Propriétés catalytiques à l'échelle nanométrique sondées par diffraction des rayons X de surface et imagerie de diffraction cohérente.

Catalytic properties at the nanoscale probed by surface x-ray diffraction and coherent diffraction imaging

Thèse de doctorat de l'Université Paris-Saclay

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I would like to thank all the person that made the completion of my thesis possible.

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Introduction

(The Introduction chapter should contain background information as appropriate, plus definitions of all special and general terms. Your topic should be: clearly stated and defined; have a clear overall purpose; and have clear, relevant and coherent aims and objectives. It is also informative to give a brief description of the contents of the remaining chapters of the thesis. This alerts the reader and prepares them for the rest of the thesis.)

1.1 The oxidation of Ammonia

Ammonia oxidation is an essential catalytic reaction used in the production of artificial fertilizers and in environmental applications. In both cases, particular focus is on two products of the reaction, namely, NO and N_2. The selectivity toward either one is dictated by reaction parameters, that is, by temperature, NH_3 and O_2 partial pressures, and the type of catalyst.

Detail and literature about the oxidation of Ammonia on Platinum nano-catalyst can be found here (Resta et al. 2020).

1.1.1 From industry to model catalysis

1.1.2 Crystal structures

1.1.3 Pt 111

1.1.4 Pt 100

1.1.5 Nanoparticles

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1.2   Aim and Scope

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1.3   Outline of the Thesis

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Chapter 2

Theory and methods

2.1 Heterogeneous Catalysis

Detail found in Corentin thesis and dutch guy thesis

2.1.1 Mechanisms

In heterogeneous catalysis, two mechanisms are generally considered : the Langmuir–Hinshelwood mechanism [44, 45, 46] and the Eley–Rideal mechanism [47]. In the first mechanism both reactants are adsorbed at the surface of the catalyst, react at the surface and then happen the desorption of the product. In Eley–Rideal mechanism, only one of the reactant is adsorbed while the other one reacts with it directly from the gas phase. The first mechanism (Langmuir–Hinshelwood) appears to be generally preferred [48] (Fig. 1.1).

Last meachanism is Mars - Van Krevelen (MvK) mechanism

The overall heterogeneous catalytic reaction generally consists of a series of elementary steps : adsorption of the reactants, diffusion on the surface, breaking of reactants bonds, creation of new bonds to form products and finally desorption of these new chemicals. Catalysts are usually complex systems in powder form (presenting different surface orientation, i.e. facets) coupled with promoters (chemicals that improve the catalytic activity). It is therefore difficult to provide a molecular-level understanding of such processes. Model catalysts can therefore be used to simplify the investigation. A well-built theory has been proposed by Hammer and Nørskov [49] and lays down the basic rules behind catalysis. Some key parameters are used to rationalize and describe a catalytic process and catalysts performances. More recent approaches involving the use of machine learning can help predict the key descriptors for catalysis [50, 51]. Hammer and Nørskov theory is more of a model theoretical approach that could be experimentally questioned by model catalysts.

Catalysis is described by key parameters such as the stability (the propensity of the catalyst to stay unchanged after the reaction), the activity and the turn-over frequency (TOF, number of mole of reactant that can be converted per mole of catalyst over time), the selectivity (for example targeting the production of one particular isomer), the propensity to deactivation of the catalyst (for instance due to its oxidation). Depending on the chemical reaction, one wishes to have an active catalyst that is very stable and very selective towards a unique product, and doing so for a long time. However, it is difficult to meet all the requirements at once. A high activity is unfortunately often

linked to a poor selectivity

Hammer and Nørskov [49] have compiled and provided a well-built theory of adsorbates surface interactions for simple transition metals. As shown in Fig. 1.2, the model predicts that as the d-band of the metal shifts up towards the Fermi level (the filling of the band is kept fixed so that as the center of the d-band is shifted up, the band width decreases), the electron density of states of the adsorbate is modified and antibonding states appear above the Fermi level. Therefore they are empty and the bonds become stronger as the number of empty antibonding states increases. In short, the closer to the Fermi level and the narrower the d-band, the stronger the bonding i.e. the chemisorption.

This model seems to work fine for simple transition metals (3d, 4d and 5d) [38, 39] for chemisorption (e.g. oxygen adsorption [49]) and also for molecular dissociation (e.g. CO dissociation [53], NO dissociation on Ru(0001) [42]). A clear linear correlation between adsorption energies and d-band position is determined both experimentally and theoretically. This is similar to the Brønsted-Evans-Polanyi linear relation between the activation and reaction energies. In the case of a monolayer of a transition metal over a substrate, a similar behavior is observed and the model still works fine (e.g. 5d metals on Pt(111) [54])

Role of strain :

Kitchin et al. 2004

Mavrikakis, Hammer and Norskov 1998

We define a system where a (metal) sample, consisting of a surface and a bulk is in contact with a gaseous environment.

Materials

Conditions

This reaction is considered as a classic example of a strongly exothermic, heterogeneous, catalytic reaction [4]. Due to the very fast kinetics of oxidation reactions, a direct experimental investigation of several reaction steps is difficult at realistic conditions.

nitrous oxide is a powerful oxidiser similar to molecular oxygen.

Selectivity to nitrous oxide at low temperature was reported in the following order: $Pt > Pd > Ni > Fe > W > Ti$[6].

N2O selectivity for us ?

NH3 oxidation requires surface sites for the adsorption of two ammonia molecules and two oxygen atoms.

Furthermore, the importance of availability of oxygen vacant sites near N-containing adspecies was demonstrated by the decrease of the reaction rate when a surface oxide was formed [31–33]. Finally, adsorbed oxygen did not block the ammonia adsorption [12]. All these facts led to the conclusion that a dual-site mechanism is operative. A similar conclusion on the reaction mechanism was made for ammonia oxidation on a supported ruthenium catalyst [34].

Relation to nanoparticle size It was also reported that the stoichiometry of oxygen chemisorption increases by a factor 2.7 with increasing platinum crystallite size. This could also lead to an increase of the reaction rate if the oxygen adsorption is the rate-determining step in this system.

2.1.2 Particle-Size Effect in Catalytic Oxidation Over Pt Nanoparticles

Alexandr Yu. Stakheev, ..., Valerii I. Bukhtiyarov, in Advanced Nanomaterials for Catalysis and Energy, 2019

Relationships between turnover frequency and the size of supported Pt clusters are discussed for oxidation of hydrocarbons, CO, and NO by molecular oxygen. Analysis of the experimental data indicates that TOF tends to increase for bigger platinum particles. This tendency is particularly pronounced for the nanoparticles smaller than 4–5 nm. According to the most realistic models, the observed tendency stems from the deactivation of edge, corner, and neighboring atoms by two processes: (1) strong oxygen adsorption on edge and corner atoms with high degree of coordinative unsaturation, and (2) oxidation of Pt to PtOx, which is facilitated over undercoordinated sites. As the metal clusters grow in size, the fraction of undercoordinated edge and corner atoms decreases leading to the increase in experimentally observed TOF.

The increase of supported platinum particle size led also to considerable changes in selectivity in the ammonia oxidation over a Pt/Al2O3 catalyst [7,22,26]. Large crystallites of 15.5 nm, for which over 98% of the surface atoms are plane atoms [28], exhibited low selectivity to nitrogen formation. Selectivity to nitrogen increased with decreasing platinum loading

2.1.3 Stability

The turnover frequency TOF quantifies the specific activity of a catalytic centre for a special reaction under defined reaction conditions by the number of molecular reactions or catalytic cycles occurring at the centre per unit time. For heterogeneous catalysts the number of active centres is derived usually from sorption methods.

