# Splitting Algorithms

# and

# Generalized Normalizing Flows

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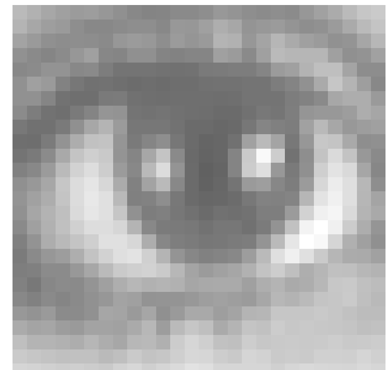
# Lectures

0. Motivation
1. Splitting Algorithms
2. Optimal Transport and SMART
3. Normalizing Flows
4. Generalized Normalizing Flows

Porter des hiboux à Athènes

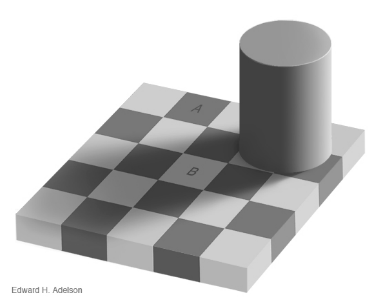
Eulen nach Athen tragen

**Gray-value images**: $x : \Omega \to \mathcal{M}$
e.g. $\Omega = [1:m] \times [1:n]$ and $\mathcal{M} = \{\underbrace{0}_{black}, \dots, \underbrace{255}_{white}\}$

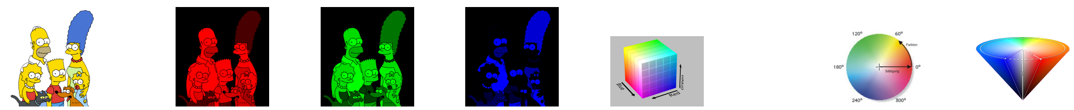



| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| 98 | 93 | 90 | 91 | 94 | 94 | 97 | 104 | 101 | 97 |
| 123 | 114 | 108 | 105 | 97 | 93 | 93 | 95 | 97 | 97 |
| 111 | 105 | 98 | 96 | 97 | 96 | 94 | 103 | 106 | 104 |
| 99 | 94 | 91 | 95 | 103 | 109 | 92 | 91 | 98 | 98 |
| 93 | 95 | 100 | 100 | 93 | 94 | 85 | 79 | 79 | 79 |
| 99 | 109 | 105 | 89 | 81 | 77 | 78 | 76 | 74 | 75 |
| 99 | 99 | 91 | 78 | 76 | 76 | 83 | 84 | 77 | 76 |
| 95 | 85 | 78 | 76 | 83 | 90 | 102 | 100 | 79 | 78 |
| 82 | 77 | 77 | 83 | 98 | 114 | 123 | 106 | 81 | 81 |
| 79 | 83 | 95 | 115 | 134 | 141 | 137 | 101 | 91 | 114 |

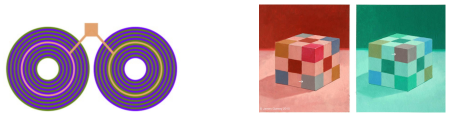
Visual system: Checkerboard shadow illusion of Adelson



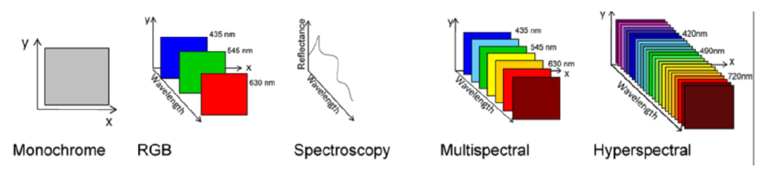
**Color images**: Many color systems, e.g. RGB system from computer screen, HSV ...



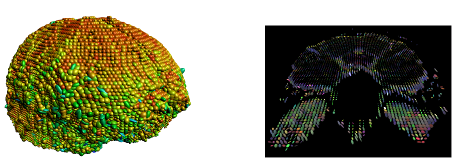
Visual system: Illustration of the lateral inhibition (Courtesy: M. Bertalmio)



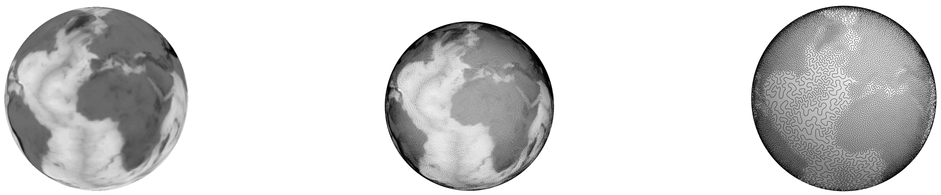
**Hyperspectral images**:




**Manifold-values images**: DT-MRI, IN-SAR



**Images on $\mathbb{R}^3$ and manifolds**:



# Motivation: Inverse Problems in Imaging

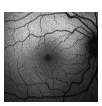
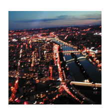
Inverse Problem: Find $x$ given $y$ with (known/unknown) forward operator $F$,

$$y = \text{noisy}(F(x))$$

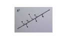
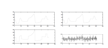
Find solution as minimizer of variational model:

$$\mathcal{J}(x) = \underbrace{\mathcal{D}_F(x,y)}_{\text{data term}} + \lambda \underbrace{\mathcal{R}(x)}_{\text{regularizer, prior}}, \qquad \lambda > 0$$

Examples:

- image restoration: denoising, (blind) deblurring, inpainting, superresolution, ...    
- computerized tomography (CT) (Video Siltanen)
- MRI (Fouriermatrix)
- FIB: Focused ion beam
- EBSD: Electron backscatter diffraction ($\mathcal{M} = \mathrm{SO}(3)/\mathcal{S}$)
- diffraction tomography
- SMLM: single molecule localization microscopy

# Motivation: Inverse Problems in Imaging

- Regularizer to make the problem well-posed, since $F$ is in general ill-posed/ill-conditioned
  - $F(x) = y$ has no solution (PCA) 
  - no unique solution (inpainting) 
  - solution does not depend continuously on input data (compact operators, deblurring, CT) 
    mildly ill-posed $\sigma_n > Cn^{-\gamma}$, $\gamma \le 1$,
    moderately ill-posed $\sigma_n > Cn^{-\gamma}$, $\gamma > 1$,
    severely ill-posed singular values decay faster than polynomial speed
- Prior for certain class of images: Bayesian (MAP) approach

$$\hat{x} \in \operatorname*{argmax}_x \log\left(p_{X|Y=y}(x)\right) \qquad \text{Bayes: } p_{X|Y=y}(x) = \frac{p_{Y|X=x}(y)p_Y(y)}{p_X(x)}$$

$$= \operatorname*{argmin}_x \left\{ -\log\left(p_{Y|X=x}(y)\right) - \log\left(p_X(x)\right) \right\}$$

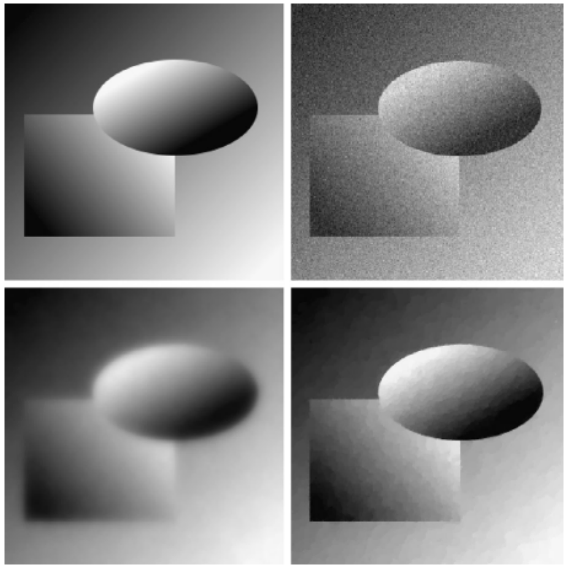
$$= \operatorname*{argmin}_x \left\{ \underbrace{\mathcal{D}_F(x,y)}_{\text{data-fidelity term}} + \lambda \underbrace{\mathcal{R}(x)}_{\text{prior}} \right\}$$

e.g. Gibbs prior

$$p_X(x) = \mathrm{e}^{-\lambda \mathcal{R}(x)} \in L_1(\mathbb{R}^d)$$

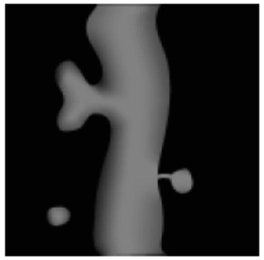
Typical regularizer/prior:

- Tikhonov regularizer:
  - continuous: $\mathcal{R}(u) = \int_\Omega |\nabla u|^2 \, \mathrm{d}\boldsymbol{x} = |u|^2_{W_2^1}$
  - discrete: $\mathcal{R}(x) = \| \, |\nabla x|^2 \, \|_1 = \sum_{i,j} (x_{i+1,j} - x_{i,j})^2 + (x_{i,j+1} - x_{i,j})^2$
- Total Variation regularization:
  - continuous: $\mathcal{R}(u) = |Du|_{TV} = \sup_{\varphi \in C_c^1(\Omega, \mathbb{R}^2), \|\varphi\|_\infty \leq 1} \langle u, \operatorname{div} \varphi \rangle = |u|_{W_2^1}$
  - discrete: $\mathcal{R}(x) = \| \, |\nabla x| \, \|_1 = \sum_{i,j} \sqrt{(x_{i+1,j} - x_{i,j})^2 + (x_{i,j+1} - x_{i,j})^2}$

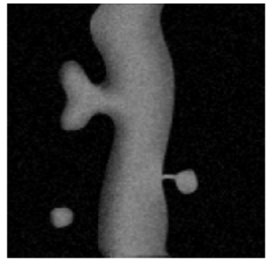


$$\underset{x}{\operatorname{argmin}} \left\{ \frac{1}{2} \|y - x\|^2 + \lambda \mathcal{R}(x) \right\}$$

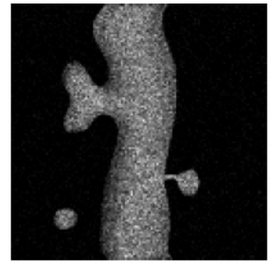
# MAP Estimation



(a) Phantom.



(b) Gaussian noise.



(c) Poisson noise

Right: Phantom of a confocal microscopy image illustrating a neuron. Middle: white additive Gaussian noise Right: Poisson noise (Courtesy: A. Jezierska, PhD thesis)

- $\operatorname{argmin}_x \left\{ -\log\left(p_{Y|X=x}(y)\right) - \log\left(p_X(x)\right) \right\}$

$$p_{Y|X=x}(y) = \begin{cases} \frac{1}{(2\pi\sigma^2)^{N/2}} e^{-\frac{\|y-F(x)\|_2^2}{2\sigma^2}} & \text{Gaussian noise,} \\ \prod_{i=1}^{N} \frac{(F(x)_i)^{y_i}\, e^{-F(x)_i}}{y_i!} & \text{Poisson noise} \end{cases}$$

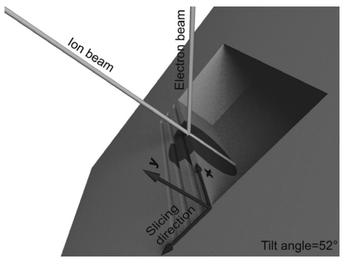
Up to a constant

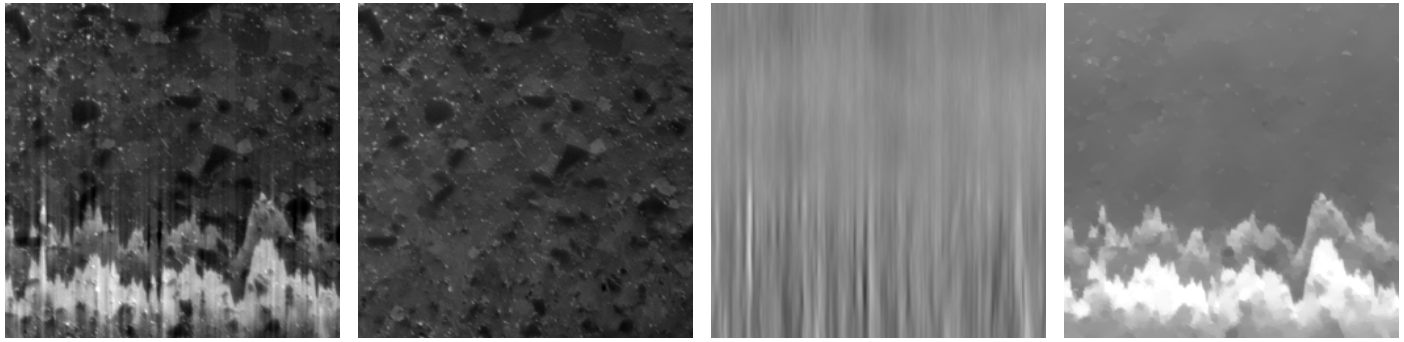
$$-\log\left(p_{Y|X=x}(y)\right) = \begin{cases} \frac{1}{2\sigma^2}\|y - F(x)\|_2^2 & \text{Gaussian,} \\ -\sum_i y_i \log(F(x)_i) + F(x)_i = \mathrm{KL}(y, F(x)) + c & \text{Poisson} \end{cases}$$

with Kullback-Leibler divergence (componentwise)

$$\mathrm{KL}(u, v) = u \log u - u \log v - u + v$$

# Example 1: Removal of Curtaining Effects in FIB



Model:

