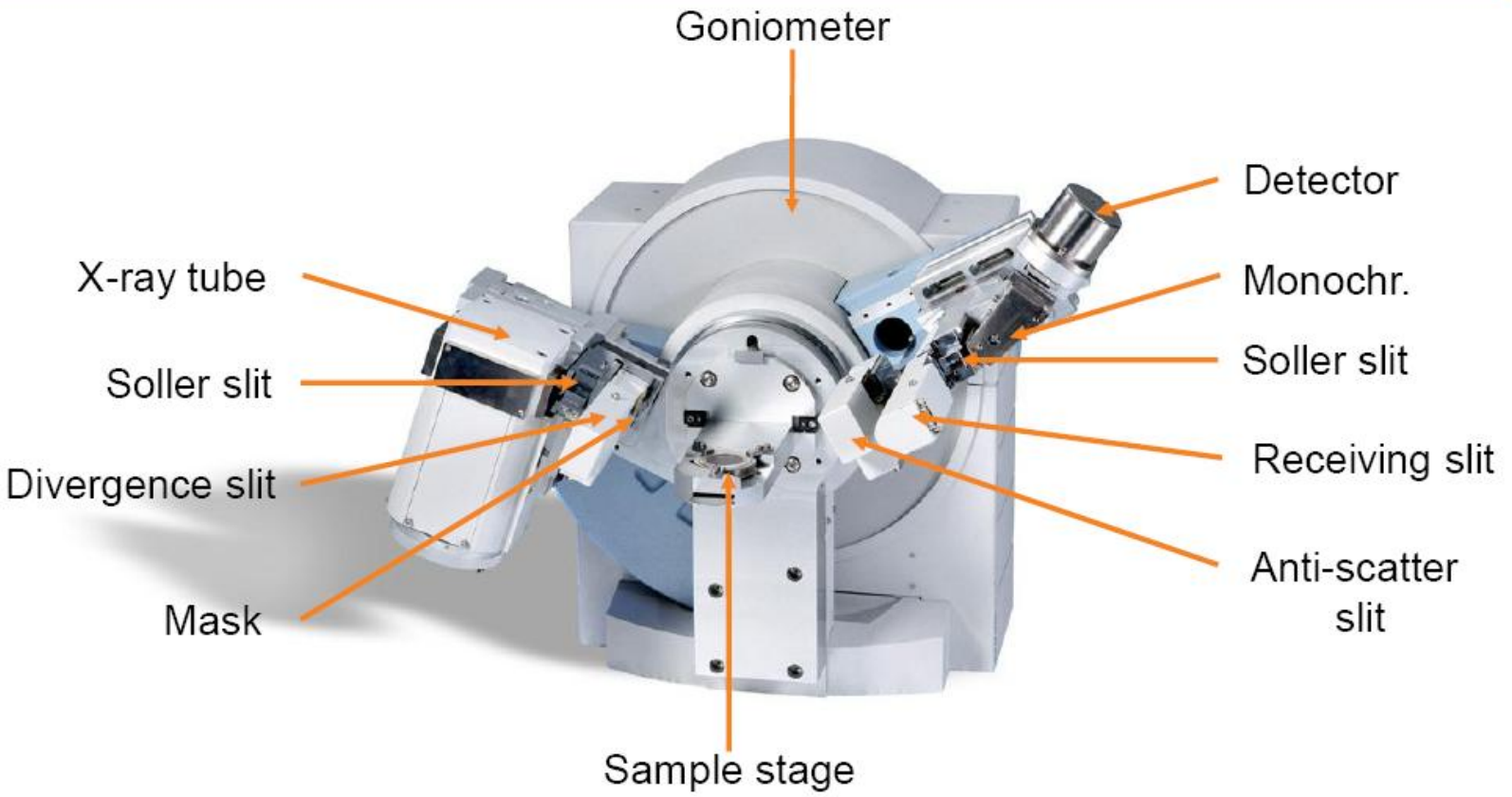
Classical Powder Diffractometer

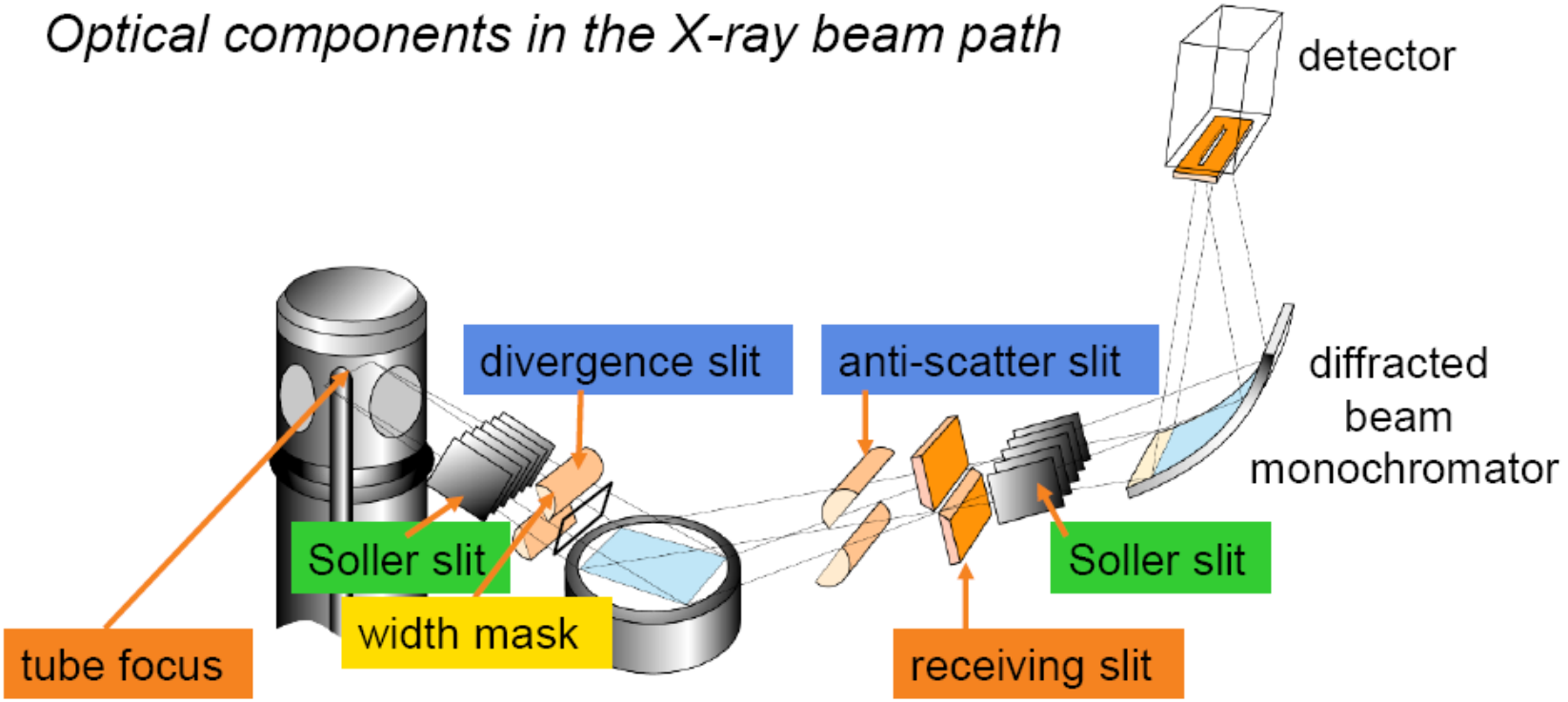


Powder Diffractometers

PANalytical

Classical Powder Diffractometer

Optical components in the X-ray beam path



How are XRD Data Collected?

样品制备

粉末衍射仪要求样品晶粒数目足够多且表面平整

- 首先，需把样品研磨成十分细小的粉末颗粒（360目的粉末 ），使试样在受光照的体积中有足够多数目的晶粒，且晶粒是随机取向。这样，才能满足获得正确的粉末衍射图谱数据的条件，才能保证用衍射仪法获得的衍射强度值有很好的重现性。
- 然后，把样品粉末制成有一个十分平整平面的试片。 最简单又常用的是“压片法” 和“涂片法” 。前者用量较大，后者用量少。

How are XRD Data Collected?