Separate from the TOF, evaluating the catalytic activity, the turnover number (TON) value is an important parameter to evaluate the stability of the catalyst. In homogeneous and heterogeneous catalysis, the TON is a dimensionless number,24,25 which is defined as the number of the molecules produced per catalytic site before deactivation under given reaction conditions. That is to say, the catalyst can achieve the total number of turnovers until it is totally dead, regardless of the reaction time.26 In this respect, an ideal catalyst should have an infinite TON. Thus, the TON represents the maximum yield of products attained from an active catalytic site up to the decay of activity for a specific reaction. The TON of a catalyst for water oxidation is calculated according to Eq. (5):

2.1.4 Linking strain and reactivity

Hammer and Noskrov blabla

2.2 X-ray interaction with matter

Understanding the different mechanism at play when photons interact with matter is of crucial importance to be able to decide how to use x-rays as a probe in material science. Each phenomena is at the source of different techniques, diffraction brings surface x-ray diffraction (SXRD) and Bragg coherent diffraction imaging (BCDI), two

techniques used during this thesis that give complementary information about the sample structure and constitution.

X-ray absorption together with the photoelectric effect explained by Einstein in 1905 are at the source of a third technique, x-ray photoelectron spectroscopy, specific to the nature of the adsorbates on the sample's surface.

In this chapter we will discuss the origin of each technique, their sensitivity and the information that we can obtain from using them.

2.2.1   Scattering from electrons and atoms

The duality between wave and particles was first mentionned by Max Planck and Albert Einstein in the early 20th century and generalized to all matter by Louis-Victor de Broglie in 1924 with the famous formula:

$$\lambda = \frac{h}{p} \tag{2.1}$$

Electromagnetic waves, i.e. light or photons can be characterized by their energy E in eV and wavelength λ in m. The conversion between both is realized thanks to Planck's constant: $h = 6.626 \times 10^{-34}$ J s with the following equation:

$$E = \frac{hc}{\lambda} \tag{2.2}$$

$c = 2.9979 \times 10^8$ m s^{-1} the speed of light in vacuum.

The properties of the photon and its use in our society depends on its energy and wavelength. If visible light is situated between 500eV and 900eV, micro-waves used in our everyday life are situated between 10^{-6}eV and 10^{-4}eV. On the other side of the electromagnetic spectrum, we have higher energy photons such as x-rays ($\in [10^2, 10^6]$eV) and γ-rays (above 10^{-6}eV).

For example, x-ray with a wavelength of 1 Å have an energy of 12384.4eV, we will see that the very fact that the wavelength of x-rays is in the range of the distance between atoms is the reason why we use x-rays for diffraction.

2.2.2   Cross-sections

When an electromagnectic beam interacts with matter it will be attenuated by absorbtion, reflection or scattering, etc ... Each process can be quantified depending on the atoms the beam interacts with and the energy on the incoming photon, this is illustrated in figure 2.2. The cross-section for a particuliar process p defined as follows:

$$\sigma_p = (\Lambda_p N_i)^{-1} \tag{2.3}$$

Λ_p is the attenuation length in m defined as the length after which the beam is reduced to $1/e$, N_i is the atomic number-density in atoms/unit volume.

In the frame of this thesis, the cross-sections of (elastic) Thomson scattering is the most important, at the origin of x-ray diffraction. This process is dominant for energies below 200keV, together with photoelectric absorption for which the K, L and M edges are shown.

Compton scattering also named inelastic scattering is a process during which some energy is transfered from the incoming electromagnetic wave to the atoms' electrons.

This results in a lower energy for the scattered photon (and therefore a higher wavelength) compared to the incoming photon. This effect has a low cross-section compared to the two other processes and is therefore not taken account during the experiments.

We begin our discussion of x-ray scattering by first considering scattering from a single free electron using classical electromagnetic theory. During elastic scattering, the oscillating electric field of the x-ray wave exerts forces ($\vec{F} = q\vec{E}_i$, q represents the charge) on the electron, causing it to accelerate and oscillate in the same direction as the incident field.

The oscillating electron then emits a spherical wave with the same wavelength as the incident beam (Thomson scattering) and this is the scattered field.

If we consider how the incident x-ray wave will interact with the different charge elements relative to the origin of the atom, you can see from Figure 1.4 that there is a path length difference of where = is the scattering vector and is equal to the change experienced by the wavevector during scattering.

Let us first consider a simple approach to neutron scattering with a system consisting of a single nucleus, one can write the nucleus-neutrons interaction potential for a single nucleus as $V(\vec{r})$.

We can then derive the Schrödinger equation as follows:

$$\left[\frac{-p^2}{2m} + V(r)\right]\psi(r) = E\psi \tag{2.4}$$

where the first term corresponds to the kinetic energy and the second to the potential energy, i.e. the nucleus-neutrons potential $V(\vec{r})$. $\psi(r)$ is the eigenfunction of the neutron. The general solution to the Schrodinger equation is given in the Born Approximation (DWBA).The incoming wave is assumed plane:

$$\phi_i(r, w) = \exp\left(-i(kx - \omega t)\right) \tag{2.5}$$

and the resulting wave is the sum of a plane wave and a spherical wave. The final particle scatters in all directions in the form of a spherical wave.

$$\phi_f(r, w) = \exp\left(-i(kx - \omega t)\right) + f(\theta)\frac{\exp\left(-i(kx - \omega t)\right)}{r} \tag{2.6}$$

Bragg's Law

In the frame of this thesis, where the all the information will be extracted from the analysis of Bragg peaks, it is mandatory to explain the physics behind Bragg peaks.

The lattice of our crystal is defined by three vectors $\vec{a}$, $\vec{b}$, $\vec{c}$. Any vector $\vec{v}$ of the unit cell can then be created by a linear combination of these three vectors:

$$\vec{v} = n_1\vec{a} + n_2\vec{b} + n_3\vec{c}, \quad with\ (n_1, n_2, n_3) \in \mathbb{Z}^3 \tag{2.7}$$

the volume of the unit cell is:

$$V = \vec{a}.(\vec{b} \times \vec{c}) \tag{2.8}$$

An important tool of crystallography is the *reciprocal space* of dimension m^{-1}, defined by the three vectors $\vec{a*}$, $\vec{b*}$, $\vec{c*}$:

$$\vec{a*} = \frac{2\pi}{V}(\vec{b} \times \vec{c}), \qquad \vec{b*} = \frac{2\pi}{V}(\vec{c} \times \vec{a}), \qquad \vec{c*} = \frac{2\pi}{V}(\vec{a} \times \vec{b}) \tag{2.9}$$

From the De Broglie wavelength (**??**), it is possible to define the wavevector k of neutrons (**??**). We can then define the momentum transfer $\vec{Q}$ as the difference between the wavevector of the incoming neutron $\vec{k}$ and the wavevector of the scattered neutron $\vec{k'}$:

$$\vec{Q} = \vec{k} - \vec{k'} \tag{2.10}$$

The figure 2.3 leads to (2.11) and illustrates the particular case of a Bragg peak. If the momentum transfer $\vec{Q}$ can be expressed as a linear combination of reciprocal vectors, here graphically verified, a Bragg peak occurs for this value of Q.

$$\vec{Q_{hkl}} = 2k \sin\theta = \frac{4\pi}{\lambda}\sin\theta \tag{2.11}$$

$\vec{Q}$ can be written as a linear combination of the reciprocal length between planes.

$$\vec{Q} = n\frac{2\pi}{d_{hkl}}, \qquad with\ n \in \mathbb{Z} \tag{2.12}$$

Combining (2.11) and (2.12), we fall back on the most famous equation of crystallography, Bragg law:

$$n\lambda = 2d_{hkl}\sin\theta \tag{2.13}$$

To summarize, a Bragg peak result from the constructive interference between coherently scattered waves at discrete values of the incident angle 2θ or of the momentum transfer $\vec{Q}$ on a specific set of crystalline planes. $\vec{Q}$ and 2θ are linked through (2.11). The condition to have constructive interference is known as Bragg law and is given by (2.13).