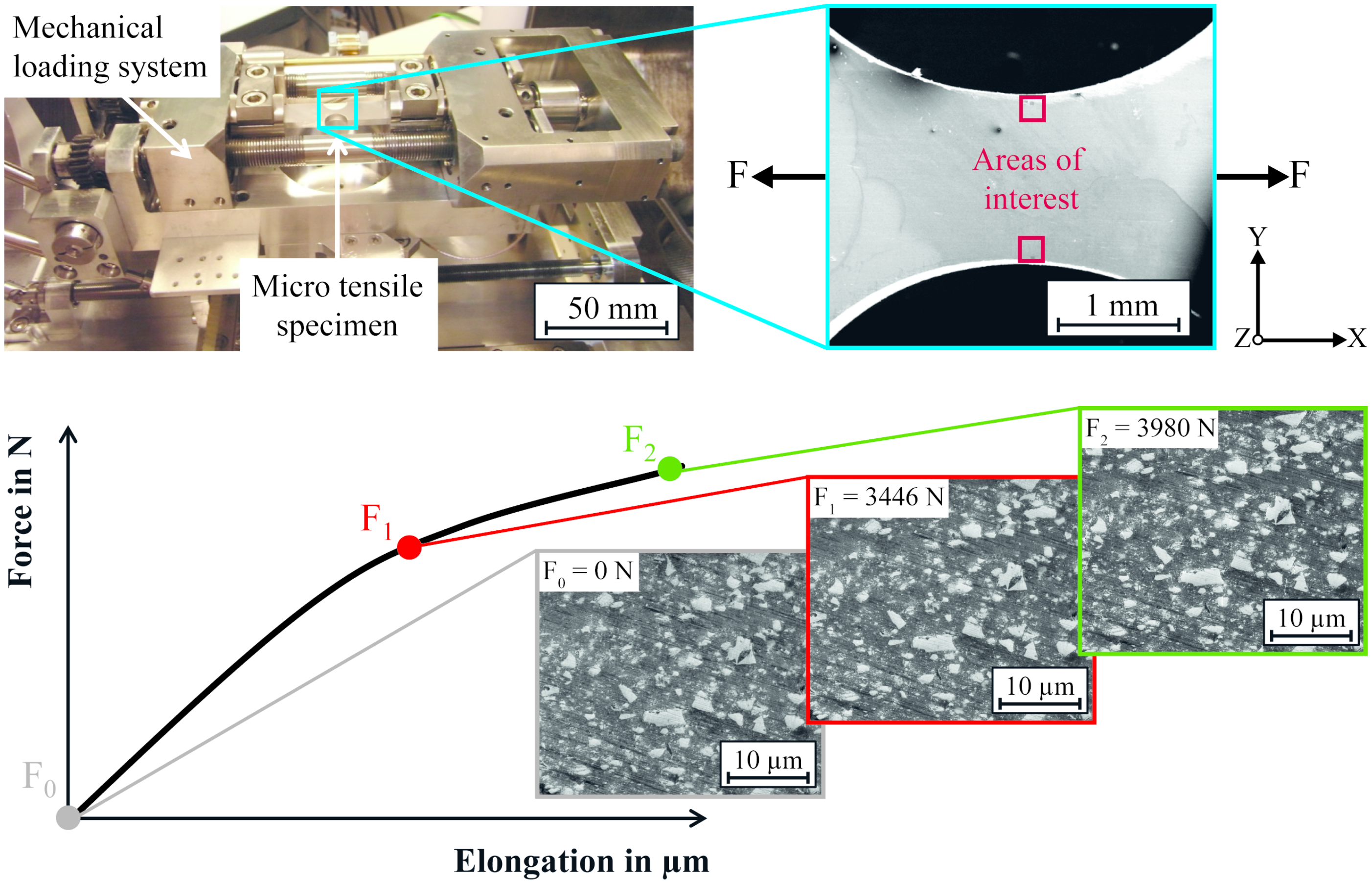
$$\mathcal{J}(u,s,l) = \|f - (u+s+l)\|_2^2 + \varphi_1(u) + \varphi_2(s) + \varphi_3(l),$$

with

$$\begin{aligned} \varphi_1(u) &:= \mu_1 \|\nabla_{x,z} u\|_{2,1} + \mu_2 \|\Delta_z u\|_1 + \iota_{[0,1]^N}(u), \\ \varphi_2(s) &:= \|\nabla_y s\|_1, \\ \varphi_3(l) &:= \mu_3 \|\nabla_{x,y} l\|_{2,1} \end{aligned}$$

- Video: J.-H. Fitschen

# Example 2: Strain Computation




Top: Experimental setup for the tensile test inside a scanning electron microscope. Bottom: Load-deformation diagram with three selected micrographs taken under increasing load.

# Example 2: Strain Computation

Model: $u = (u_1, u_2)^\top$ vector field

$$\mathcal{J}(u) := \|A_{f_2}u + c_{f_1,f_2}\|_1 + \mathrm{TGV}(u)$$

where the data term arises from linearizing the brightness invariance assumption:

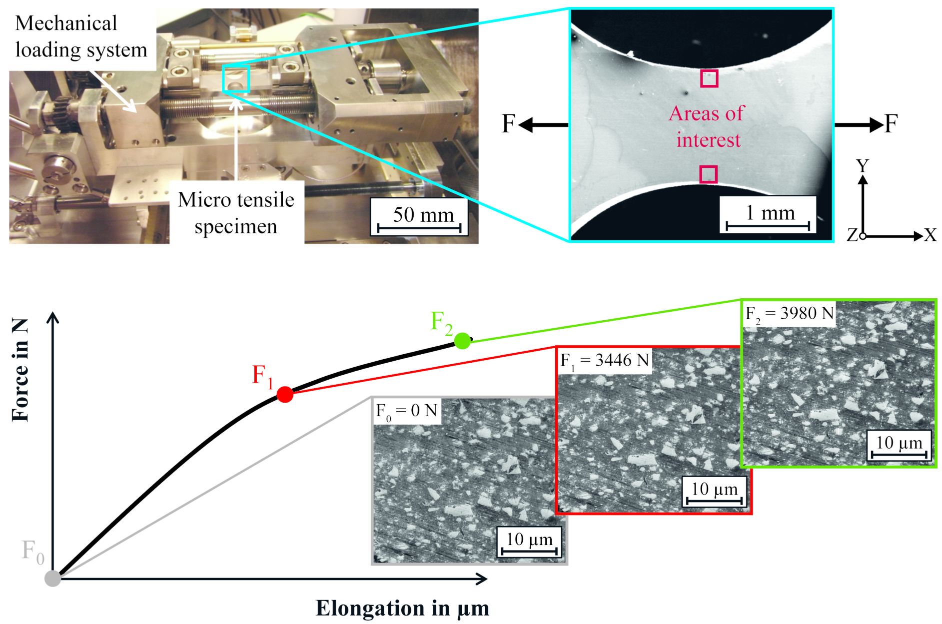
$$\begin{aligned} 0 &\approx f_1(x) - f_2\big(x + u(x)\big) \\ &\approx f_1(x) - f_2(x + \bar{u}(x)) - \big\langle \nabla f_2(x + \bar{u}(x)), u(x) - \bar{u}(x)\big\rangle \end{aligned}$$

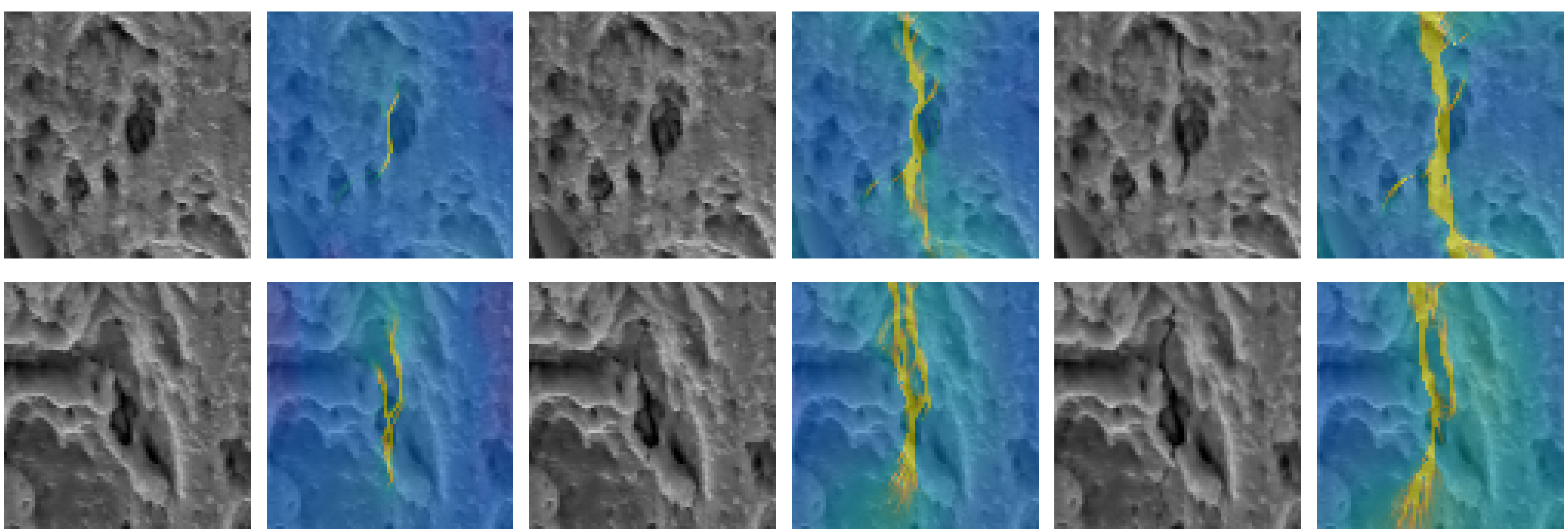
and the regularizer is

$$\mathrm{TGV}(u) := \inf_a \left\{ \int_\Omega \lambda_1 \underbrace{\|\nabla u - a\|_F}_{\text{local feature}} + \lambda_2 \underbrace{\|\nabla a\|_F}_{\text{global feature}} \, dx \right\}$$

Reference: Bredies, Kunisch, Pock 2010, Setzer, Steidl 2008

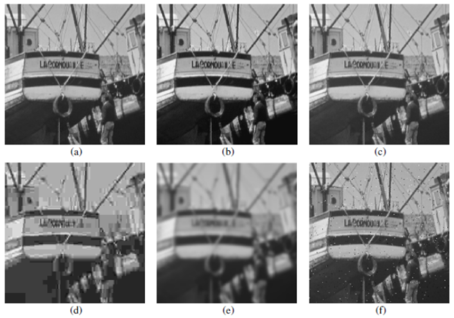
# Example 2: Strain Computation



# Quality Measures

- MSE: $\mathrm{MSE}(u,f) := \frac{1}{N}\|u-f\|_2^2$
- PSNR: Peak signal to noise ratio $\mathrm{PSNR}(u,f) := 10\log_{10}\frac{|\max f - \min f|^2}{\frac{1}{N}\|u-f\|_2^2}$,
- MAE: Mean absolute error $\mathrm{MAE}(u,f) := \frac{1}{N}\|f-u\|_1$.
- SSIM: Structure similarity measure (Simoncelli et al. 2004)
- Sharpness index (Moisan et al. 2011)
- LPIPS: Learned Perceptual Image Patch Similarity (Zhang/Efros 2018)



Different type of distortions, all with MSE = 210. (a) Original image, (b) Contrast-stretched image, SSIM = 0.9168, (c) Mean-shifted image, SSIM = 0.9900, (d) JPEG compressed image, SSIM = 0.6949, (e) Blurred image, SSIM = 0.7052, (f) Salt-pepper noise contaminated image, SSIM = 0.7748. Image: Simoncelli et al 2004.

# Motivation: Neural Networks and Deep Learning ϟ

M. Elad (2017) SIAM News: **Deep, deep trouble**:
Deep learning's impact on image processing, mathematics, and humanity
Change to: **High, high challenge**

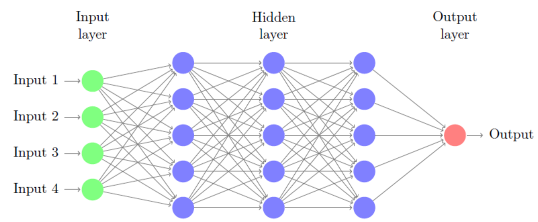



Figure 1: Model of a NN with three hidden layers, i.e., $d = 4$, $K = 4$, $n_1 = n_2 = n_3 = 5, n_4 = 1$.

NN: $\Phi(\cdot\,;\theta) : \mathbb{R}^d \to \mathbb{R}^{n_K}$ of the form

$$\Phi\left(\cdot;\theta\right) := A_K\sigma \circ A_{K-1}\sigma \circ \ldots \sigma \circ A_1$$

with non-linear activation $\sigma : \mathbb{R} \to \mathbb{R}$ acting componentwise and affine functions

$$A_k(x) := W_k x + b_k, \qquad W_k \in \mathbb{R}^{n_k, n_{k-1}},\ b_k \in \mathbb{R}^{n_k}$$

Training of a NN by minimizing

$$\mathcal{J}(\theta) := \sum_{i=1}^{N} \ell\big(\Phi(x_i;\theta); y_i\big),$$

Minimization Algs: stoch. gradient descent algorithm (filtered backprojection, automatic differentiation), inertial stoch. PALM Refs: Hertrich/Steidl 2022

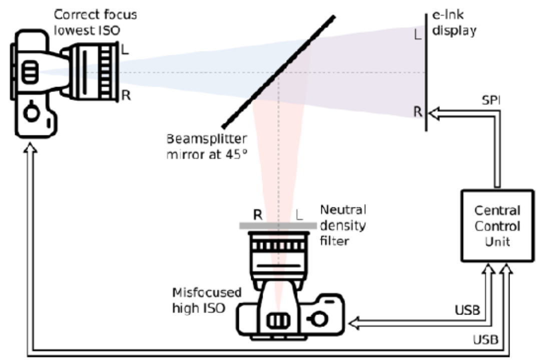
Fitschen: ,,most stupid method to solve problems"

# Example 1: Deblurring

Helsinki Deblur Challenge 2021 organized by the Finish Inverse Problem Society

Winner: Genzel, MacDonald, März (PhD), T. Trippe (Master thesis) TUB

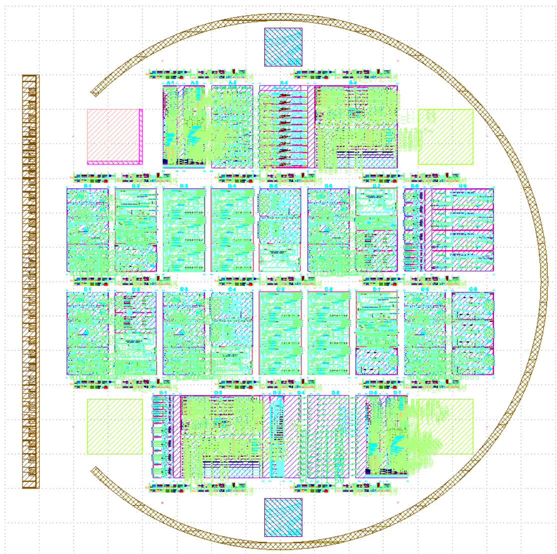
- Goal: deblurring of text images obtained by an optical aperture



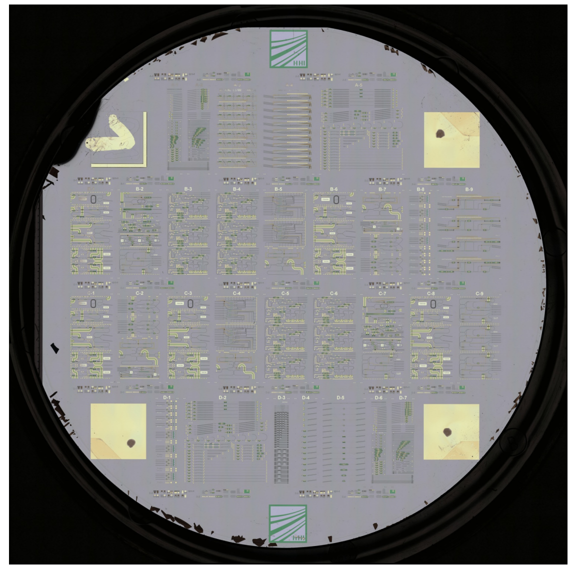

- 20 levels of increasing defocus blur, 200 samples per level
- Results:

# Example 2: Photo Integrated Circuit Design

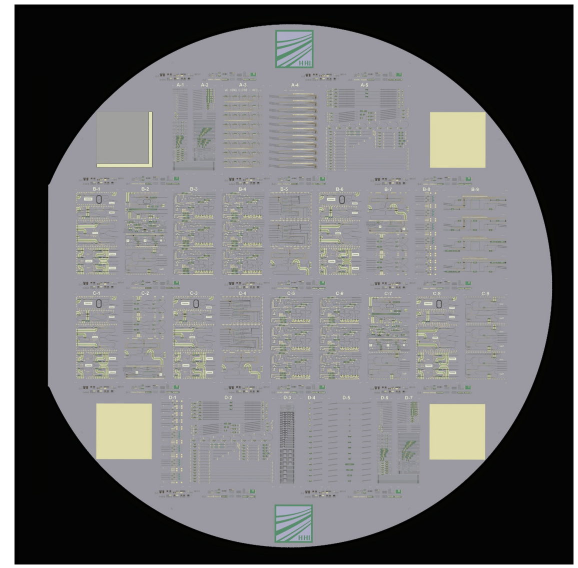
Master thesis C. Wittmann (with Hertz Institute Berlin)



plan



photo



NN simulation

- LPIPS as loss function

How to model and minimize variational models in inverse problems and how NNs can be incorporated?