扫描方式

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Definition: Gonio Scan

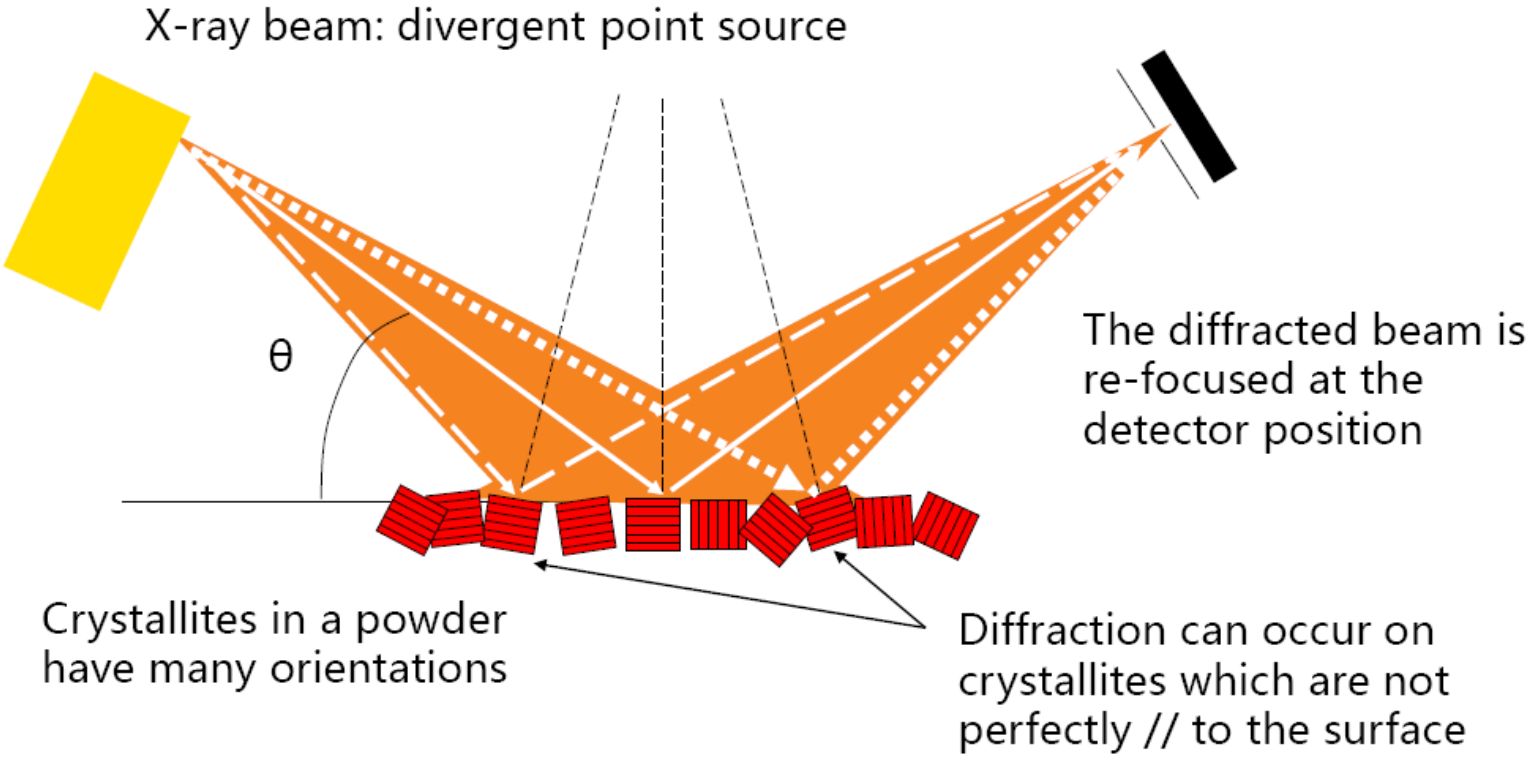
- Also known as 'Powder scan', '2θ-θ scan', 'Symmetric scan', 'Bragg-Brentano geometry'
- θ is kept as half the value of 2θ
- Only diffraction from planes parallel to the sample surface is collected
- Applications:
  - Phase analysis (qualitative and quantitative)

How are XRD Data Collected?

扫描方式

PANalytical

Definitions: Para-focusing Geometry(准聚焦几何)



How are XRD Data Collected?

扫描方式

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Definition: 2θ-ω Scan

- The angle of incidence is defined as ω
  - It is kept as half the value of 2θ + an offset

$\omega = \theta + \theta_{offset}$ （只测量与平面有夹角的晶面，它的夹角是θ_{offset}）

- While 2θ is scanned, ω follows with half the speed
- Applications:
  - Phase analysis
  - Analysis of polycrystalline thin film on single crystal
  - Stress analysis

How are XRD Data Collected?

扫描方式

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2θ Scan

- The incidence angle ω is kept at a fixed value, while the detector moves to cover a 2θ range

- Applications:
  - Thin film measurement
    - Grazing Incidence scan (usually ω < 10°)

How are XRD Data Collected?

扫描方式

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ω Scan

- 2θ is kept at a fixed value (usually equal to a Bragg angle of an expected reflection), while the incident beam (or the sample) moves to cover an ω range
  - Also called rocking curve

- Applications:
  - Polycrystalline samples with highly preferred orientation and/or low crystal statistics
  - Single crystals with epitaxial layer grown on it

How are XRD Data Collected?