From (2.12), one can define the general reciprocal-space metric tensor for any crystalline system:

$$\frac{(2\pi)^2}{d_{hkl}^2} = h^2\,(\vec{a^*}.\vec{a^*}) + k^2\,(\vec{b^*}.\vec{b^*}) + l^2\,(\vec{c^*}.\vec{c^*}) + 2hk\,(\vec{a^*}.\vec{b^*}) + 2hl\,(\vec{a^*}.\vec{c^*}) + 2kl\,(\vec{b^*}.\vec{c^*}) \tag{2.14}$$

$$\frac{(2\pi)^2}{d_{hkl}^2} = h^2\,a^{*2} + k^2\,b^{*2} + l^2\,c^{*2} + 2hk\,a^*.b^*\cos\gamma^* + 2hl\,a^*.c^*\cos\beta^* + 2kl\,b^*.c^*\cos\alpha^* \tag{2.15}$$

$$\frac{(2\pi)^2}{d_{hkl}^2} = Ah^2 + Bk^2 + Cl^2 + Dhk + Ehl + Fkl \tag{2.16}$$

Equation (2.14) can be simplified as (2.17) for a simple cubic system, defining the interplanar spacing between the crystalline planes:

$$d_{hkl} = \frac{2\pi}{|\vec{a^*}|\sqrt{h^2 + k^2 + l^2}} = \frac{|\vec{a}|}{\sqrt{h^2 + k^2 + l^2}} \tag{2.17}$$

Moreover, for each peak, indexed by its *hkl* miller indices that specify the orientation of the crystalline planes, the momentum transfer can be written as a linear combination of reciprocal space vectors, for a cubic lattice:

$$\vec{Q_{hkl}} = h\vec{a*} + l\vec{b*} + k\vec{c*} \tag{2.18}$$

Inelastic scattering

One can also write for the momentum transfer:

$$\omega = \frac{\hbar k_f^2}{2m} - \frac{\hbar k_i^2}{2m} \tag{2.19}$$

We have elastic scattering if $|\vec{Q}| = 0$, energy is not transferred (to or from the material) in this case, we lose all dynamical information about the sample and study the structural information alone.

For inelastic scattering, when $|\vec{Q}| \neq 0$, energy is transferred, given or received from the sample. In that case we measure neutrons as a function of both energy and momentum transfer. It can lead to a dispersion relation giving more insight in the geometry of the phenomena that lead to the loss or gain of energy.

2.2.3   Intensity of a nuclear Bragg peak

Neglecting absorption, very weak for most of the elements, and considering only a non-magnetic structure factor; the intensity of a Bragg peak I_{nuc} as a function of its miller indices hkl and of 2θ can be written as:

$$I_{nuc} = A \times |F_{hkl}|^2 \times j_{hkl} \times L(2\theta) \times \exp(-2W) \tag{2.20}$$

where A is an instrument constant.

Structure factor

F_{hkl} is known as the structure factor, it is given by:

$$F_{hkl} = \sum_{j=0}^{n} b_j \exp(-2\pi i \vec{Q}.\vec{r_{j0}}) \tag{2.21}$$

The structure factor is the summation of the contribution to the scattering energy of each atoms at the position $\vec{r_{j0}}$ of scattering length b_j in our unit cell for a given $\vec{Q}$. The position of the atom $\vec{r_{j0}}$ is given by:

$$\vec{r_{j0}} = x_j \vec{a} + y_j \vec{b} + z_j \vec{c} \tag{2.22}$$

Debye-Waller factor

The position $\vec{r_j}$ of the atom j is not static but should be rather understood as the instantaneous position of the atom. In a crystal, atoms vibrate around their equilibrium position $\vec{r_{j0}}$, we have:

$$\vec{r_j}(t) = \vec{r_{j0}} + \vec{u}(t) \tag{2.23}$$

$\vec{u} = \vec{u}(t)$ is the thermal displacement, accounting for thermal vibrations in the crystal. These oscillations around the equilibrium position can be understood following the model of a harmonic oscillator at low temperature, with discrete frequencies of vibrations. The frequency of the vibrations, that increase with temperature, are linked to quasi-particles named *phonons*. Another contribution to the thermal displacement is the zero-point displacement, if one could lower the temperature of the crystal in a

perfect vacuum down to absolute zero, one would have expected the system to not show any motion. However, quantum physics tells us that even at absolute zero there is a probability for the atom to not be in at its equilibrium position, called zero-point displacement. Moreover, the Debye-Waller factor also takes into account the static displacement in the lattice that is linked to disorder. This will be discusses further in chapter 2.

The exponential in (2.21) can be rewritten as:

$$\exp\left(-2\pi i \vec{Q}.\vec{r_j}\right) = \exp\left(-2\pi i \vec{Q}.(\vec{r_{j0}} + \vec{u})\right) \tag{2.24}$$

The average of this equation is given by:

$$\langle \exp\left(-2\pi i \vec{Q}.\vec{r_j}\right) \rangle = \exp\left(-2\pi i \vec{Q}.\vec{r_{j0}}\right) \times \langle \exp\left(-2\pi i \vec{Q}.\vec{u}\right) \rangle \tag{2.25}$$

The second term of this expression can be expanded as the second order Taylor series for $\exp x_0$ with $x_0 = -2\pi i \vec{Q}.\vec{u}$ at zero, we loose the (2π) for clarity:

$$\langle \exp\left(-i\vec{Q}.\vec{u}\right) \rangle = 1 - \langle\, i\vec{Q}.\vec{u}\, \rangle - \frac{1}{2}\langle\, (\vec{Q}.\vec{u})^2\, \rangle + o\left(\langle\, (\vec{Q}.\vec{u})^2\, \rangle\right) \tag{2.26}$$

Since the displacement are random, the average of $i\vec{Q}.\vec{u}$ is equal to zero. However the average of the square of $\vec{Q}.\vec{u}$ is non zero and can be further developed as:

$$\langle\, (\vec{Q}.\vec{u})^2\, \rangle = Q^2\, \langle\, u^2\, \rangle\, \langle\, \cos\theta^2\, \rangle = \frac{1}{3}\, Q^2\, \langle\, u^2\, \rangle \tag{2.27}$$

which leads to:

$$\langle \exp\left(-i\vec{Q}.\vec{u}\right) \rangle = 1 - \frac{1}{6}\, Q^2\, \langle\, u^2\, \rangle \tag{2.28}$$

that corresponds to the first order Taylor series for $\exp x_0$ with $x_0 = \frac{1}{6}\, q^2\, \langle\, u^2\, \rangle$ at zero, we can write:

$$1 - \frac{1}{6}\, Q^2\, \langle\, u^2\, \rangle = \exp\left(\frac{1}{6}\, Q^2\, \langle\, u^2\, \rangle\right) \tag{2.29}$$

The final intensity contribution of the Debye Waller factor is the square of (2.29) given by:

$$\exp\left(\frac{1}{3}\, Q^2\, \langle\, u^2\, \rangle\right) \tag{2.30}$$

The last two terms of (2.20), respectively j_{hkl} and $L(2\theta)$ are the multiplicity of a Bragg peak and the Lorentz factor. They will be studied in a section covering the instrument used for powder diffraction for they both relate more to the collection of the data than to the theoretical intensity of a Bragg peak.

2.3   X-Ray diffraction

Laboratory X-Ray powder diffractometers commonly use Cu-Kα radiation and a Bragg-Brentano geometry for which the incoming beam diverges onto the sample and the diffracted beams is focused on the detector, both beams are at a fixed radius from the sample position. Focussing the diffracted beam leads to better resolution. It is then

possible to either fix the source and move the sample and detector by respectively θ and 2θ or to fix the sample and move the source by respectively $-\theta$ and θ. This second configuration is more adapted to liquid sample for example.

The advantages of using neutrons over X-ray in general are summarized in the table 2.1. For powder diffraction, the main differences hold in the scatterer, in the necessity to account more thoroughly for absorption and in the creation of polarization corrections while using X-ray (which is only possible for the spin in the case of neutrons, no polarization factor for neutrons) at a synchrotron (due to how the X-Rays are emitted). Laboratory sources are unpolarized and in the case of a Bragg-Brentano geometry where the incident beam constantly covers the entire sample the absorption correction is also negligible. The structure factor dependence on q can be seen in the atomic form factor that measures the scattering power of an isolated atom:

$$f(\vec{q}) = r_0 \int \rho(\vec{r}) \exp\left(-i\vec{q}.\vec{r}\right) d^3\vec{r}, \tag{2.31}$$

$$\text{with} \quad r_0 = \frac{e^2}{mc^2} \tag{2.32}$$

with r_0 the Thomson scattering length, e the charge of the electron, m the mass of the electron and c the speed of light. Magnetic neutron scattering depends also on q but the intensity falls off faster than for X-ray for which we do not consider only the unpaired electrons but the whole electronic cloud around an atom of atomic number Z. The structure factor is therefore also proportional to Z. Finally, the angular resolution of X-ray diffraction is higher than for neutron diffraction.