Let's do some MATH.

A. Maslow (1966):
"If the only tool you have is a hammer,
you treat everything as if it were a nail."

Berlin Mathematics Research Center

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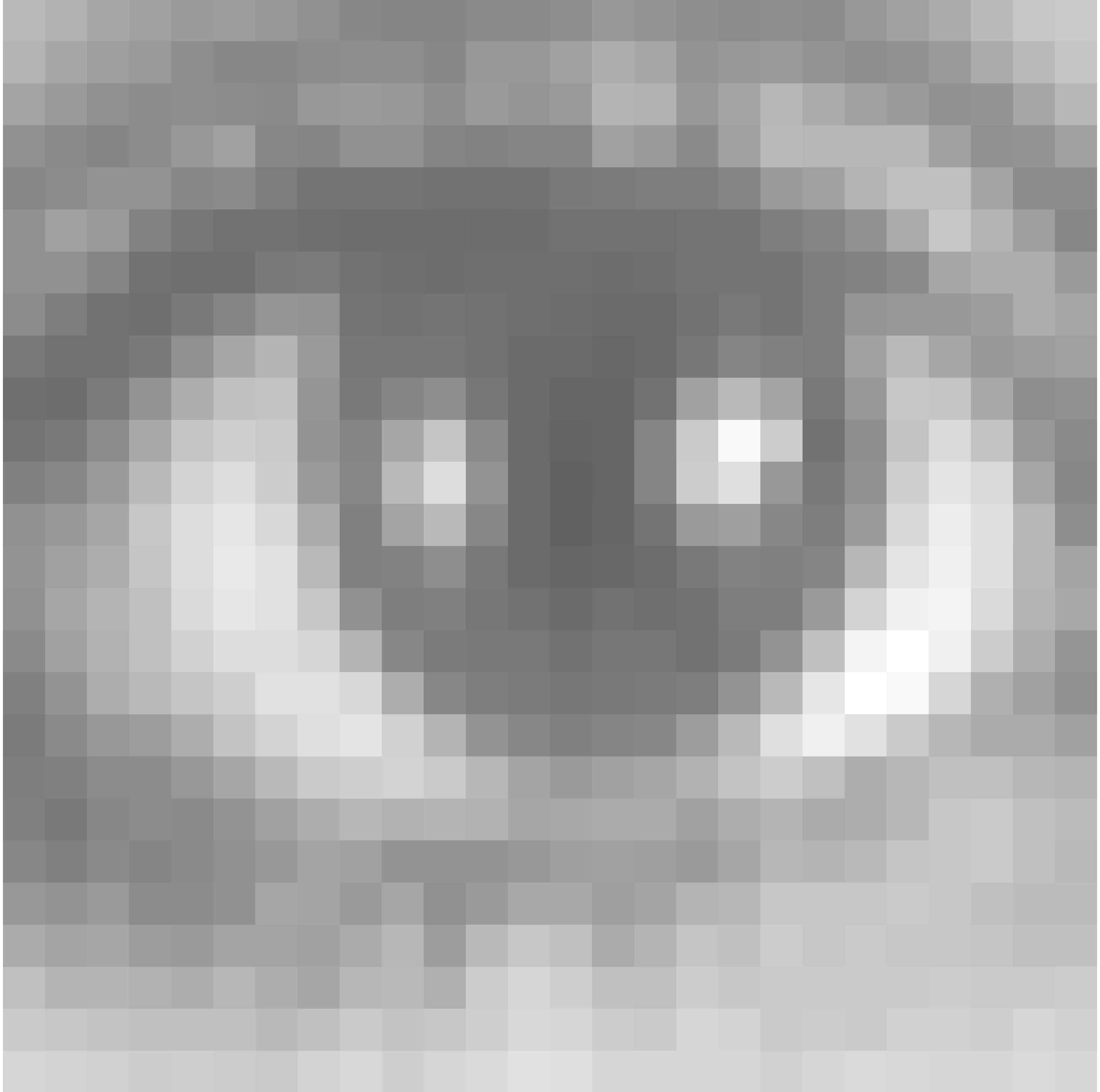
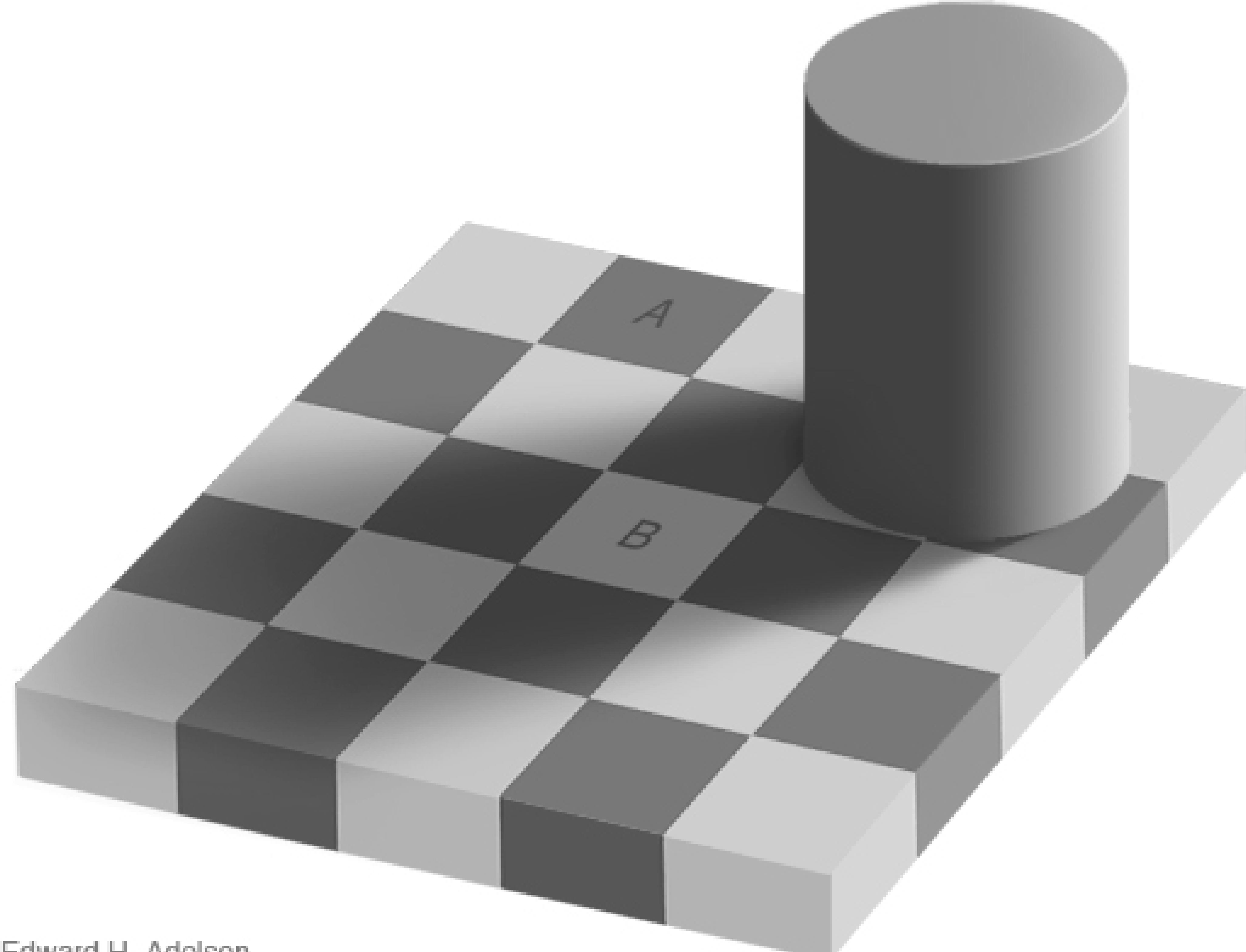
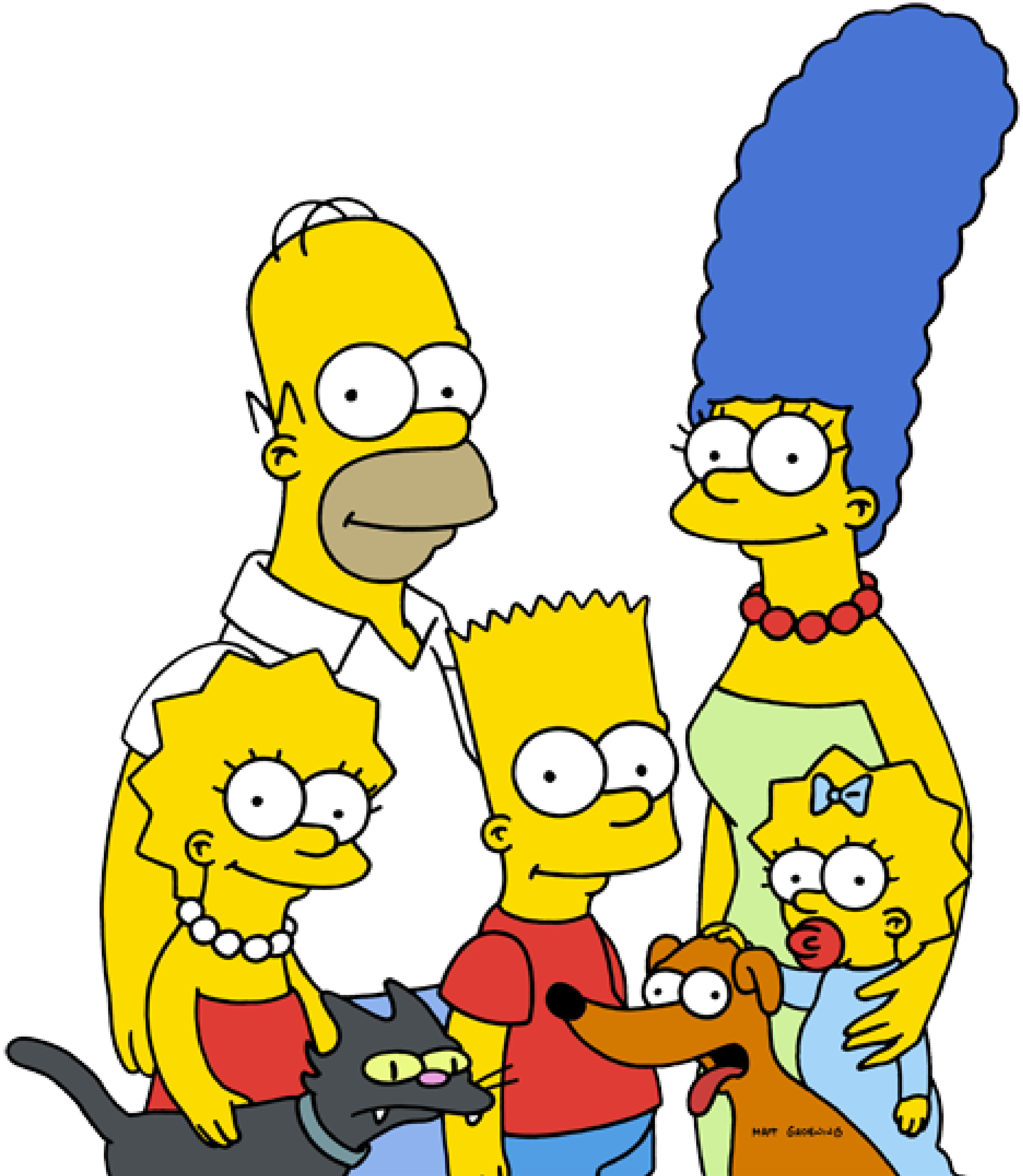
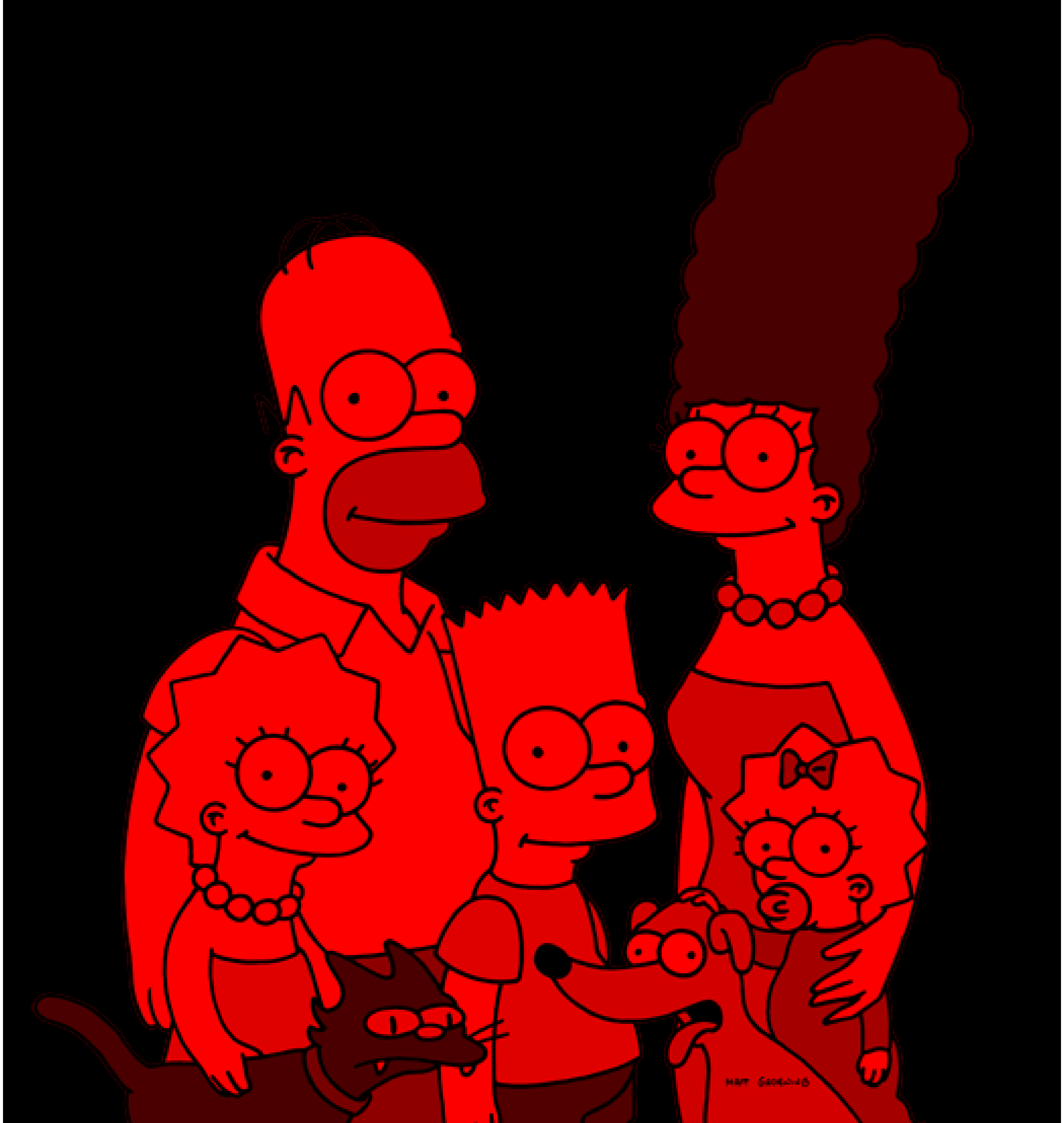
DFG Deutsche Forschungsgemeinschaft