扫描方式

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Summary

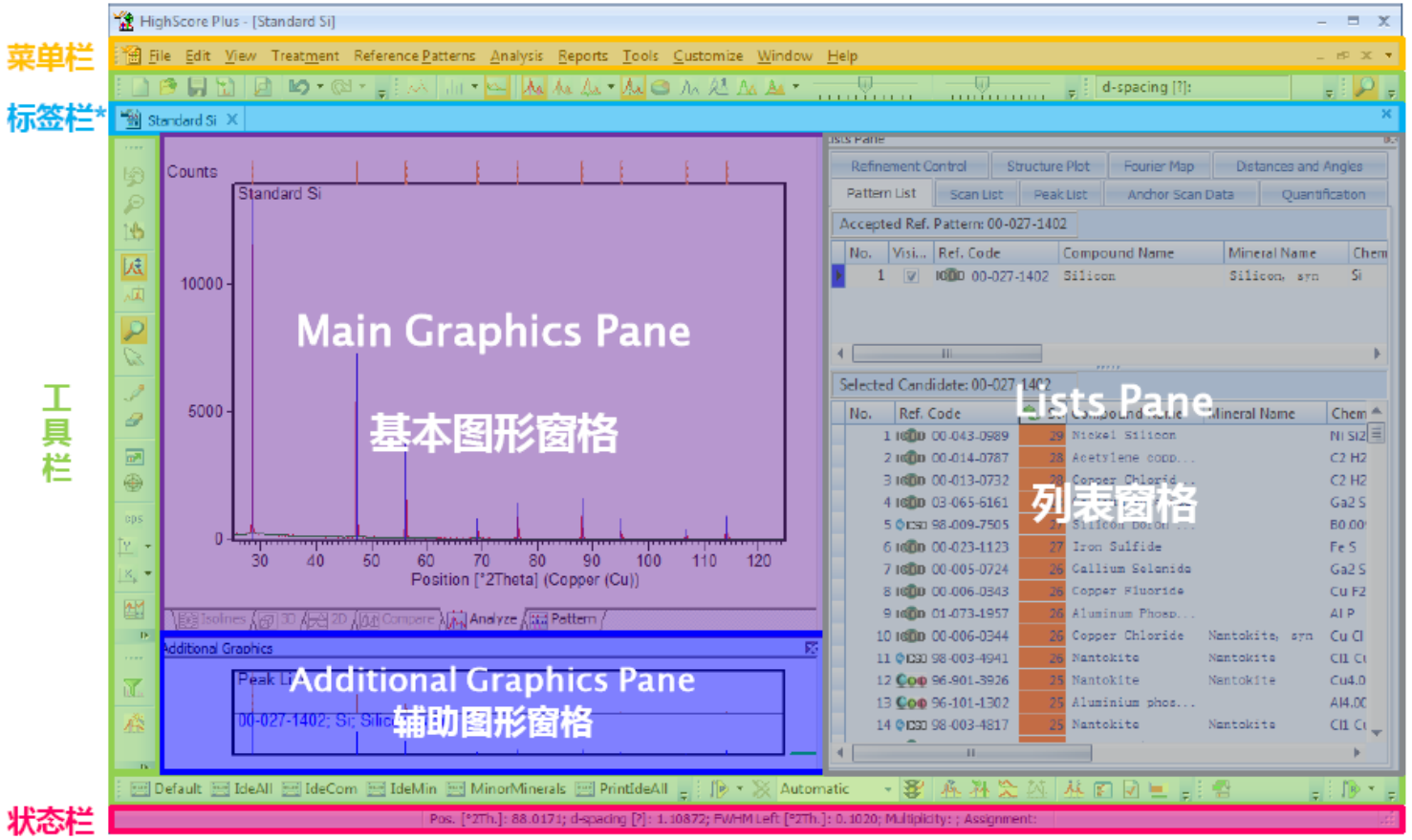
- Different crystallites are observed depending of the type of scan used
  (观察不同的晶体用不同的扫描方式）
- Each type of scan has its specific application
  (每种类型的扫描都有其特定的应用)

X’Pert HighScore (Plus) 软件应用

强大友好的分析软件

X’Pert HighScore (Plus) 软件应用

HighScore (Plus) 界面总览



X’Pert HighScore (Plus) 软件应用

- 物相定性和定量分析
- 晶粒大小和点阵畸变计算
- 结晶度计算
- 点阵参数精确计算
- 全谱拟合
- 解晶体结构

Malvern Panalytical

X-ray diffractometry certificate




This is to certify that

Ms. Rui Feng

has successfully completed the

XRD-basic

Held at MALVERNPANALYTICAL, APAC Application Laboratory, Shanghai, China

Signature of course leader:

陈永一 黄德翠

Date: 23 March 2018

2018.3.19 - 2018.3.23

SPECTRIS

谢　谢！