	Neutrons	X-rays
Dependence on q	Constant with q	Decreases for high q
Sample size	Huge, cm^3	Small, between 0.1 and 1 mm
Availability	Only at nuclear facilities	Lab and synchrotrons
Ability to discriminate neighbouring elements	Yes, depending on b	No
Ability to discriminate isotopes	Yes	No
Ability to "see" light elements	Yes	No
Radiation damage	No, but activation	Yes, but no activation
Possibility to investigate magnetic structures	Yes	Yes, in development
Acquisition time	Long due to low flux and low efficiencies	Fast, possibly ultrafast (sub second resolution)
Resolution	Low $\Delta\theta$ resolution	Moderate $\Delta\theta$ resolution

*Table 2.1: Summary of the main perks and disadvantages of using neutrons or X-ray for diffraction (**borfecchia_gianolio_agostini_bordiga_lamberti**).*

2.4 SXRD

2.4.1 Crystal truncation rods

Thus the diffraction intensity of the finite-sized crystal has diffuse streaks connecting all the Bragg points. The diffuse intensity far from the nodes is of order of magnitude N^4 compared with N^6 at the nodes.

Scattering that is sharp in two directions and diffuse in the third (referred to as a "rod" of scattering) must arise from a crystalline object that is localized in one dimension and extended in the other two.

We are then left with only the sixth component due to the sharply truncated surface. We will call these features "crystal truncation rods. '

We now wish to estimate the strength of the truncation rods in the Bragg geometry. We must first modify Eqs. (1) and (2) by including the x-ray coherence length, m (measured in unit cells), of the experimental configuration. This broadens all the diffraction features to $\frac{1}{m}$ reciprocal units. The Bragg points then have intensity of order $N_1 N_2 N_3 m^3$, while the diffuse intensity is $N_1 N_2 m^2$

A typical penetration depth is $1\mu m$ so $N_3 = 10^3$ unit cells (perpendicular to the face). With $m \approx 100$ unit cells, this gives a relative intensity $\frac{I(Braggpeak)}{I(truncationrod)} = N_3 m \approx 10^5$

More roughness means wider Bragg peaks and deeper valleys between the BP.

It is not clear that different detailed models of roughness could be distinguished at this level of accuracy. One central concept to all descriptions of crystal truncation rods, however, is the continuation of the crystal lattice into the roughened region (not defects, keeping symmetry).

2.4.2   Reciprocal space mapping

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2.4.3   Reflectively

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2.4.4   Computer programs

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2.5 BCDI

2.5.1 Coherent diffraction

Bragg coherent diffractive imaging (BCDI) is a lensless x-ray imaging technique that uses computational algorithms in place of physical lenses to achieve high-resolution imaging. It can be used to visualize the Bragg electron density and atomic displacement fields of crystalline materials in three-dimensional (3D) detail and with nanometer resolution.

We focus only on elastic scattering as that is the main process exploited when studying the structure of materials (the x-ray photon is elastically scattered (energy is conserved) and both the incident and scattered photons have the same wavelength).

By adding up the scattered amplitudes of an arrangement of atoms, we can then get the diffracted amplitude for a crystal. Note that the following derivations only apply if the diffraction pattern is viewed at a distance far away from the diffracting object. This region is known as the far-field or Fraunhofer region.

2.5.2 Phase retrieval

Basic algorithm is Error-Retrieval (ER), quick but can converge towards local minimum. The support corresponds to a shape when the object is included. The density of the object is thus equal to zero outside the support. (Fienup, 1978).

In practice, a slow convergence of the ER algorithm is often observed. The error-metric does not evolve and the algorithm is sort of stuck in a local minimum.

To overcome the problem of stagnation in local minima from ER, (FIenup, 1982) introduced the Hybrid-Input-Output algorithm, that differs in its application of real space constraints. Feedback parameter β, In practice, this adaptation is efficient and significantly enhances the convergence speed. It can be seen as a little perturbation that allows to leave a local minimum.

However, the HIO algorithm still fails sometimes, and this explains why the ER and HIO algorithms are generally used in combination.

Support determination

There are several techniques to estimate the support. In some cases, the shape and dimensions of the object have been already determined by other techniques (such as SEM or AFM for instance), and a support can be built from this knowledge.

Patterson function

When the shape of the object is unknown, a rough estimate of the support can be obtained from the diffraction signal using the autocorrelation function (Marchesini 2003). It is based on the Patterson function which can be defined as the invert Fourier transform of the diffracted intensity. This function can be expressed as the convolution of the complex electron density.

The size of the crystal is overestimated by the Patterson function, since it provides its autocorrelation. In practice, a non uniform density leads to a non-trivial shape of the autocorrelation. The function needs to be threshold to start with a reasonable approximation. In most of the reconstructions in this manuscript, the threshold was set to 2% of the maximum of the Patterson function. As discussed by Vaxelaire (2011), the method is not adapted to highly strained objects.

For large strain, the diffraction pattern has a large extent in the reciprocal space (Beutier et al. 2013a). As a consequence, the Patterson function underestimates the size of the object, preventing any chance of success in the phase-retrieval procedure. In summary, if the shape and size of the object is unknown, it is not recommended to use the autocorrelation function as a first estimate of the support in the case of an highly strained system.

In combination of the ER and HIO algorithms, a third algorithm is routinely used for CDI. It is known as the shrink wrap (SW) algorithm and allows to update the support during the reconstruction. It was first introduced by Marchesini (2003) and has proven to greatly improve the convergence of the procedure.

In practice, the estimate is smoothed by convolution with a Gaussian. After convolution, a thresholding is applied to the smoothed image to a typical value of 10% of the maximum value of the amplitude. Values above the threshold are set to 1 and values below are set to 0. The threshold is generally set to such low values to avoid to suppress too large parts of the support. Nevertheless, the convolution step allows to recover from a support that has been reduced

2.5.3 Accessing strain and displacement

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2.5.4   Computer programs

PyNX

Coherent X-ray imaging techniques developed during the last 20 years thanks to high brilliance in synchrotrons. Wide range of techniques:

- Phase Contrast Imaging

- Coherent Diffraction Imaging, allowing to reconstruct single objects from their diffraction pattern alone, including strain imaging of crystalline nano-objects in the Bragg geometry.

- X-ray Ptychography, used in both near and far field regime, developed for imaging extended objects (larger than the incident beam), both in small angle and Bragg geometry, also usable in the Fourier regime by scanning the transmitted beam.

These techniques all provide high resolution 2D or 3D imaging, down to 5 to 15 nm resolution, depending on the instrumental setup.

Requires a coherent X-ray beam, readily available at synchrotrons facilities. Will benefit from upgrades of synchrotrons rings, which promises 2 orders of magnitude increase in the available coherent X-ray flux thanks to higher brilliance. This will enable faster dynamics and imaging experiments as well as reaching higher resolutions. Higher energy coherent X-ray ($20keV$) will enable data collection for thicker samples and allow to mitigate radiation damage with lower absorption.

PyNX has open-source coherent X-ray imaging modules (Favre-Nicolin et al. 2020). All calculations for coherent imaging modules (`cdi, ptycho, wavefront`), respectively for Coherent Diffraction Imaging, Ptychography and coherent wavefront propagation (mostly used for simulation purposes) are executed on the GPU by using pyCUDA or pyOpenCL libraries. Language and GPU automatically selected based on tests.

Autocorrelation

The CDI technique consists of reconstructing an object from a far-field diffraction pattern alone, a technique which has been expanded to 3D reconstruction by collecting multiple (> 100) projections around a rotation axis, either in the small angle, or in the Bragg geometries - the latter approach yielding information about strain in the reconstructed object (Li et al. 2020).

In order to recover the object from non-redundant diffraction data, it is necessary to recover the lost phases of the measured amplitude (c.f. phase loss problem).