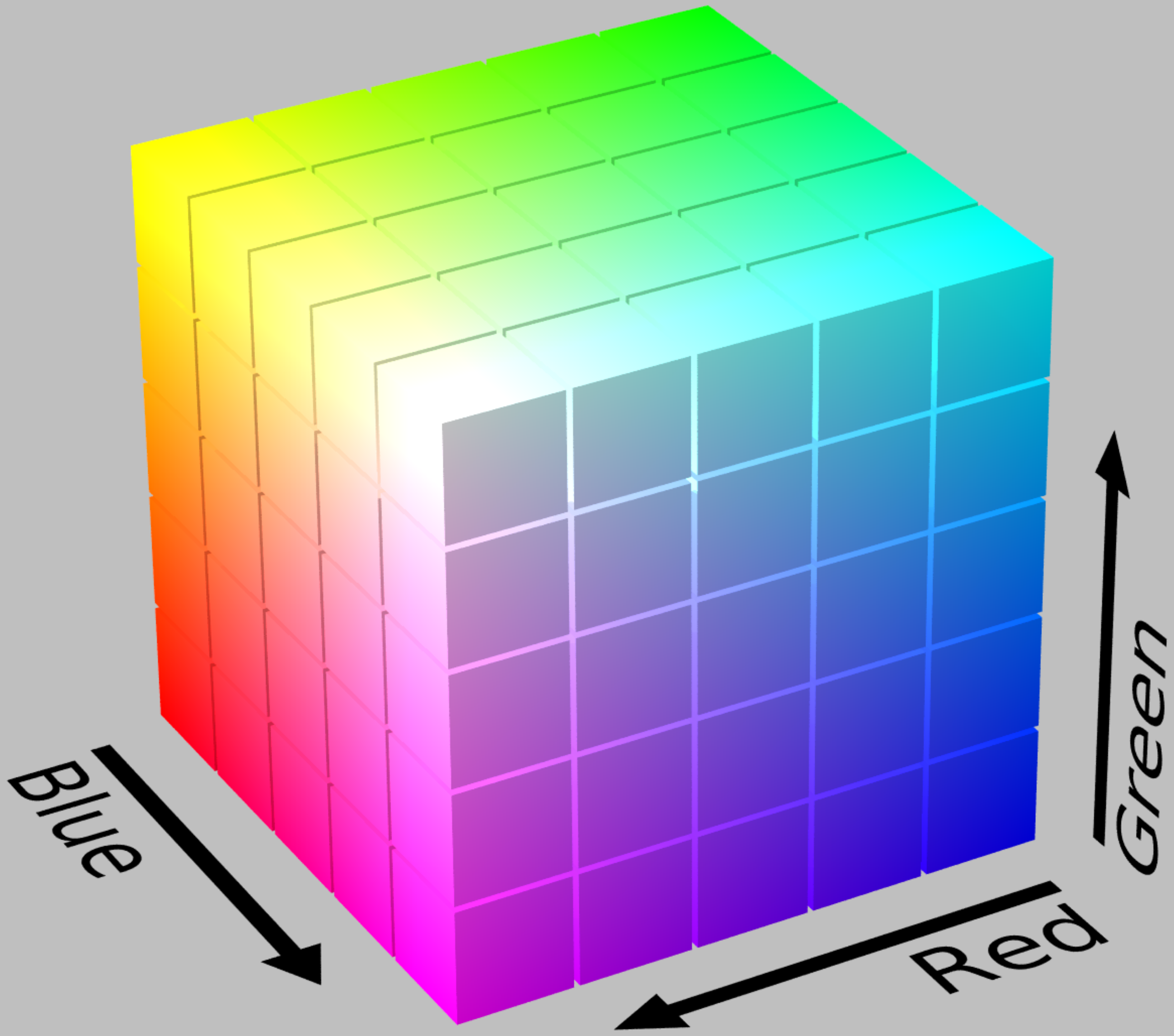





Edward H. Adelson






Blue
Red
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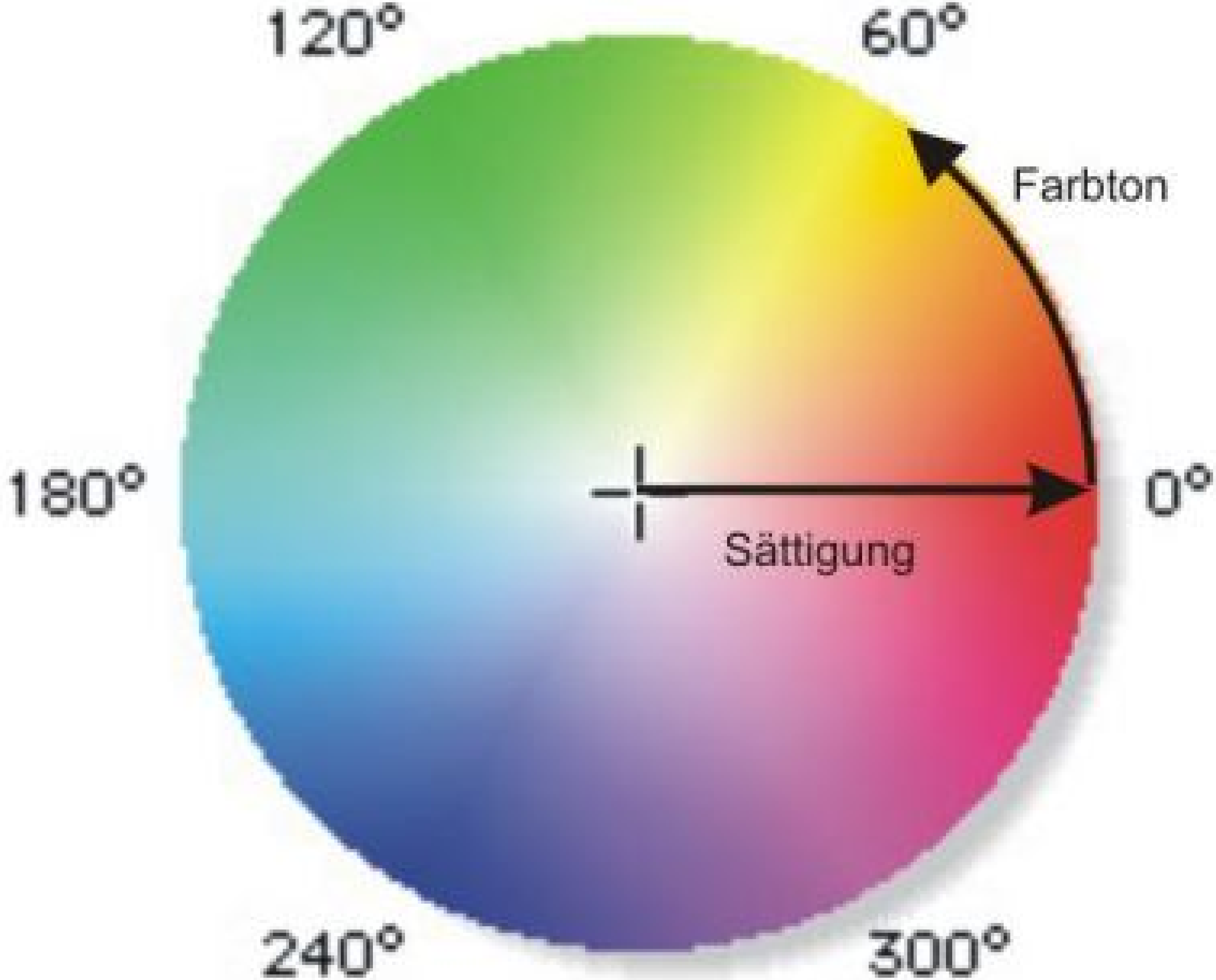
120°
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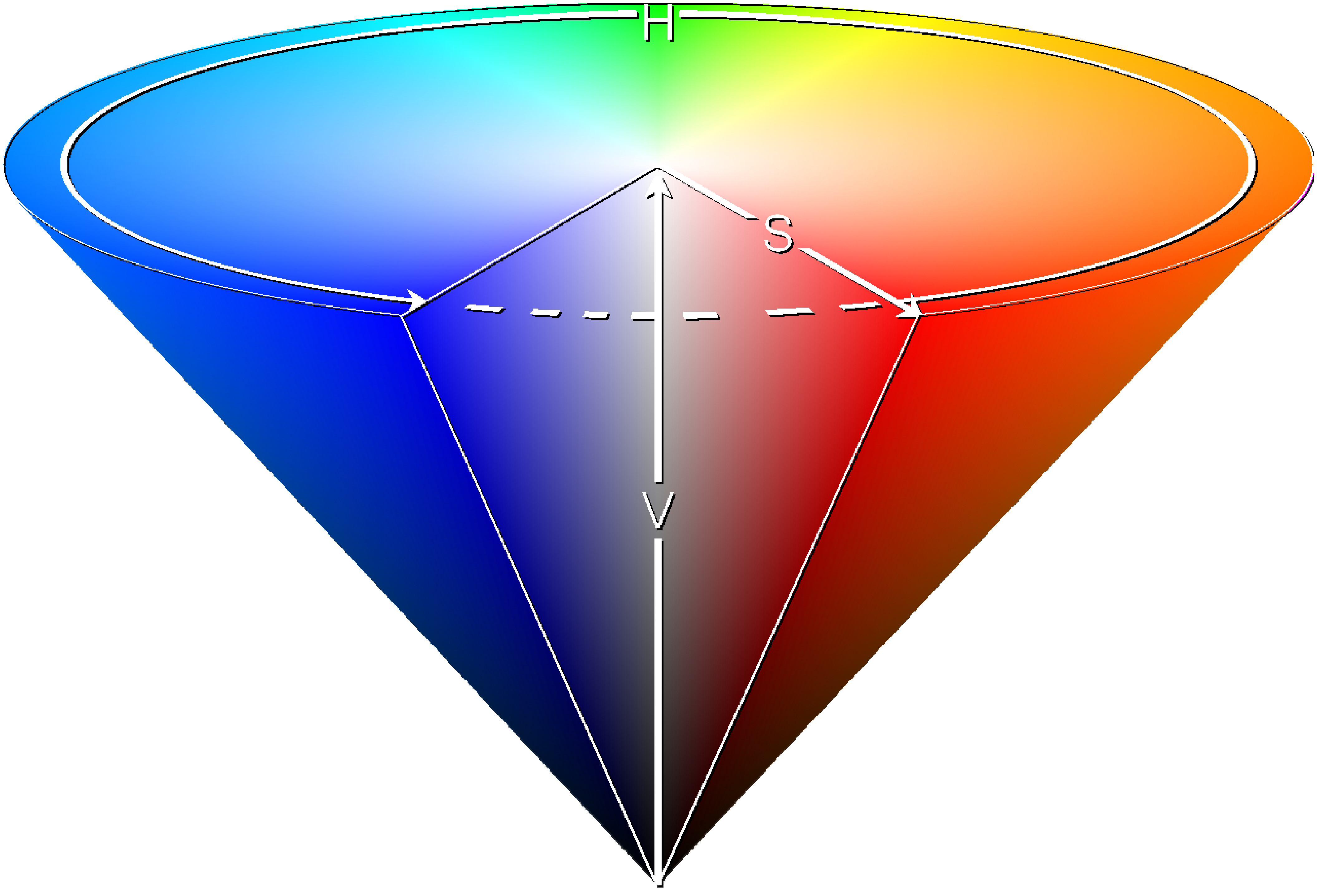
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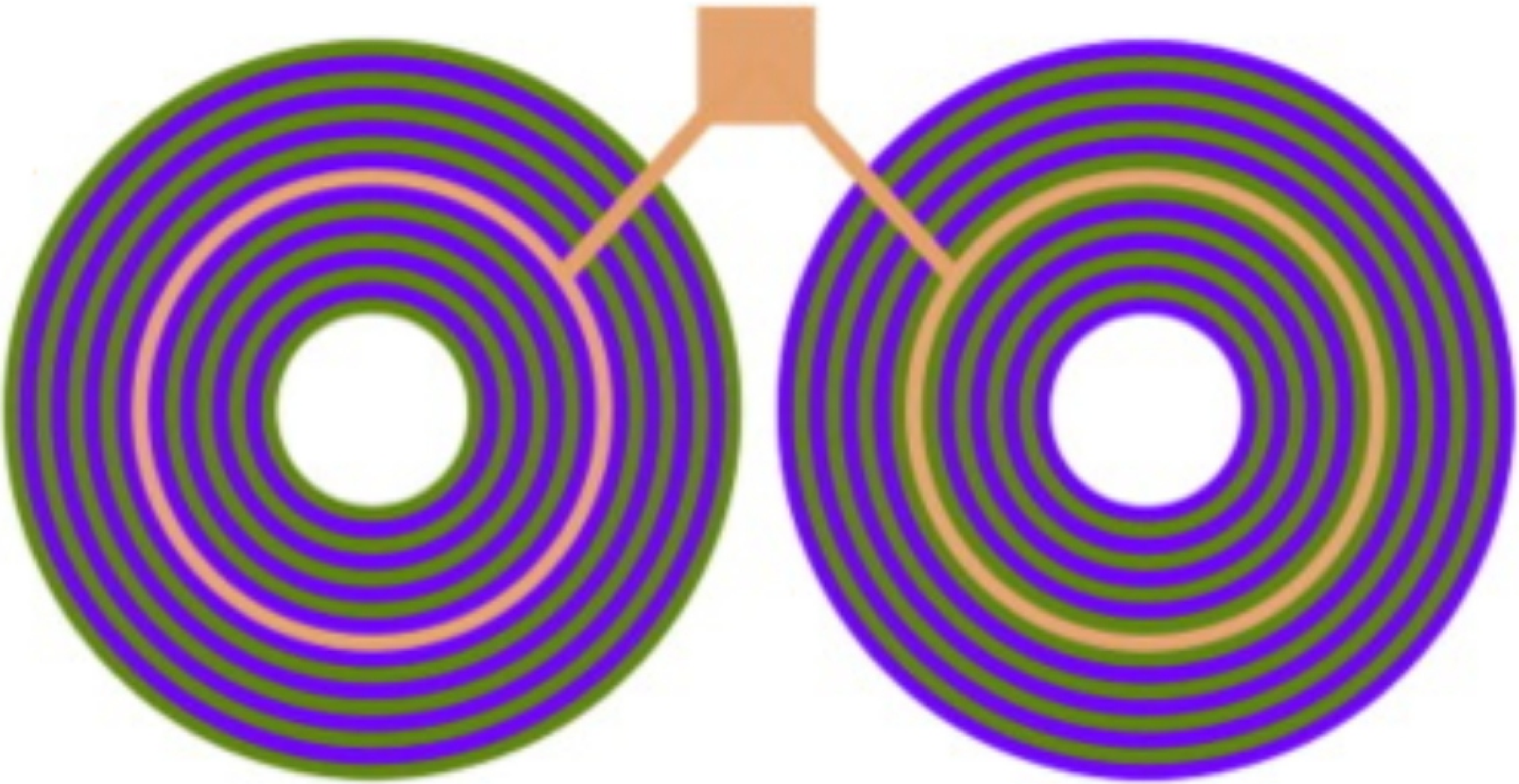
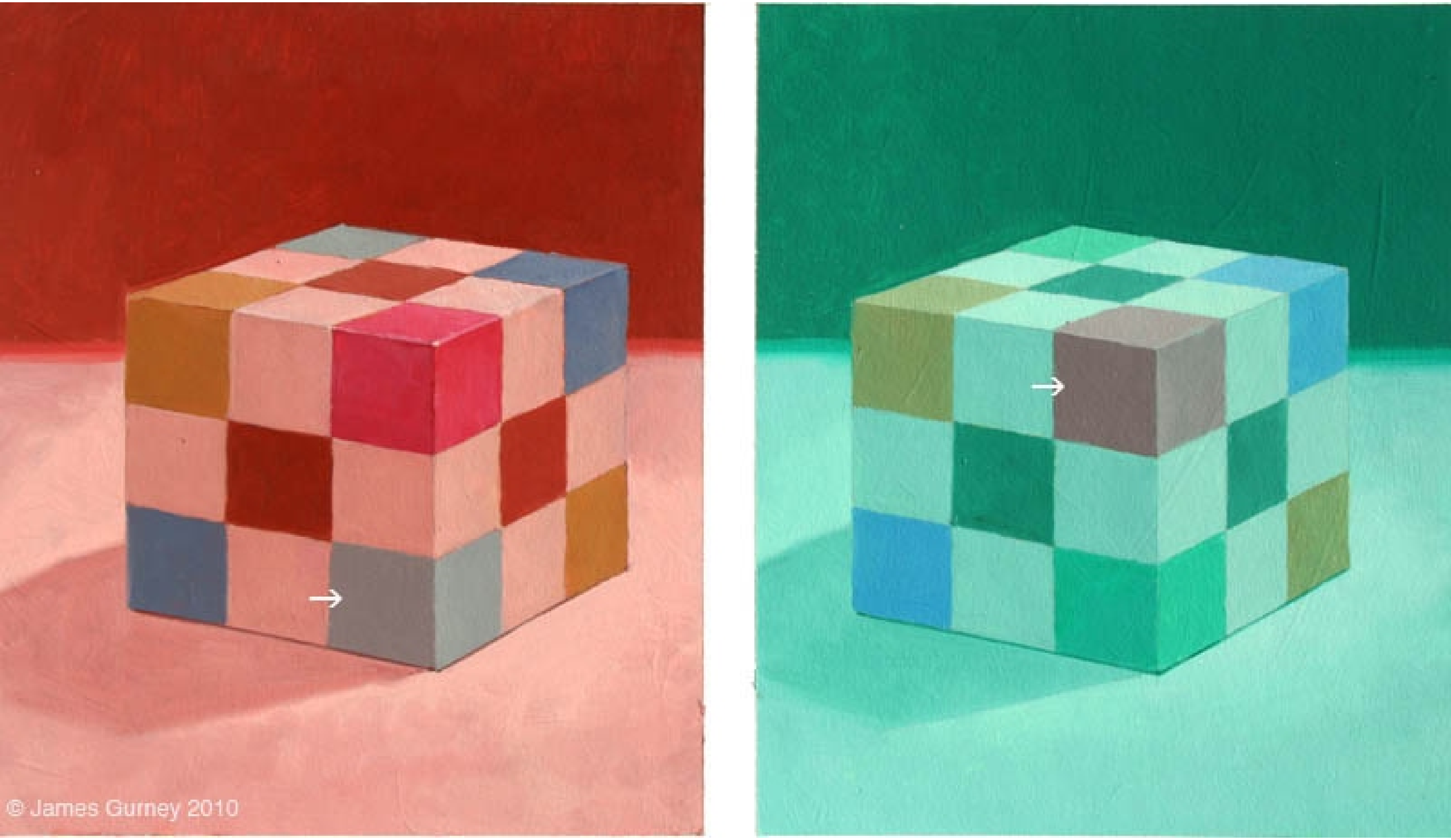
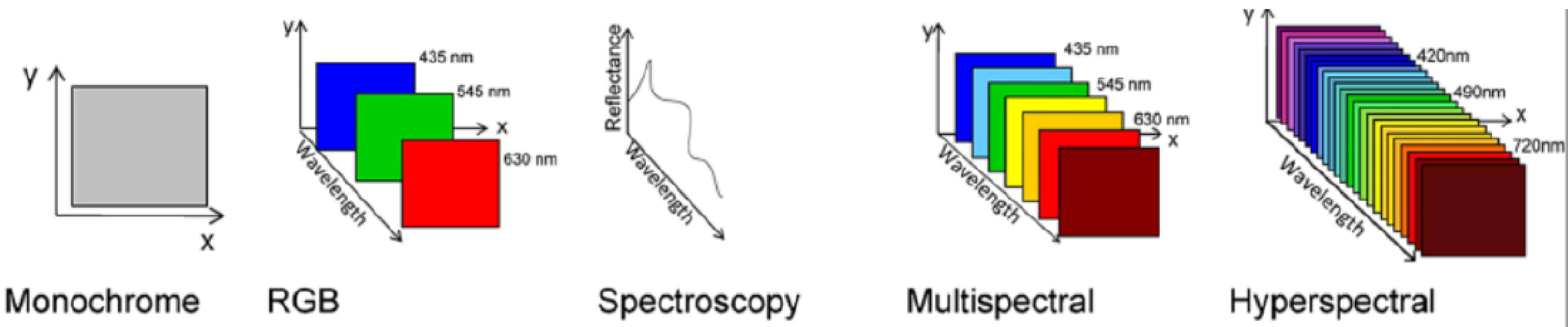



