



DISSERTATION

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submitted by

Someone

performed at

Institution

supervised by

Supervisor(s)

Address

Place, Month Year

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(Institution)

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(Institution)

date

student's signature

Short description

Short description

Kurzbeschreibung

Description in another language

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Nomenclature

$\langle \quad \rangle$		symbol to indicate averaging
$*$		convolution operator
$f(Q)$		atomic form factor of atom i ; it is dimensionless
$F(Q)$		The crystallographic structure factor. It is a complex quantity and its modulus is called the structure or scattering amplitude and the expression $ F(\mathbf{Q}) ^2$ gives the intensity $I(\mathbf{Q})$
$F(Q)$		The reduced and normalised structure function which is transformed into $G(R)$ by sine-FT. Unfortunately it has the same notation as the crystallographic structure factor, $F(\mathbf{Q})$
FT		Abbreviation for: Fourier transformation
\mathcal{F}		Symbol for FT
\mathcal{F}^{-1}		Symbol for inverse FT
\mathcal{F}_S		Symbol for sine FT
$G(r)$	$[\text{\AA}^{-2}]$	PDF, pair distribution function; reduced radial distribution function. $G(r)$ can be seen as a derivative of $R(r)$
$I(Q)$		intensity of the scattered radiation at \mathbf{Q} or Q
\mathbf{k}_i	$[\text{\AA}^{-1}]$	the wave vector which describes the direction and properties of the incident photons
\mathbf{k}_o	$[\text{\AA}^{-1}]$	the wave vector which describes the direction and properties of the scattered photons

Nomenclature

λ	[Å]	wavelength of the applied radiation
$P(\mathbf{r})$ or $P(r)$	[Å ⁻¹]	density-density or auto-correlation function; it is also called (3D)Patterson function; it contains all interatomic vectors \mathbf{r} or r but they are shifted to the origin of the Patterson map
$p(\mathbf{x})$	[Å ⁻¹]	total distribution of atoms throughout the sample
Q_{broad}	[r^{-1}]	parameter asserted to account for the influences of the limited experimental resolution on the PDF
Q_{damp}	[r^{-1}]	parameter asserted to account for the influences of the limited experimental resolution on the PDF
Q_{max}	[Å ⁻¹]	upper limit of the FT of the diffractogram to $G(r)$
Q_{min}	[Å ⁻¹]	lower limit of the FT of the diffractogram to $G(r)$
\mathbf{Q}	[Å ⁻¹]	Scattering vector; defined by the relation $\mathbf{Q} = 2\pi(\mathbf{K}_o - \mathbf{K}_i)$
Q or $ \mathbf{Q} $	[Å ⁻¹]	Modulus of the scattering vector \mathbf{Q}
ρ_0	[distances.Å ⁻³]	averaged auto-correlation; in literature this quantity is also denoted by the term <i>atom number density</i> which defines the mean number of atoms per unit volume at large values of R
$\rho(r)$	[distances.Å ⁻³]	density-density correlation function $C(R)$ from which the self reference of each atom is subtracted
\mathbf{r}_{ij} or r_{ij}	[Å]	distance between two atoms $\mathbf{x}_j - \mathbf{x}_i$; it is also the Patterson vector; its magnitude is interpreted as a radius r

$S(Q)$	[au]	reduced total scattering structure function (in some literature given in terms of the classical scattering of one electron)
$S(r)$	[au]	Patterson self-correlation
θ	[rad]	scattering angle; the theoretically possible range is from 0 to 180; due to the experimental setup this can never be reached
$T_i(Q)$		Debye-Waller factor of atom i (see section ??)
$W(r)$		rectangle function the PDF is multiplied with in order to account for the measurement range (section ??)
\mathbf{x}_i	[Å]	position vector of atom i

Introduction

“But finally, of course, small devices are more delicate! (And if they are not small, why bother?) Why do we want smaller devices? So that we can make many more of them, within a given system. That means it won’t be enough to have the smaller devices as reliable as the larger ones. They have to be more reliable. [...]

Pessimism is, unfortunately, unpopular. But excessive optimism can only cause a premature and excessive counter-reaction when the optimistic promises are not speedily fulfilled.”

— Rolf Landauer (1989), ‘Nanostructure physics: fashion or depth’

The aim of this template is to provide something useful.