A variety of algorithms are available, all of which rely on alternating between a real-space estimate of the object and diffraction (Fourier) space, where an amplitude constraint can be applied from the measured intensity.

bcdi

Preprocessing

Signal to noise ratio that influence FFT window size for cropping
  Oversampling ratio
  Poisson (Shot) noise

Postprocessing

This section tries to detail the postprocessing of the phase and amplitude following the phase retrieval.

The 3D diffraction pattern is centered on its center of mass, and cropped to fit the FTT requirements. Its center is the center of the FFT array, which becomes the center of the reconstructed object. Phase and displacement can be inverted ??

```python
if invert_phase:
    phase_fieldname = "disp"
else:
    phase_fieldname = "phase"
```

The shape of the object that is post processed is determined by a threshold, here 0.05, with a 10 padding.

```python
nz, ny, nx = obj.shape

zrange, yrange, xrange = pu.find_datarange(
        array=obj, amplitude_threshold=0.05, keep_size=prm.get("keep_size", False)
)

numz = zrange * 2
numy = yrange * 2
numx = xrange * 2
```

Firstly, the phase outside a certain threshold (default value 0.05) is set to zero. A different threshold, lower than the isosurface threshold, is used on the amplitude to compute the support so that surface voxels aren't accidentally excluded from the correction. The phase is then unwrapped, thanks to the skimage method (see figure 2.4). It is then wrapped properly between the maximum and minimum of the phase.

```python
    phase, extent_phase = pu.unwrap(
        avg_obj,
        support_threshold=threshold_unwrap_refraction,
        debugging=debug,
        reciprocal_space=False,
        is_orthogonal=is_orthogonal,
    )
```

```
extent_phase = phase.max() - phase.min()

phase = (obj - start_angle + range_angle) \% range_angle + start_angle
```

Secondly, the phase ramp is removed before phase filtering. To do so, the gradient of the phase is computed in three directions. It returns a set of ndarrays corresponding to the derivatives of the phase with respect to each dimension. Each derivative has the same shape as f. The points for which the gradient is higher than the threshold (≈ 1) are ignored. The mean of the other points is returned as the ramp along that direction.

```
# Detail below
amp, phase, rampz, rampy, rampx = pu.remove_ramp(
    amp=abs(avg_obj),
    phase=phase,
    initial_shape=original_size,
    method="gradient",
    amplitude_threshold=isosurface_strain,
    threshold_gradient=threshold_gradient,
)

# Define the support from the amplitude
support = np.where(amp > amplitude_threshold * abs(amp).max(),
                   1, 0)

# Compute gradient
gradz, grady, gradx = np.gradient(phase, 1)

# Remove points lower than threshold
threshold_gradient = 1.0
supportz = np.where(abs(gradz) < threshold_gradient, 1, 0)

# Make sure there  are no points outside the support
supportz = supportz * support

# Ramp is the mean value
rampz = gradz[supportz == 1].mean()

# Create mesh grid
myz, myy, myx = np.meshgrid(
    np.arange(0, nbz, 1),
    np.arange(0, nby, 1),
    np.arange(0, nbx, 1),
    indexing="ij",
)

# Remove phase gradient
phase = phase - myz * myrampz - myy * myrampy - myx * myrampx
```

Example of gradient computation in python, using the nearest neighbours, see example applied to object phase in figure 2.5.

```python
f = np.array([1, 2, 4, 7, 11, 16], dtype=float)
np.gradient(f) = array([1. , 1.5, 2.5, 3.5, 4.5, 5. ])
```

Thirdly, the phase offset is removed. Careful here, the threshold used is `isosurface_strain`, the offset is either the value at the COM of the amplitude, or the mean value of the phase.

```python
# Phase offset removal, detail below
support = np.where(amp > isosurface_strain * amp.max(), 1, 0)
phase = pu.remove_offset(
    array=phase,
    support=support,
    offset_method=offset_method, # usually mean, or COM
    phase_offset=phase_offset, # usually 0
    offset_origin=offset_origin, # usually not pre-determined
    title="Phase",
    debugging=debug,
)


# COM
if offset_method == "com":
    zcom, ycom, xcom = center_of_mass(support)
    array = array - array[zcom, ycom, xcom] + phase_offset
# mean
elif offset_method == "mean":
    array = array - array[support == 1].mean() + phase_offset

 # wrap again
 phase = (phase - start_angle + range_angle) \% range_angle + start_angle
```

Once that the phase is unwrapped, and that the phase ramp and offset are removed, the phase is averaged over a window and apodized to reduce noise in strain plots. The phase is averaged using a kernel of half-width `half_width_avg_phase`. For the apodization, the diffraction pattern is recomputed with `numpy.fft.fftn()`. This function computes the N-dimensional discrete Fourier Transform over any number of axes in an M-dimensional array by means of the Fast Fourier Transform (FFT). The zero-frequency component is shifted to the center of the spectrum using `numpy.fft.fftshift()`. An apodization window

```python
# compute support
support = np.where(amp < isosurface_strain, 1, 0)

# Average phase with nearest neighbours
phase = pu.mean_filter(
    array=phase, support=support,
    half_width=half_width_avg_phase, # usually 1
```

```python
# Apodization
amp, phase = pu.apodize(
    amp=amp,
    phase=phase,
    initial_shape=original_size,
    window_type=prm.get("apodization_window", "blackman"),
    sigma=prm.get("apodization_sigma", [0.30, 0.30, 0.30]),
    mu=prm.get("apodization_mu", [0.0, 0.0, 0.0]),
    alpha=prm.get("apodization_alpha", [1.0, 1.0, 1.0]),
    is_orthogonal=is_orthogonal,
)


# Compute electronic density
avg_obj = amp * np.exp(1j * phase)
```

The phase is now corrected. The following steps are the centering of the object, as well as the interpolation of the arrays in the orthogonal reference frame where $\vec{q_{com}}$ is aligned onto the reference axis.

```python
# Centering of array
if centering_method == "max":
    avg_obj = pu.center_max(avg_obj)
    # shift based on max value,
    # required if it spans across the edge of the array before COM
elif centering_method == "com":
    avg_obj = pu.center_com(avg_obj)
elif centering_method == "max_com":
    avg_obj = pu.center_max(avg_obj)
    avg_obj = pu.center_com(avg_obj)


# Calculate q of the Bragg peak in the laboratory frame
q_lab = (
    setup.q_laboratory
)  # (1/A), in the laboratory frame z downstream, y vertical, x outboard
qnorm = np.linalg.norm(q_lab)
q_lab = q_lab / qnorm


# Find Bragg peak
bragg_peak = bu.find_bragg(
    data=data,
    peak_method="maxcom",
    roi=detector.roi,
    binning=None,
)


# Compute atomic planar distance
planar_dist = 2 * np.pi / qnorm   # qnorm should be in angstroms
planar_dist = planar_dist / 10   # switch to nm
```

```python
# Find inplane and outofplane angles from setup
# and Bragg peak
setup.correct_detector_angles(bragg_peak_position=bragg_peak)
prm["outofplane_angle"] = setup.outofplane_angle
prm["inplane_angle"] = setup.inplane_angle

# Orthogonalise object
obj_ortho, voxel_size, transfer_matrix = setup.ortho_directspace(
    arrays=avg_obj,
    q_com=np.array([q_lab[2], q_lab[1], q_lab[0]]),
    initial_shape=original_size,
    voxel_size=fix_voxel,
    reference_axis=axis_to_array_xyz[ref_axis_q],
    fill_value=0,
    debugging=True,
    title="amplitude",
)
```