© James Gurney 2010


y
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Monochrome
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435 nm
545 nm
630 nm
Wavelength
RGB
Reflectance
Wavelength
Spectroscopy
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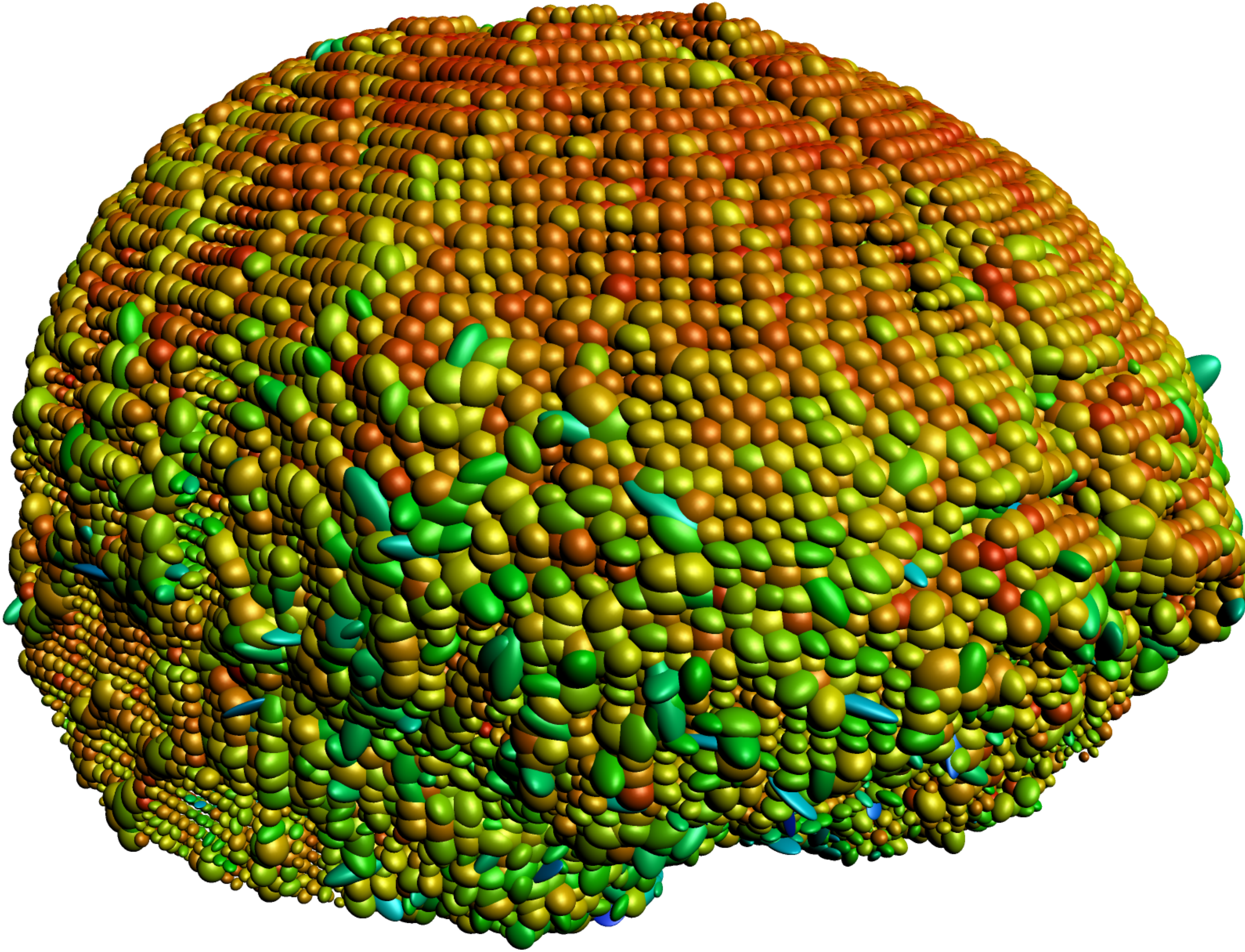
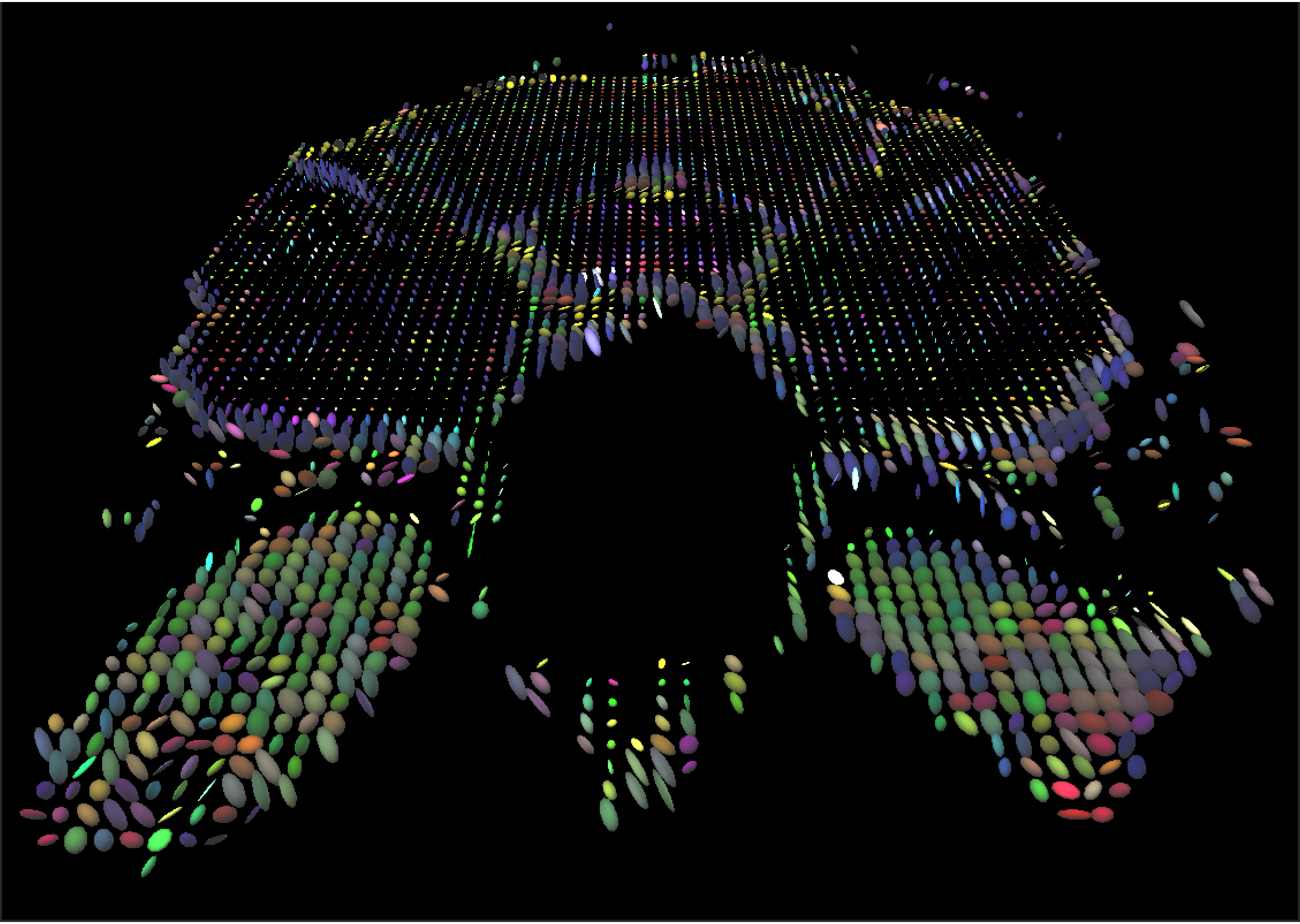
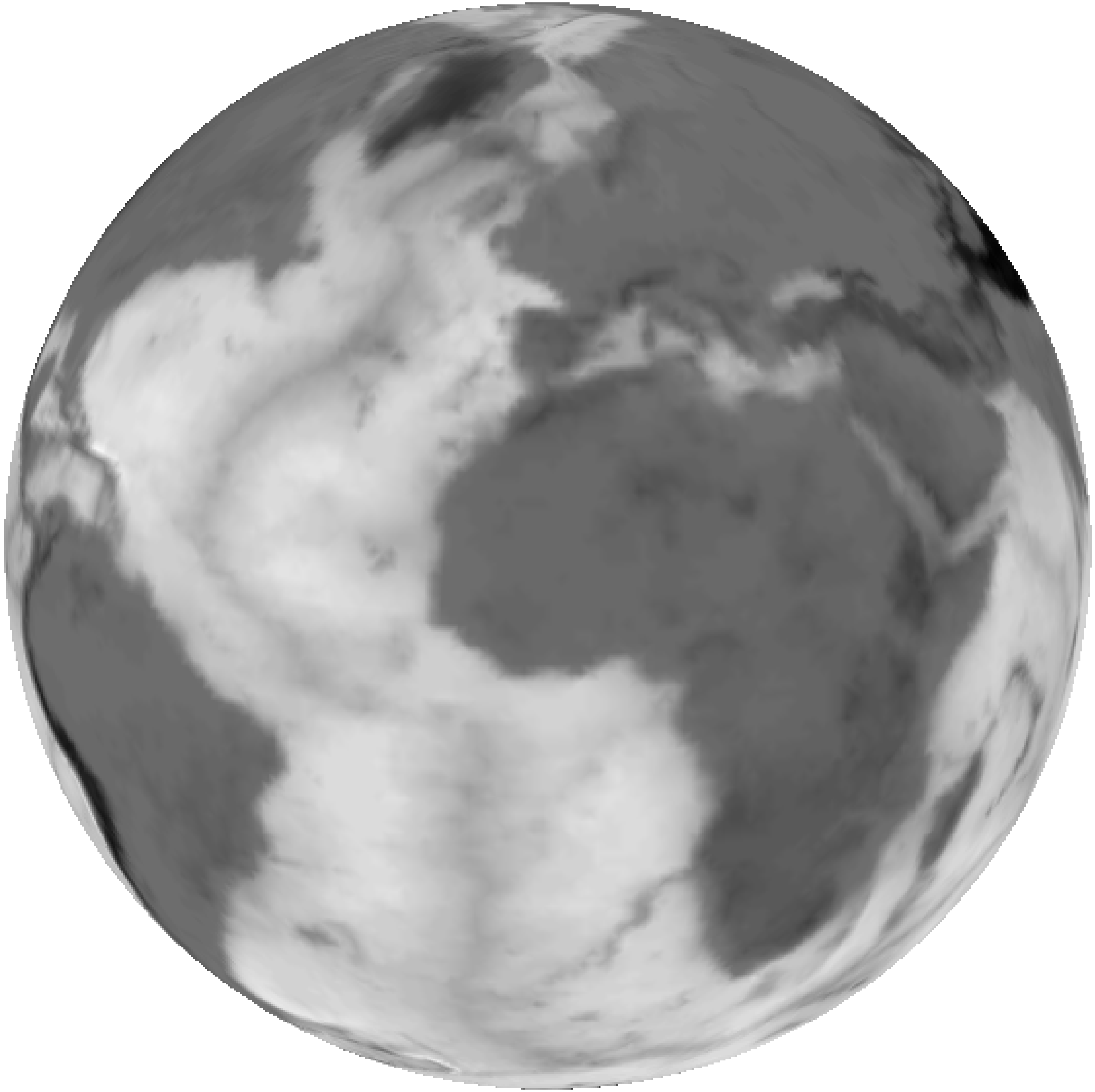
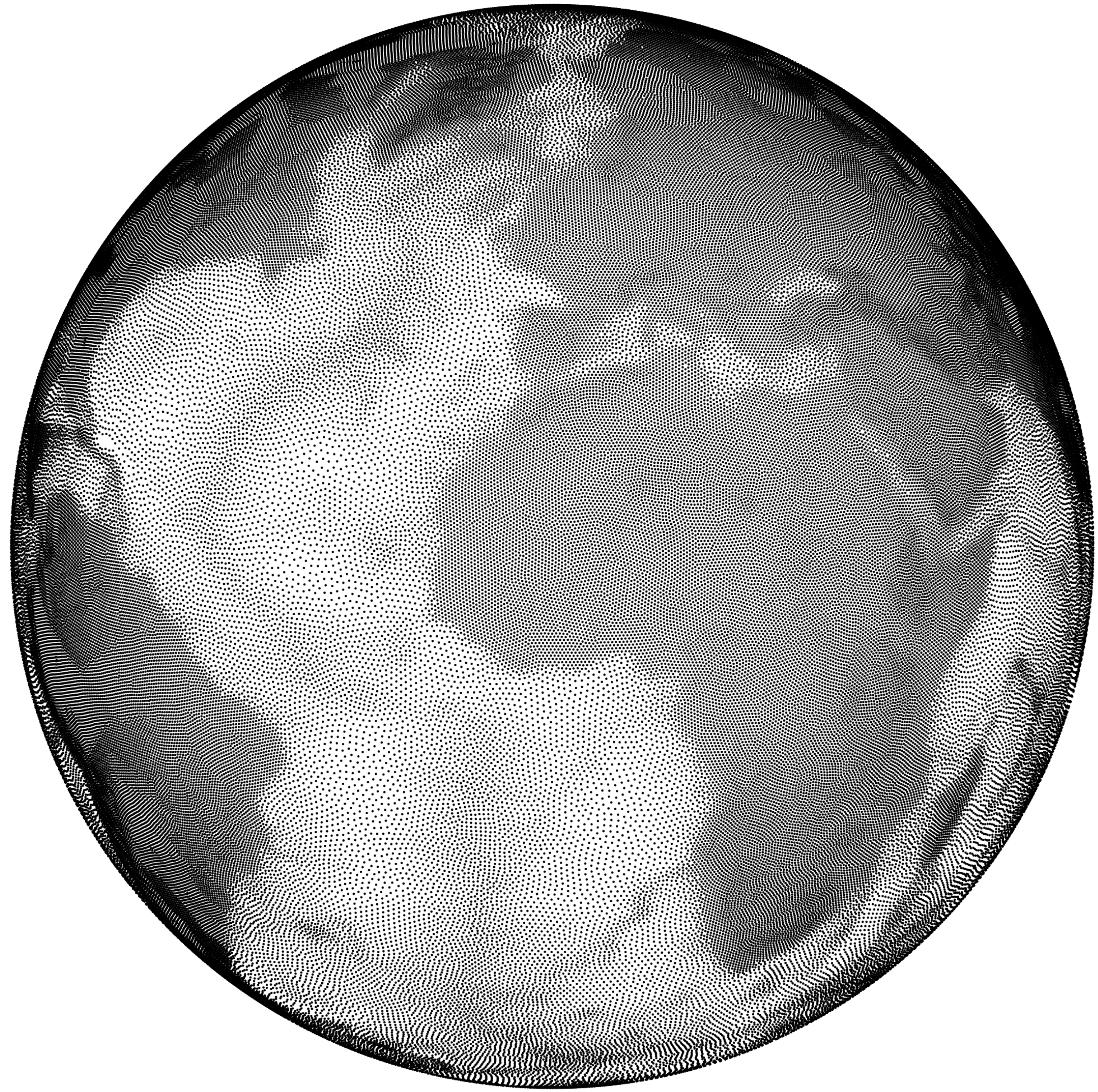
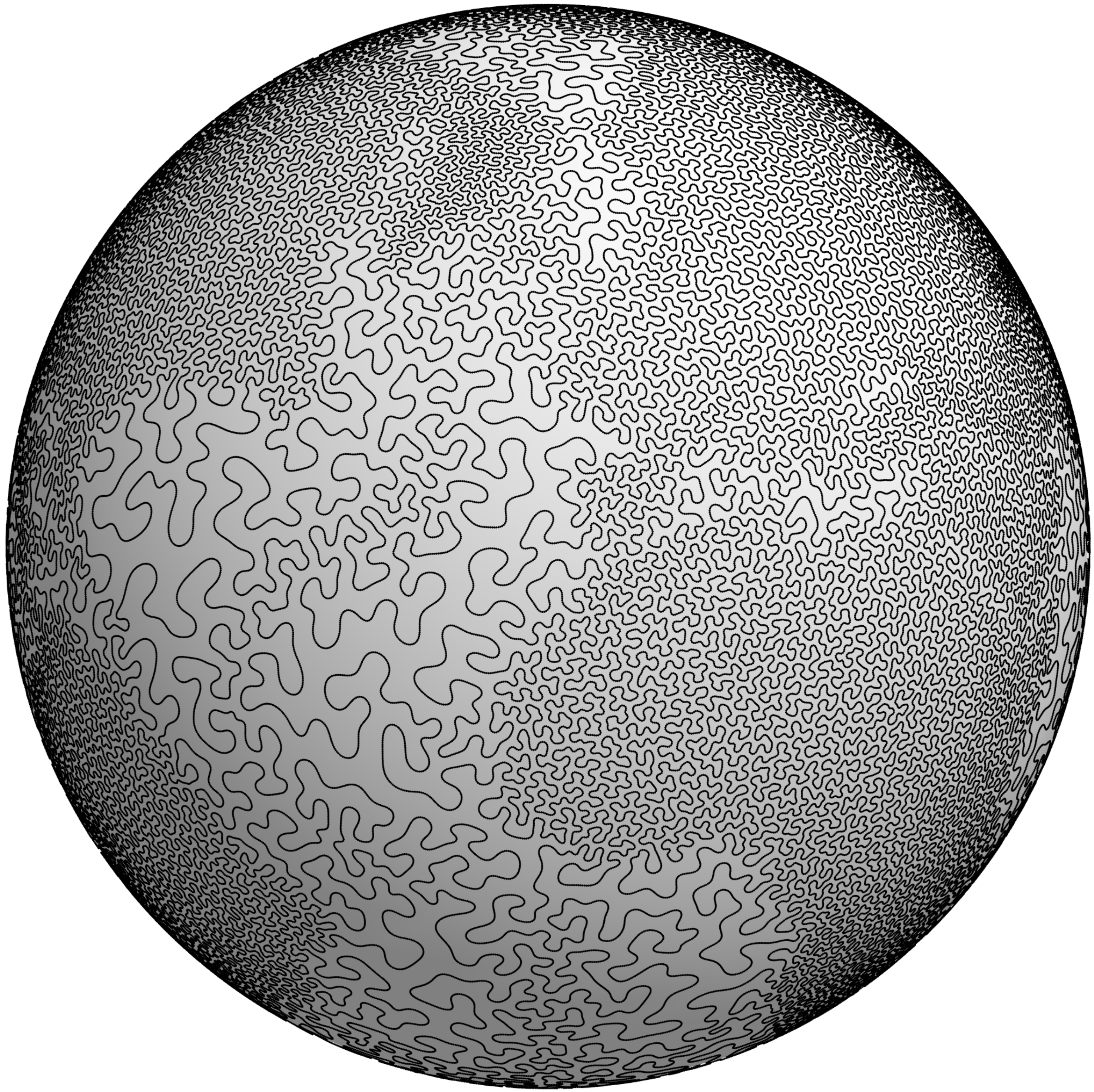
720nm
Wavelength
Hyperspectral