Place, Month Year
Philipp Hans

Chapter 1

Coarse intro

1.1 Some important facts

$$G_{calc}(r) = \frac{1}{r} \sum_i \sum_{j \neq i} \left[\frac{f_i(Q)f_j(Q)}{\langle f(Q) \rangle^2} \delta(r - r_{ij}) \right] - 4\pi r \rho_0 \quad (1.1)$$

$$G_{exp}(r) = 4\pi r [\rho(r) - \rho_0] = \frac{2}{\pi} \int_{Q_{min}}^{Q_{max}} Q(S(Q) - 1) \sin(Qr) dQ \quad (1.2)$$

Table 1.1: Composition of the samples according to XRF measurements

sample	Transition	Si as SiO ₂ [wt%]	Ti as TiO ₂ [wt%]	Si [mol%]	Ti [mol%]
SF154 XRF	Ka	92.86	7.14	94.5	5.5
SF155 XRF	Ka	70.36	29.64	75.9	24.1

Chapter 2

Technical details

text

Chapter 3

Experimental Aspects

test

Chapter 4

Progress

test

Chapter 5

Future Developments

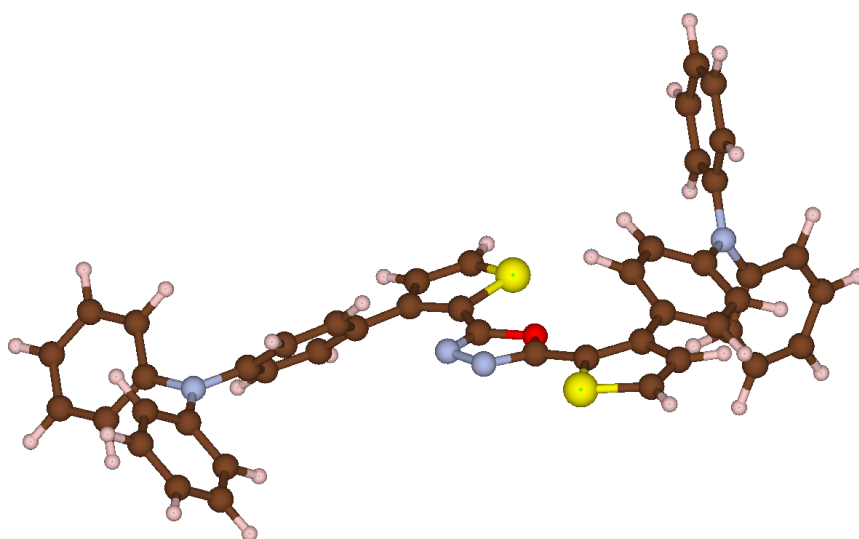


Figure 5.1: Overall caption

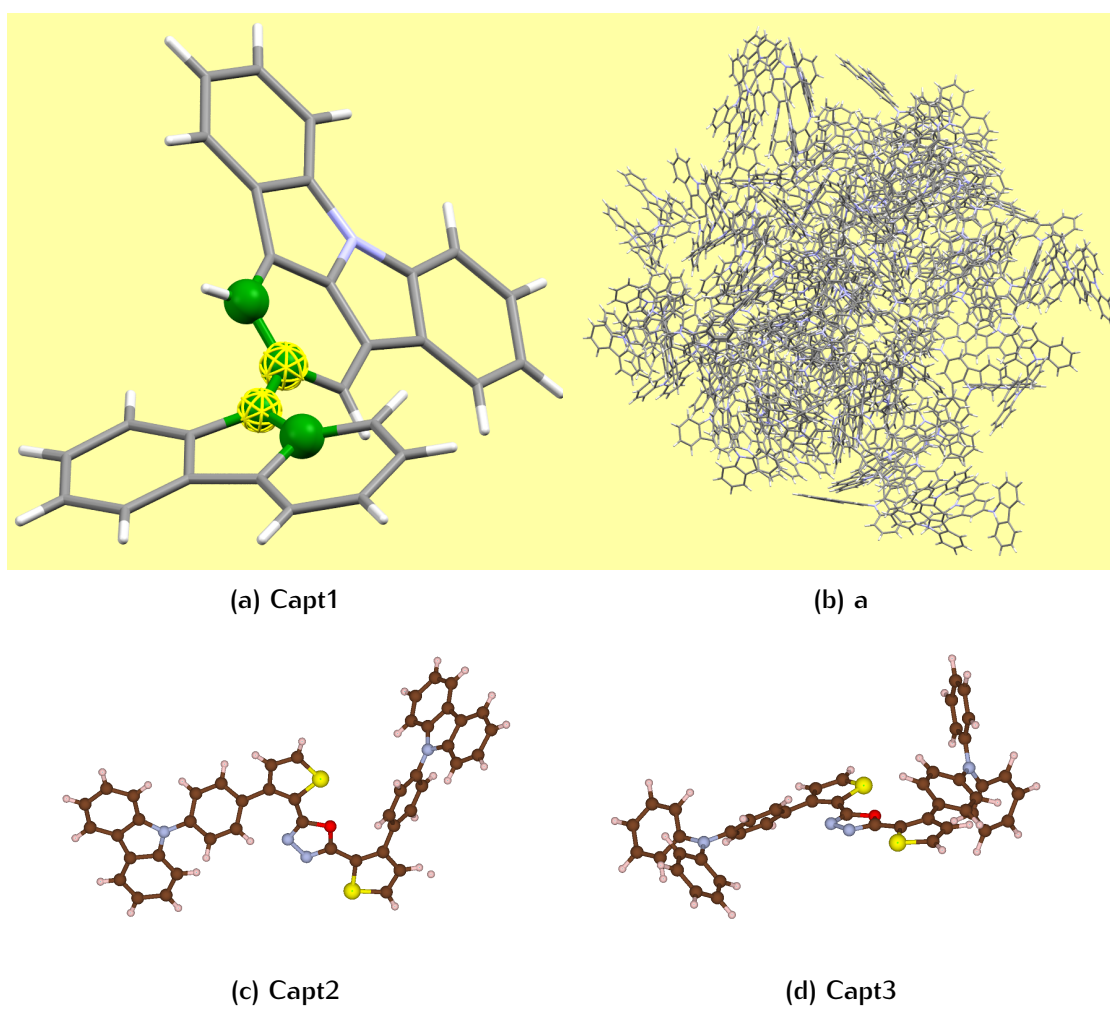


Figure 5.2: Overall caption

Final conclusions and outlook

“Relative to the potential structural information procurable, it is fair to say that the quantity and quality of the results are a direct reflection of the pains that have been exercised in measuring and processing the experimental intensities.”

— Klug and Alexander (1974, p. 853), *X-Ray Diffraction Procedures for Crystalline and Amorphous Solids*.

In contrast to giving striking new ‘insights’ into the atomic arrangement of nano-materials, this dissertation is critically assessing the PDF methodology. This means: investigating effects caused by measurement artefacts, data "correction" and applications of PDF analysis where it is not valid according to the theory.

Some other thoughts

Write what you think. But be diplomatic.

APPENDIX

A.1 Script to merge files

```
1 #!/usr/bin/env python3
2
3 import numpy as np
4 import matplotlib.pyplot as plt
5 from scipy.interpolate import interp1d
6 import bisect
7
8 def index_le(a, x):