The orthogonalised object is re-centered on its center of mass, the phase unwrapping, the phase ramp removal and the phase offset removal are repeated. To resume, `threshold_unwrap_refraction` is only used for the phase unwrapping, whereas `isosurface_strain` is used for both the phase ramp removal and the phase offset removal. In order to facilitate the analysis of data-sets collected on the same object, the values of these two parameters should be the same as much as possible. In any case, they should be kept in mind when analysing the data. Do not forget the -1 sign in the phase if the phasing algorithm is python or matlab-based. Finally, the strain is computed from the phase.

```python
# Add offsets if defects
if method == "defect":
    offsets = 2 * np.pi / 10 * np.linspace(-10, 10, num=11)
else:
    offsets = (0,)


for offset in offsets:
    # offset the phase
    if method == "defect":
        temp_phase = np.copy(phase)
        temp_phase = temp_phase + offset
        # wrap again the offseted phase
        temp_phase = util.wrap(
            obj=temp_phase,
            start_angle=-extent_phase / 2,
            range_angle=extent_phase
        )
    else:  # no need to copy the phase, offset = 0
        temp_phase = phase

    # calculate the strain for this offset,
```

```python
    # disp = planar_distance / (2 * np.pi) * temp_phase,
    if reference_axis == "x":
        _, _, temp_strain = np.gradient(
            planar_distance / (2 * np.pi) * temp_phase,
            voxel_size[2],
        )  # q is along x after rotating the crystal
    elif reference_axis == "y":
        _, temp_strain, _ = np.gradient(
            planar_distance / (2 * np.pi) * temp_phase,
            voxel_size[1],
        )  # q is along y after rotating the crystal
    else:  # "z"
        temp_strain, _, _ = np.gradient(
            planar_distance / (2 * np.pi) * temp_phase,
            voxel_size[0],
        )  # q is along z after rotating the crystal

    # update the strain values
    strain = np.where(abs(strain) < abs(temp_strain), strain, temp_strain)
```

Gwaihir

2.6   XPS

2.6.1   Spectroscopy

2.6.2   Peak shape

Read thesis on XPS

2.7   SixS beamline

Presentation of the MED environment ...

2.7.1   Mass flow controller

2.7.2   Residual Gas Analyser

2.7.3   Diffractometer

Horizontal or vertical setup.

Reaction scheme and rate coefficients in form, $k = A \exp(-E/RT)\exp(\varepsilon\theta_i/RT)$

Step	Reaction	A^a	E (kJ mol^{-1})	ε (kJ mol^{-1})	Reference
R1	$NH_3 + \{\} \rightarrow \{NH_3\}$	**2.0×10^8**	**0.0**	–	**[43]**
		–	112.0	–	[43]
		–	108.0	–	[44]
R2	$\{NH_3\} \rightarrow NH_3 + \{\}$	–	**96.0**	–	**[43,45]**
		1.0×10^9	75.2	–	[45]
		–	69.8	–	[46]
		1.3×10^6	0.0	–	[47]
R3	$O_2 + 2() \rightarrow 2(O)$	**2.0×10^6**	**0.0**	–	**[38]**
		3.3×10^6	0.0	–	[48]
R4	$2(O) \rightarrow O_2 + 2()$	–	**213.2**	**−60.0**	**[49]**
		–	213.2	−133.8	[50]
R5	$\{NH_3\} + (O) \rightarrow \{NH_2\} + (OH)$	**1.7×10^{15}**	**157.0**	–	**[36]**
R6	$\{NH_2\} + (O) \rightarrow \{NH\} + (OH)$	–	**0.0**	–	**[44]**
R7	$\{NH\} + (O) \rightarrow \{N\} + (OH)$	–	**0.0**	–	**[44]**
		–	58.5	–	[33]
R8	$\{N\} + (O) \rightarrow \{NO\} + ()$	–	**121.2**	–	**[33]**
R9	$\{NH\} + (O) \rightarrow \{NHO\} + ()$	–	**73.0**	–	**[51]**
R10	$\{NHO\} + (O) \rightarrow \{NO\} + (H_2O)$	–	**0.0**	–	**[51]**
		2.0×10^{15}	118.0	–	[52]
R11	$\{NO\} + () \rightarrow \{N\} + (O)$	**1.6×10^{13}**	**116.8**	–	**[21]**
			115.0	10.5	[20]
		3.0×10^5	79.1	–	[21]
R12	$\{N\} + \{N\} \rightarrow N_2 + 2\{\}$	**1.0×10^{11}**	**79.1**	–	**This study**
		1.4×10^9	92.9	–	[21]
R13	$\{N\} + \{NO\} \rightarrow N_2O + 2\{\}$	**1.0×10^{11}**	**92.9**	–	**This study**
R14	$N_2O + () \rightarrow N_2 + (O)$	**2.5×10^8**	**72.2**	–	**[21]**
		1.7×10^{14}	154.7	–	[19]
		–	**151.0**	–	**[43]**
R15	$\{NO\} \rightarrow NO + \{\}$	1.0×10^{16}	140.0	–	[53]
		–	139.2	−19.2	[20]
		4.3×10^8	54.3	–	[21]
R16	$\{NH\} + (OH) \rightarrow \{N\} + (H_2O)$	–	**46.0**	–	**[44]**
		1.0×10^{11}	79.0	−79.0	[50]
R17	$(OH) + (OH) \rightarrow (O) + (H_2O)$	–	**75.3**	–	**[54]**
		–	48.2	–	[49]
		–	**41.8**	–	**[54]**
R18	$(H_2O) + (O) \rightarrow (OH) + (OH)$	1.0×10^{11}	52.7	89.9	[50]
		–	129.6	–	[55]
R19	$(H_2O) \rightarrow H_2O + ()$	–	**40.3**	–	**[56]**
		–	41.8	–	[50]

Values in bold were used for sensitivity analysis (see Fig. 2).

[a] Pre-exponential factors of steps R1, R3, and R14 are in (s^{-1} atm^{-1}), the rest of pre-exponential factors are in (s^{-1}). Value of 1.0×10^{13} s^{-1} for the pre-exponential factors of surface steps is assumed if not otherwise mentioned.
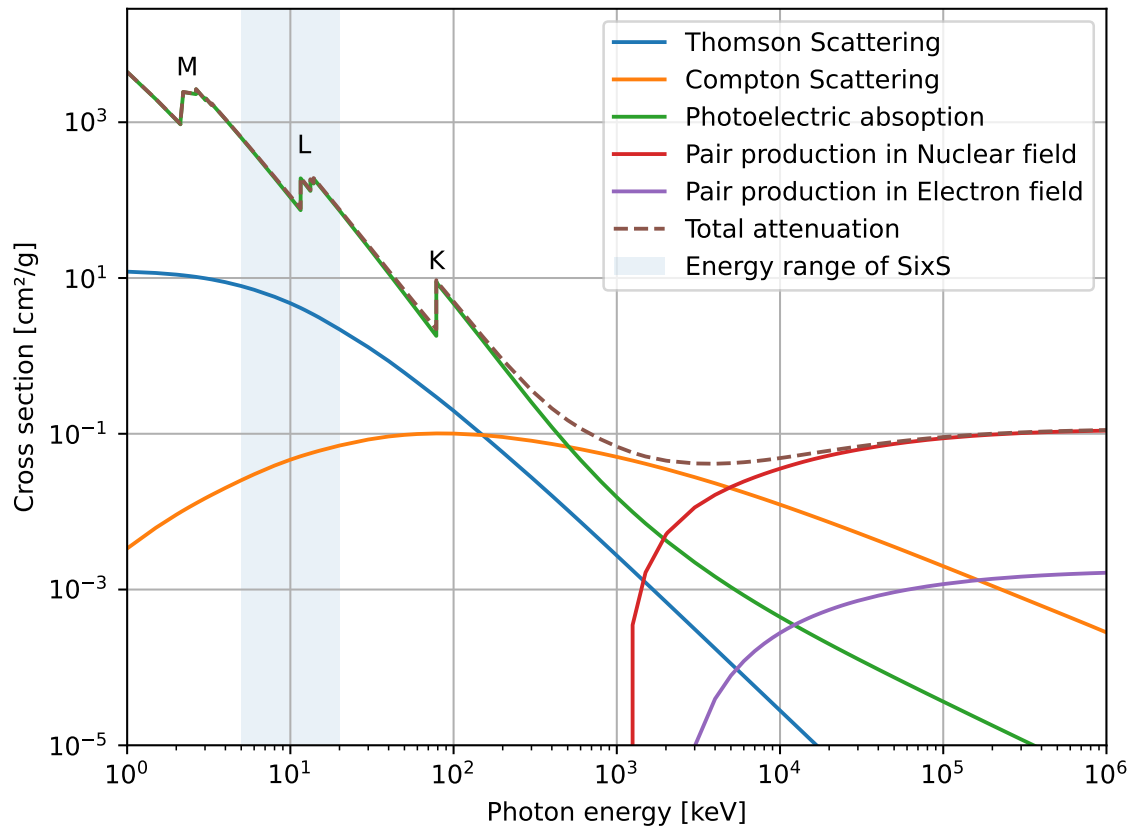
Figure 2.1: Rebrov, De Croon and Schouten 2002