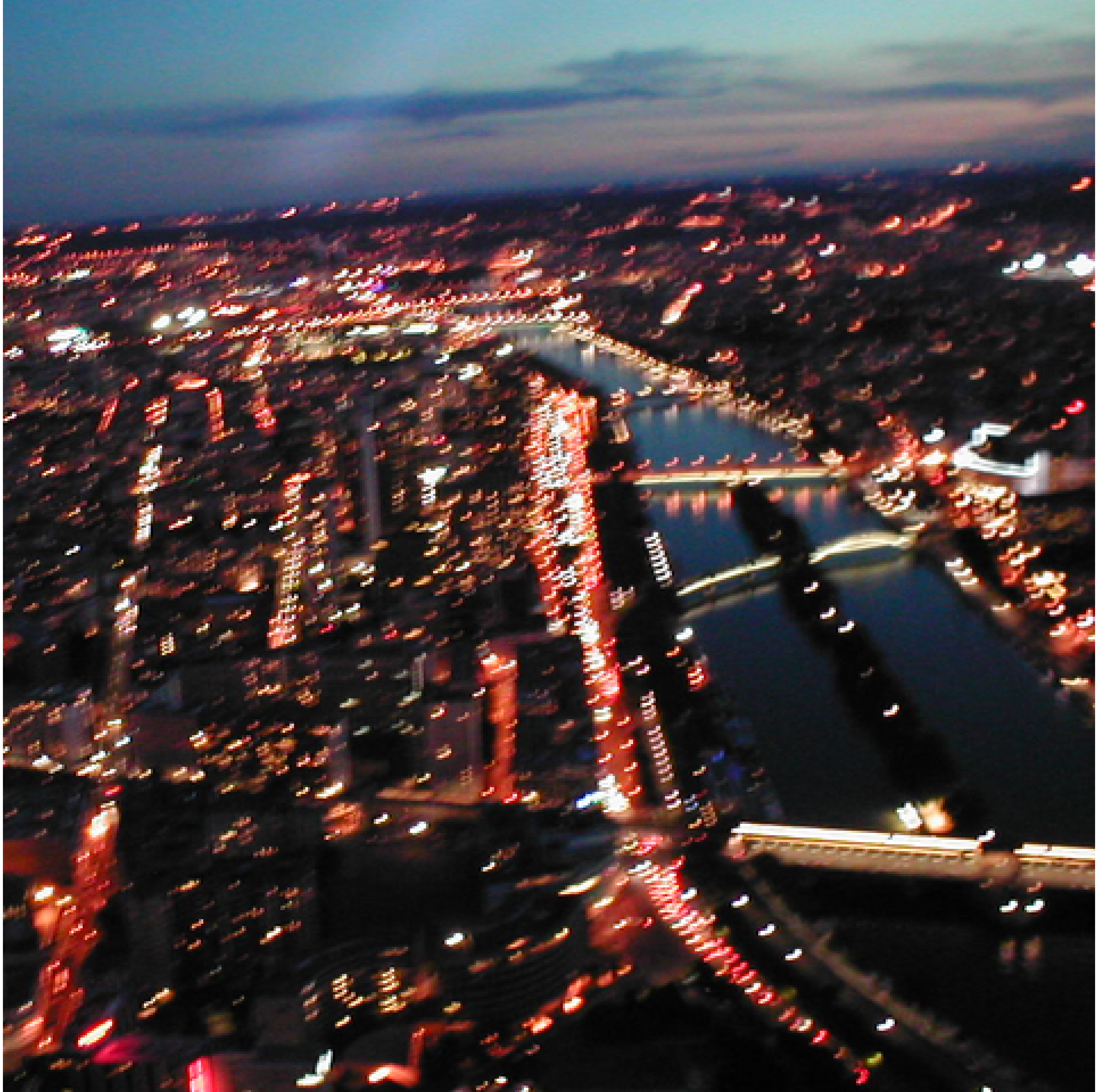


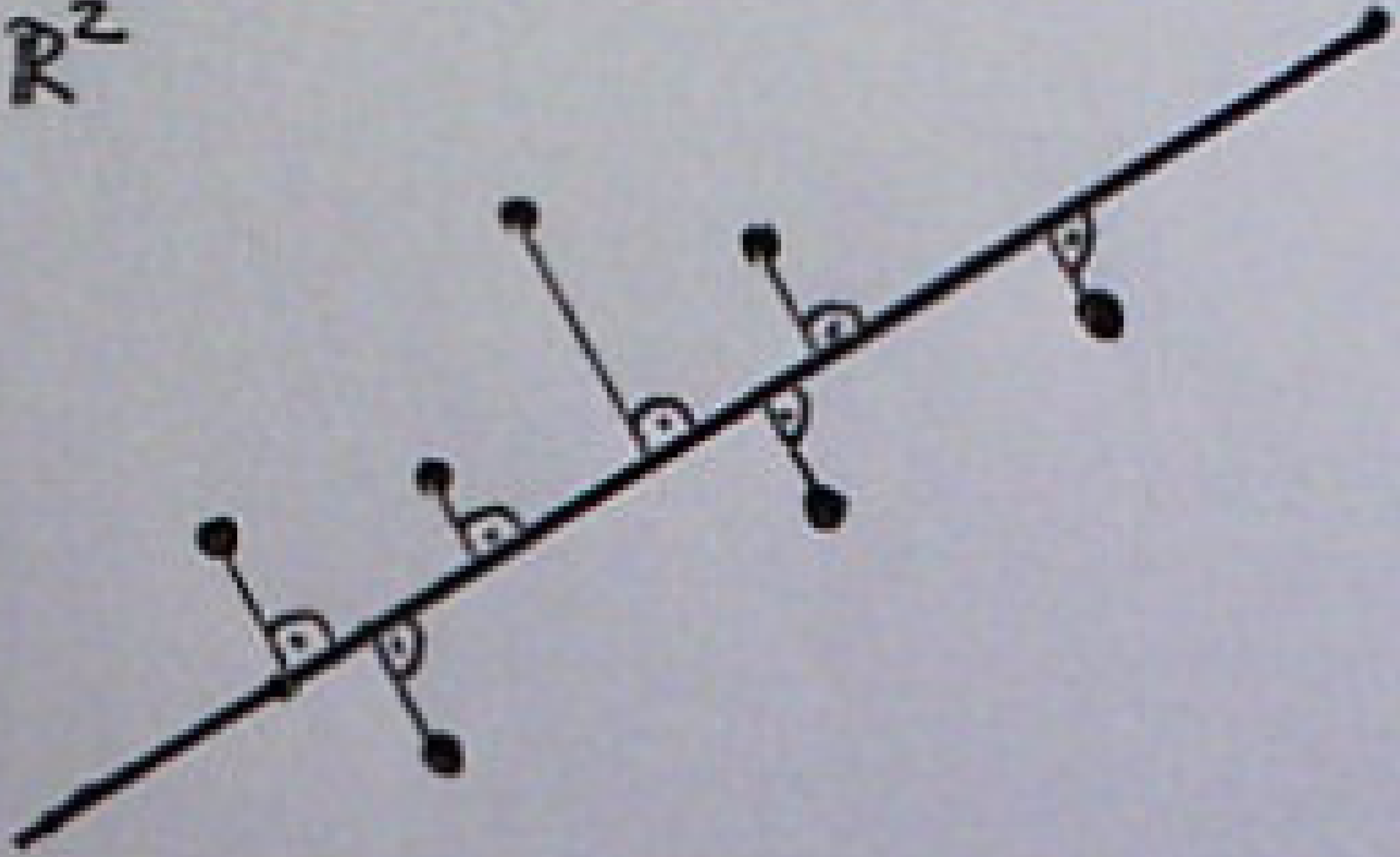


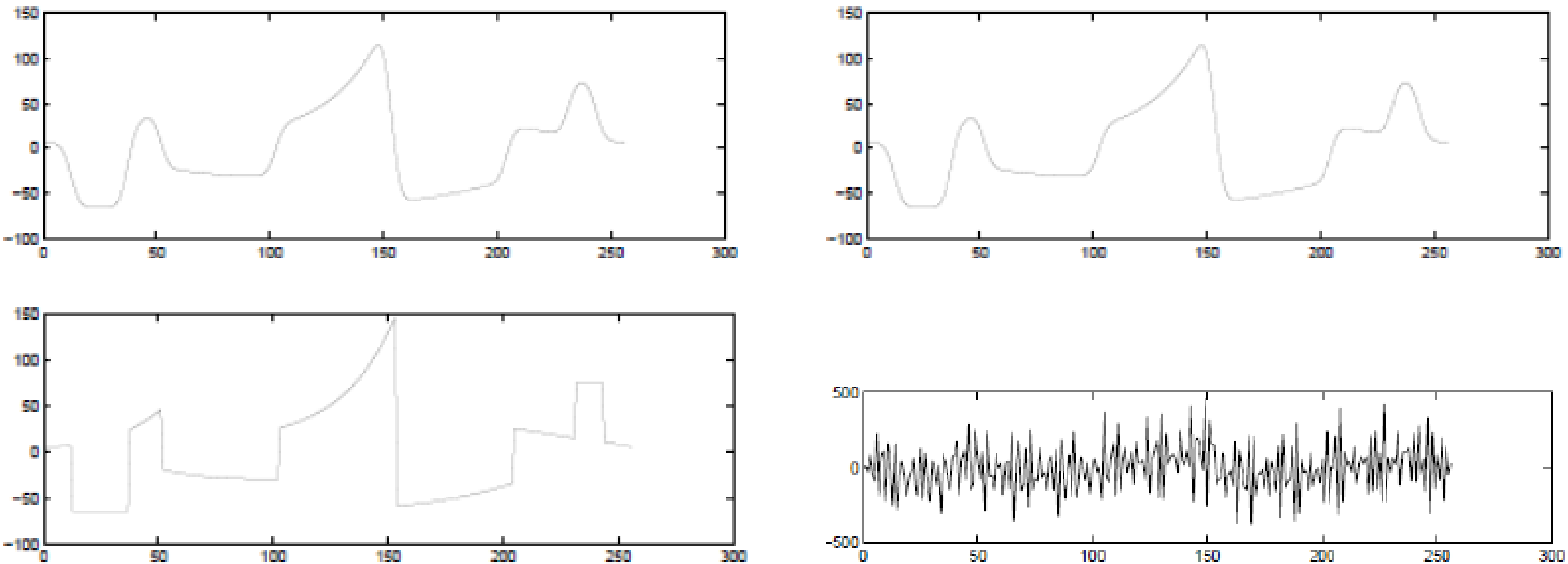









$\mathbb{R}^2$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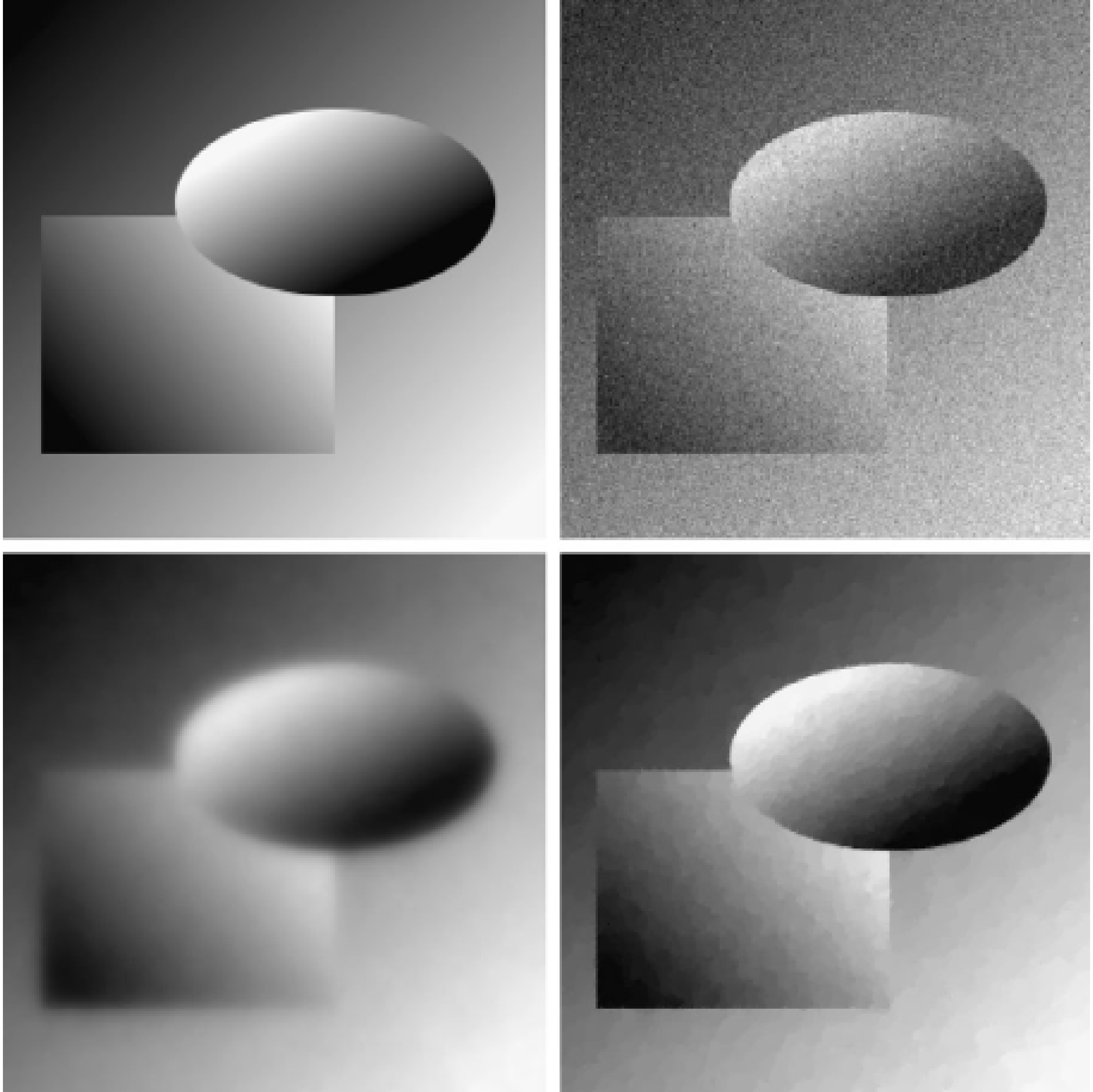