9     'Find rightmost value less than or equal to x'
10    i = bisect.bisect_right(a, x)
11    if i:
12        return i-1
13    raise ValueError
14
15 data_directory= './'
16 data_working1 = '1'
17 data_working2 = '2'
18 data_working3 = '3'
19 headerSkip = 0
20
21 # load data
22 d01 = np.genfromtxt(data_directory+ data_working1+'.xy',
    skip_header=headerSkip, dtype=float ,usecols=(0,1),
    comments='#')
```

APPENDIX

```
23 d02 = np.genfromtxt(data_directory+ data_working2+'.xy',
    skip_header=headerSkip, dtype=float ,usecols=(0,1),
    comments='#')
24 d03 = np.genfromtxt(data_directory+ data_working3+'.xy',
    skip_header=headerSkip, dtype=float ,usecols=(0,1),
    comments='#')
25
26 # split data
27 X1 , I1 = d01.T
28 X2 , I2 = d02.T
29 X3 , I3 = d03.T
30
31 # remove overlaps with worse signal-to-noise ration
32 last = index_le(X1, X2[0])
33 X1 = X1[:last]
34 I1 = I1[:last]
35 last = index_le(X2, X3[0])
36 X2 = X2[:last]
37 I2 = I2[:last]
38 last = index_le(X3, 150)
39 X3 = X3[:last]
40 I3 = I3[:last]
41
42 # add and convert section
43 Xtot = list(X1) + list(X2) + list(X3)
44 Itot = np.array( list(I1/15) + list(I2/35) + list(I3/70) )/125.25
45
46 # interpolate on equidistant grid --- could be omitted
47 helperFunction = interp1d(Xtot, Itot)
48 Xtot = np.linspace(Xtot[0], Xtot[-1], num=len(Xtot), endpoint=True,
    retstep=False)
49 Itot = helperFunction(Xtot)
50
```

```
51 # save merged data set with specifications
52 outp = np.array([Xtot,Itot]).T
53 name = 'merged_wOutInt'
54 np.savetxt(name+'.xy', outp, fmt='%.3f')
```

Bibliography

- Klug, H. and Alexander, L. E. (1974). *X-Ray Diffraction Procedures for Crystalline and Amorphous Solids*. Wiley-Interscience New York, NY, USA.
- Landauer, R. (1989). 'Nanostructure physics: fashion or depth'. In: *Nanostructure Physics and Fabrication*, pp. 17–30.