Figure 2.2: Cross-sections for Platinum (Z=78) for various processes that occur when photons interact with matter. The data was taken from the NIST (national Institute of Standards and Technology) (Berger et al. 2010) website.
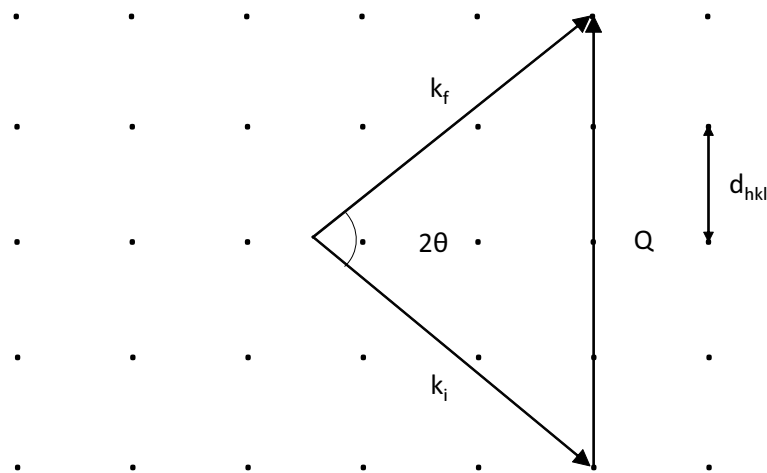

Figure 2.3: Geometry of the momentum transfer $\vec{Q}$ in reciprocal space, 2θ is the scattering angle.
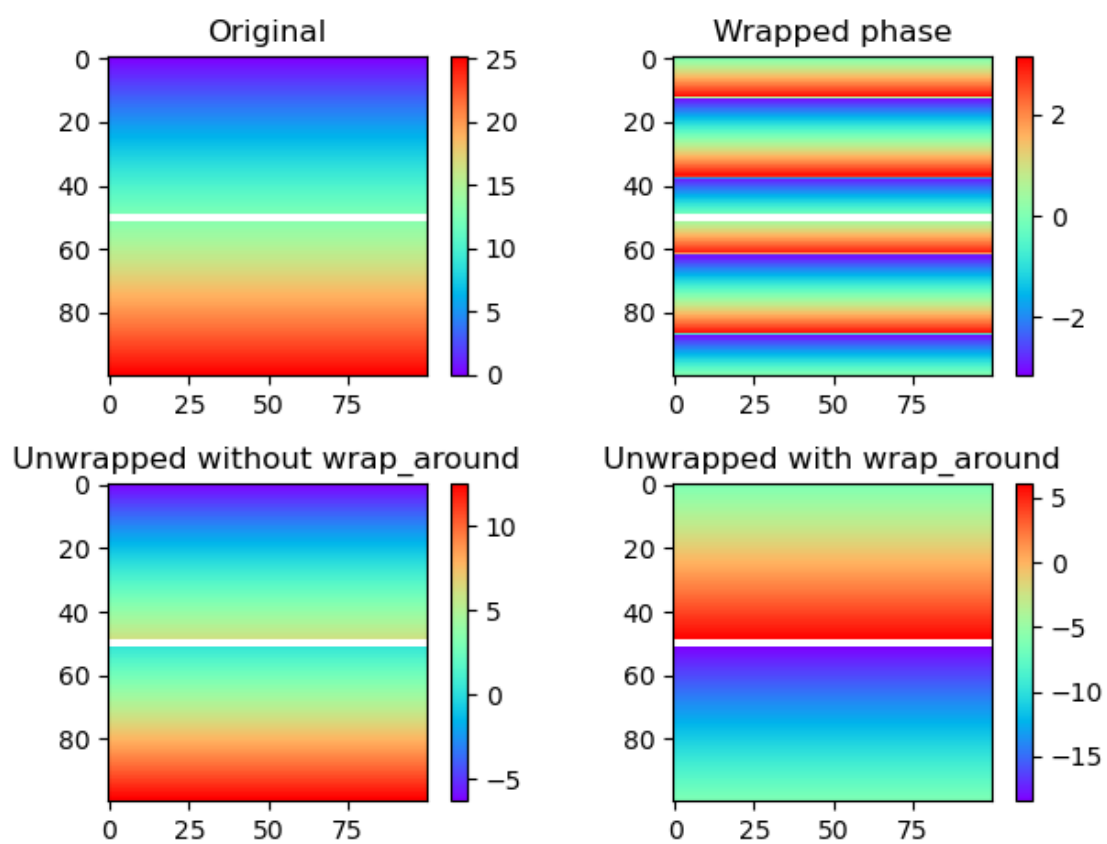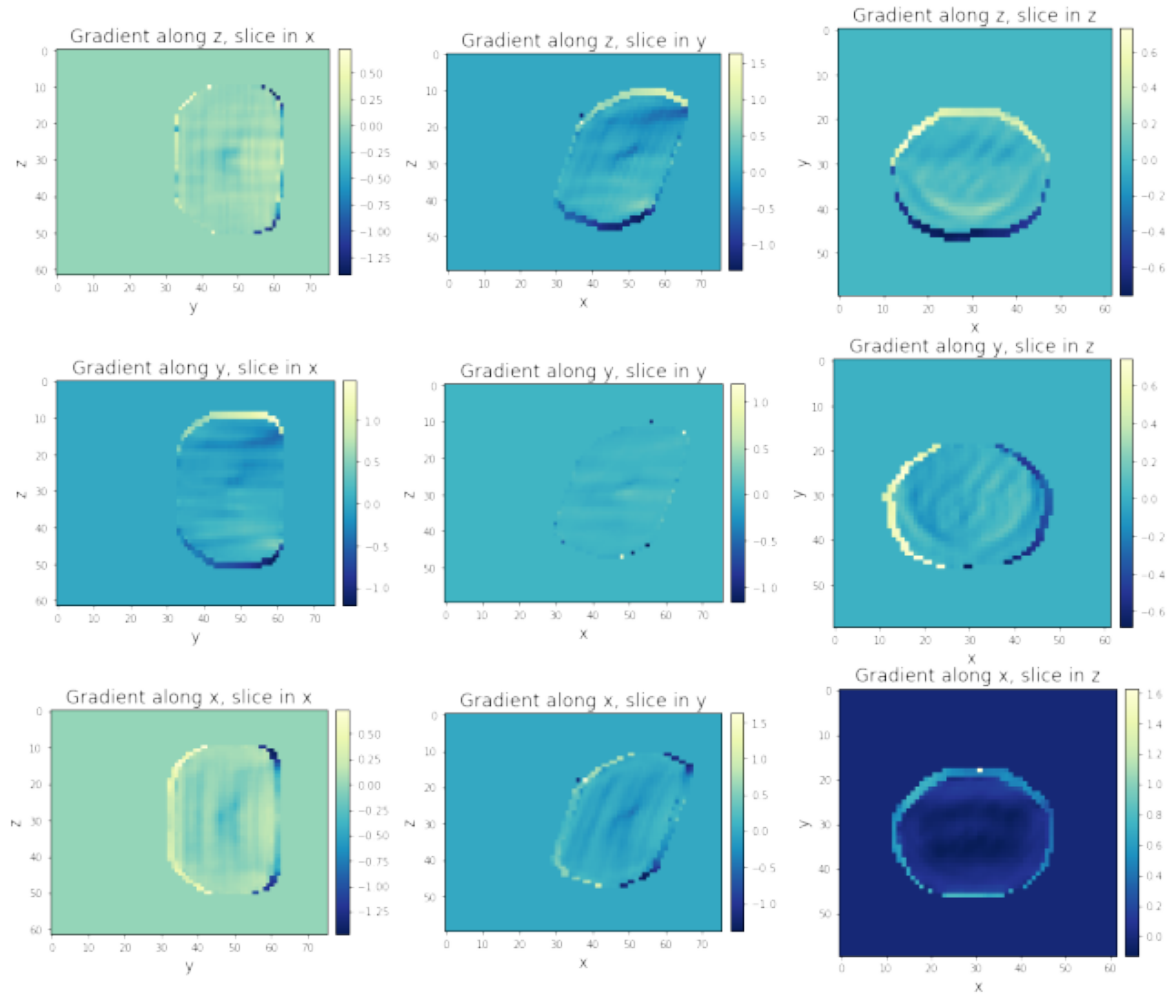
Figure 2.4: Phase unwrapping with skimage package.