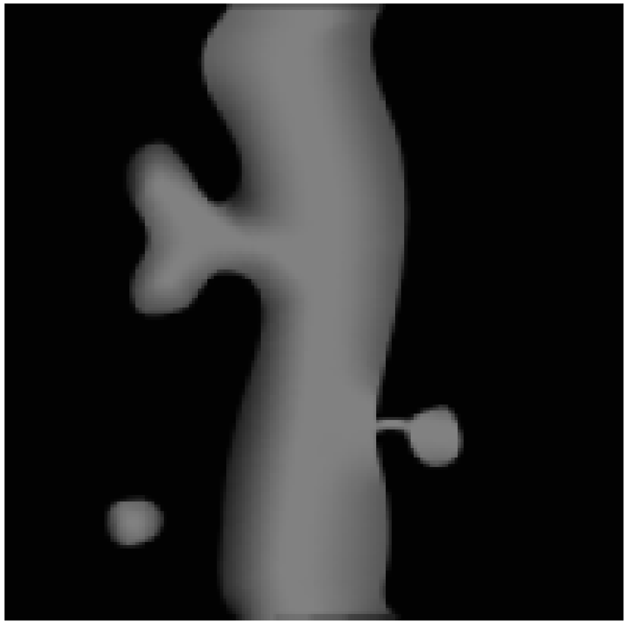
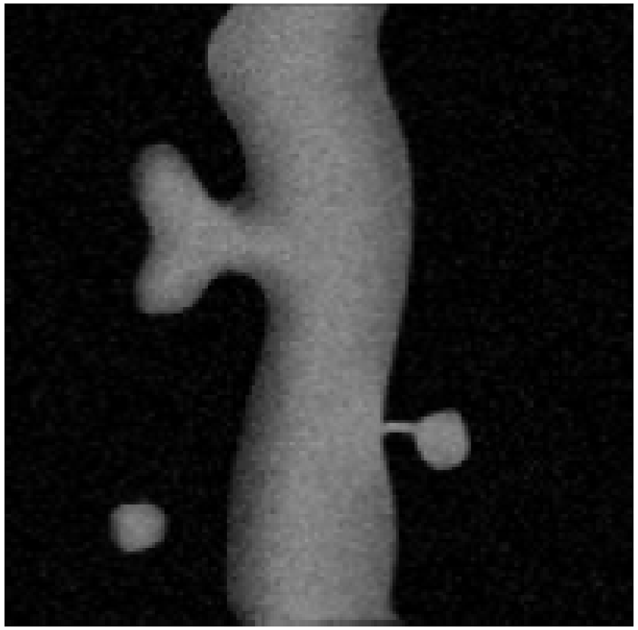
-500

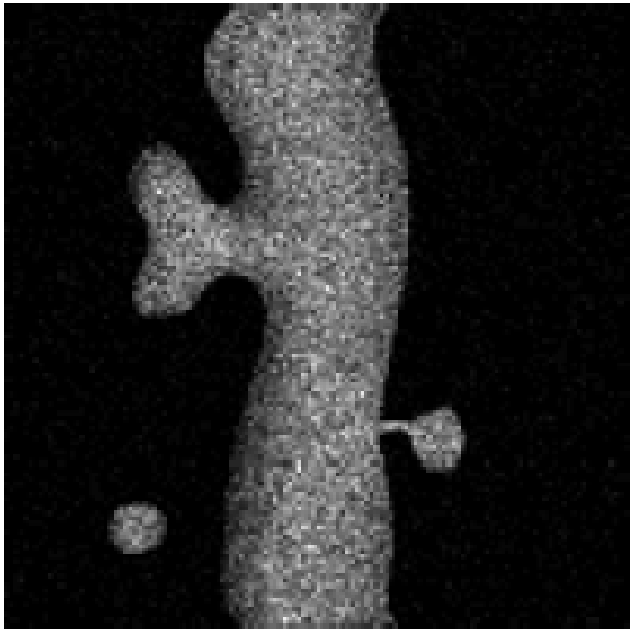




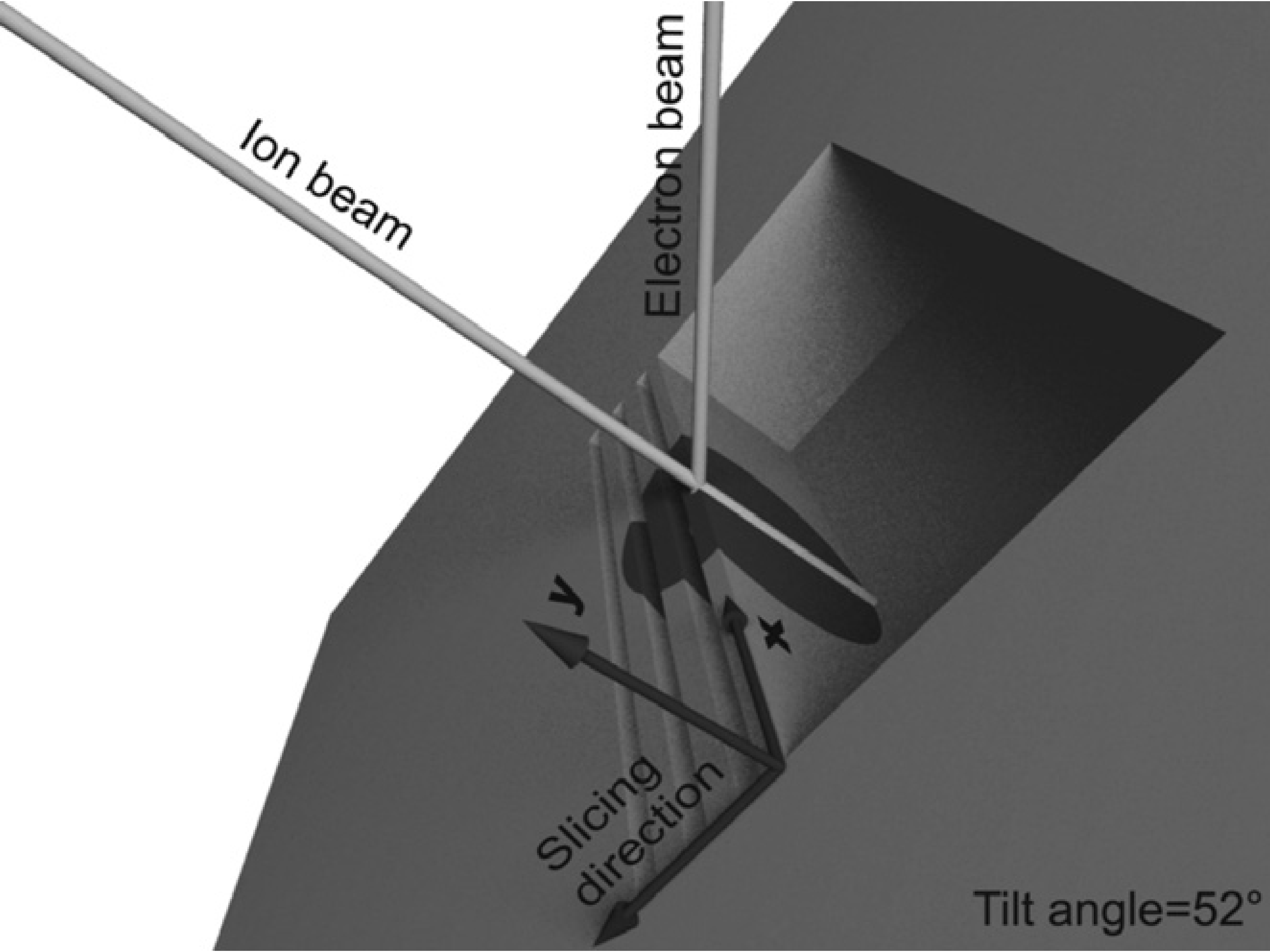
(a) Phantom.