Figure 2.5: Phase gradients

Chapter 3

Results

3.1   Operando and in-situ experiments at SixS

3.2   BCDI on isolated Pt nanoparticles

Here, we will evaluate the metal-support interaction during reaction by monitoring the activity and structure evolution of the Pt NPs dewetted on three different support materials: sapphire, MgO and TiO2 [6]. This will allow examining the effect of the support on the metal catalyst. A careful in situ analysis of the properties of the nanoparticles (size, shape, strain, refaceting, support interaction, etc) in 3D is of essential importance to gain more understanding of the behaviour of these nanocrystals during a catalytic reaction.

We want to evaluate the strain evolution of Pt particles and probe the impact of the support during CO oxidation.

3.2.1   Preliminary test on gas reactor

We performed several test on the small gas reactor to see how high we could go in temperature, which reactions happen at which temperature, etc ... The data is in *PhDScripts/test_reactor_cell*

On 20/01, we confirmed that batch were usefull ? (long batch stochio) and that products of both reactions (for the production of CO2, and then of nitrogen oxides respectively from CO and NH3 can be detected !)

Atmospheric pressure : $\approx$ 1 bar = 1 013.25 mbar = 1 013.25 hPa

uhv = 10 -9 mbar, 10-7 pascal

near ambient pressure ($>$ 1 mbar)

DATA ACQUISITION

Rotating the sample results in rotating the reciprocal space Whenever this happens, a diffracted beam is originated in the center of the Ewald sphere and passes through the reciprocal point that lies on the Ewald spherical surface... In these circumstances the so-called Bragg law is fulfilled. The set of all diffracted beams constitute the so-called diffraction pattern, which is subject to detection and evaluation. The reader should be aware that a complete diffraction pattern can contain a highly variable number of diffraction beams, from hundreds (simple inorganic compounds) to hundreds of thousands (proteins or viruses).

Ewald sphere is centered on the sample, reciprocal lattice on where $\vec{k_i}$ (from the sample) meets the sphere

Larger q -> higher hkl indexes

3.2.2   Measurements

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3.2.3   Reaction

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3.3 SXRD on Pt 100 and Pt 111

3.3.1 Surface reconstruction

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3.3.2   CTR and roughness

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3.4   Ambient pressure XPS

3.4.1   Multi component analysis at ambient pressure

3.5   Empirical Analysis

This chapter covers three areas: analysis of the data; discussion of the results of the analysis; and how your findings relate to the literature. The analysis of the data can be discussed here but the details of any analysis, such as statistical calculations, should be shown in the appendices. You should present any discussion clearly and logically and it should be relevant to your research questions/hypotheses or aims and objectives. Insert any tables or figures that you decide are important in a relevant part of the text not in the appendices, and discuss them fully. Make sure that you relate the findings of your primary research to your literature review. You can do this by comparison: discussing similarities and particularly differences. If you think your findings have confirmed some literature findings, say so and say why. If you think your findings are at variance with the literature, say so and say why.

3.5.1   Results

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When placing tables () within the body of the text, the citation is placed above the table.

3.5.2   Discussion

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When placing figures (illustrations, pictures, graphs, diagrams, charts, maps etc.) within the body of the text, the citation is placed below the figure (

Chapter 4

Transitioning to big data at Synchrotrons

4.1 Jupyter Notebook

interface

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4.2   Standards for data reproducibility

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4.3   Parallelism

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4.4 Machine Learning

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Chapter 5

Conclusion

State the main conclusions of your study. State explicitly how and to what extent you have fulfilled your aims and objectives/answered your research questions/proved your hypotheses (whichever is appropriate). Your conclusions should follow logically from your findings and not contain any new material.

5.1   Research Aims

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5.2   Research Objectives

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5.3 Practical Implications

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5.4   Future Research

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5.5 Chapter Summary

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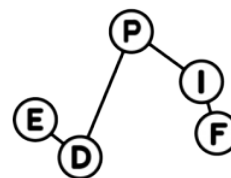
Appendix A

(Appendix A)

Gwaihir
Paper Ammonia
Paper MIR on strain and nano-twin ?
Paper Corentin on CO adsorption ?

Titre: Propriétés catalytiques à l'échelle nanométrique sondées par diffraction des rayons X de surface et imagerie de diffraction cohérente

Mots clés: Diffraction, Catalyse, Surface, Structure, Déformation

Résumé: Le principal objectif est d'imager des nanostructures pour sonder les conditions in situ et operando ; mesurer la structure à l'échelle nanométrique et révéler également les effets de masse, de surface et d'interface ainsi que les défauts. Viser à terme à comprendre les phénomènes structurels importants pour les nanocatalyseurs et les relier à leur activité, sélectivité, réutilisabilité et durabilité. En complément des études cohérentes aux rayons X sur des particules individuelles, des techniques étudiants la moyenne des ensembles comme la diffraction des rayons X à incidence rasante seront employées pour voir si l'évolution des formes d'ensemble sont similaires à celles des nanoparticules uniques et sondent s'il y a une déconnexion entre les particules uniques et l'activité catalytique sur des billions de particules. La catalyse des nanomatériaux est apparue comme un moyen efficace d'exposer une surface plus élevée et d'accélérer les processus catalytiques en maximisant le rapport surface-volume. Le développement d'une catalyse hétérogène avec une sélectivité ciblant les 100% est un défi constant ainsi que la compréhension de la durabilité et du vieillissement du catalyseur lui-même. Dans un procédé réel (réacteur d'usine de catalyseur, échappement de voiture, pile à combustible), l'évolution de la forme et de la déformation des nanoparticules catalytiques dans des conditions de réaction contribue au vieillissement du catalyseur et a un impact sur la durée de vie du dispositif. Cependant, le processus catalytique et les changements structurels associés restent encore mal compris. Comprendre comment la structure du catalyseur est affectée par la couche adsorbée dans des conditions de réaction est donc de la plus haute importance pour formuler des relations de performance de structure de catalyseur qui guident la conception de meilleurs catalyseurs.

Title: Catalytic properties at the nanoscale probed by surface X-ray diffraction and coherent diffraction imaging

Keywords: Diffraction, Catalysis, Surface, Structure, Strain

Abstract: The main objective is to image nanostructures to probe in situ and operando conditions; measure the structure at nanoscale and to reveal bulk, surface and interface effects, as well as defects. Ultimately aiming to understand the structural phenomena important for the working nanocatalysts and link them to their activity, selectivity, reusability and sustainability. In complement to coherent x-ray studies on individual particles, ensemble-averaging techniques like grazing incidence x-ray diffraction will be employed to see if the evolution of ensemble shapes is similar to the one of single nanoparticles and probe if there is a disconnect between single particles and the catalytic activity over trillions of particles. Catalysis of nanomaterials has emerged as an efficient way to expose higher surface area and accelerate catalytic processes by maximizing the surface-volume ratio. The development of heterogeneous catalysis with selectivity targeting the 100% is a constant challenge as well as understanding the durability and ageing of the catalyst itself. In a real process (catalyst plant reactor, car exhaust, fuel cell) the shape and strain evolution of catalytic nanoparticles under reaction conditions contributes to the ageing of the catalyst and impact the lifetime of the device. However, the catalytic process and the associated structural changes remain poorly understood. Understanding how catalyst structure is affected by the adsorbed layer under reaction conditions is therefore of utmost importance to formulate catalyst structure performance relations that guide the design of better catalysts.

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