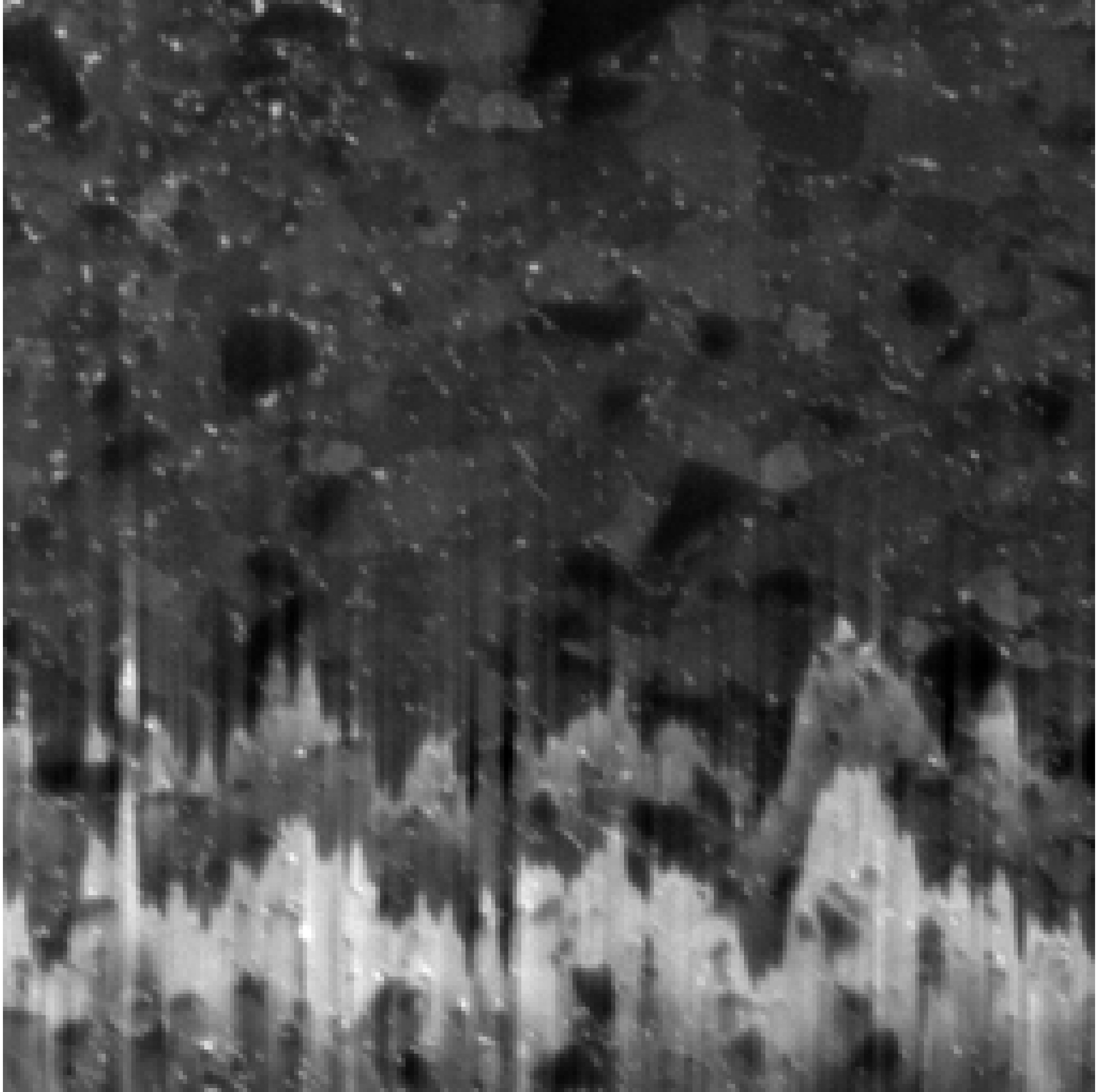


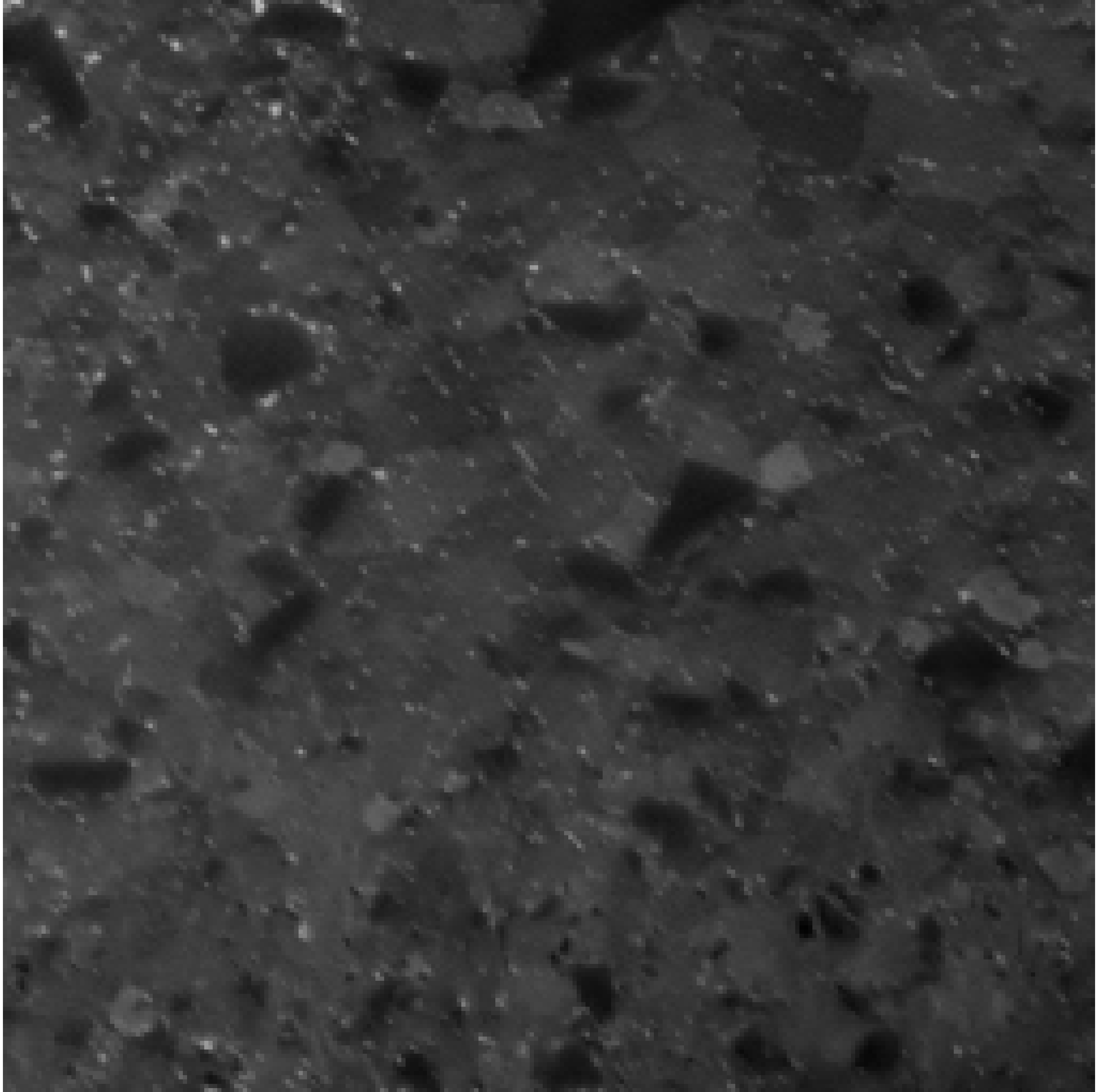
(b) Gaussian noise.

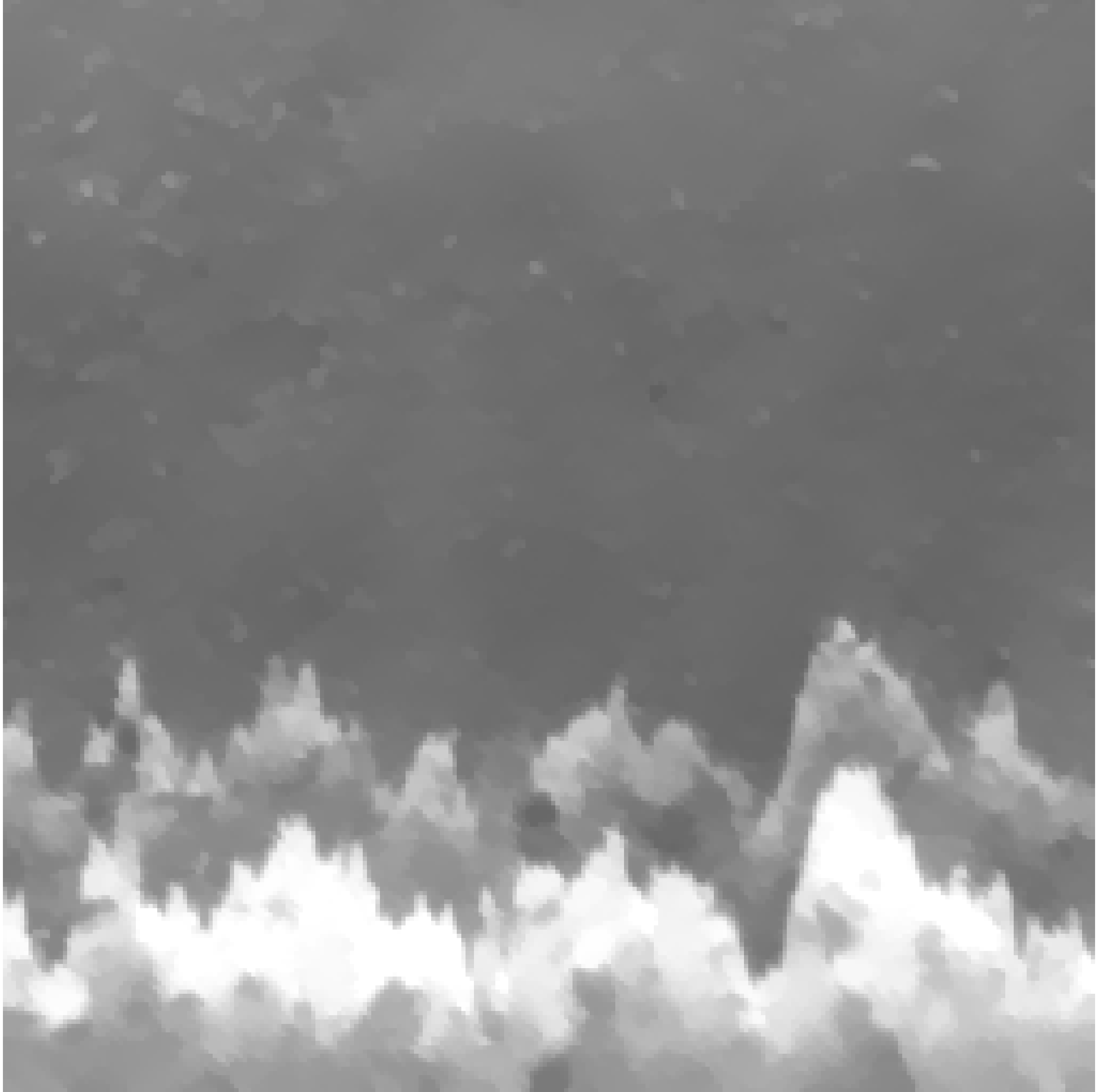


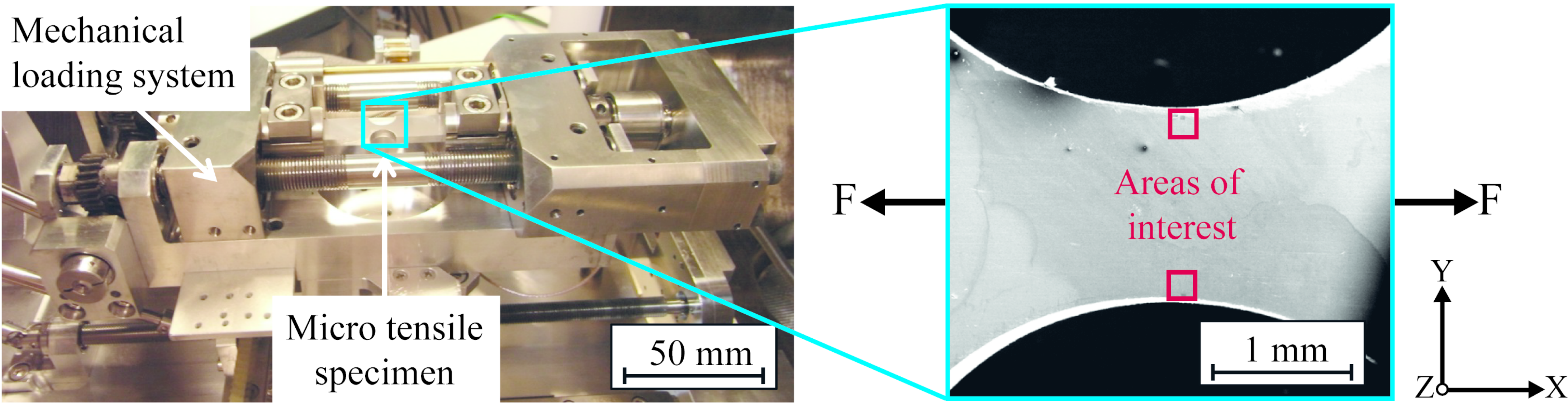
(c) Poisson noise


Ion beam
Electron beam
y
x
Slicing direction
Tilt angle=52°

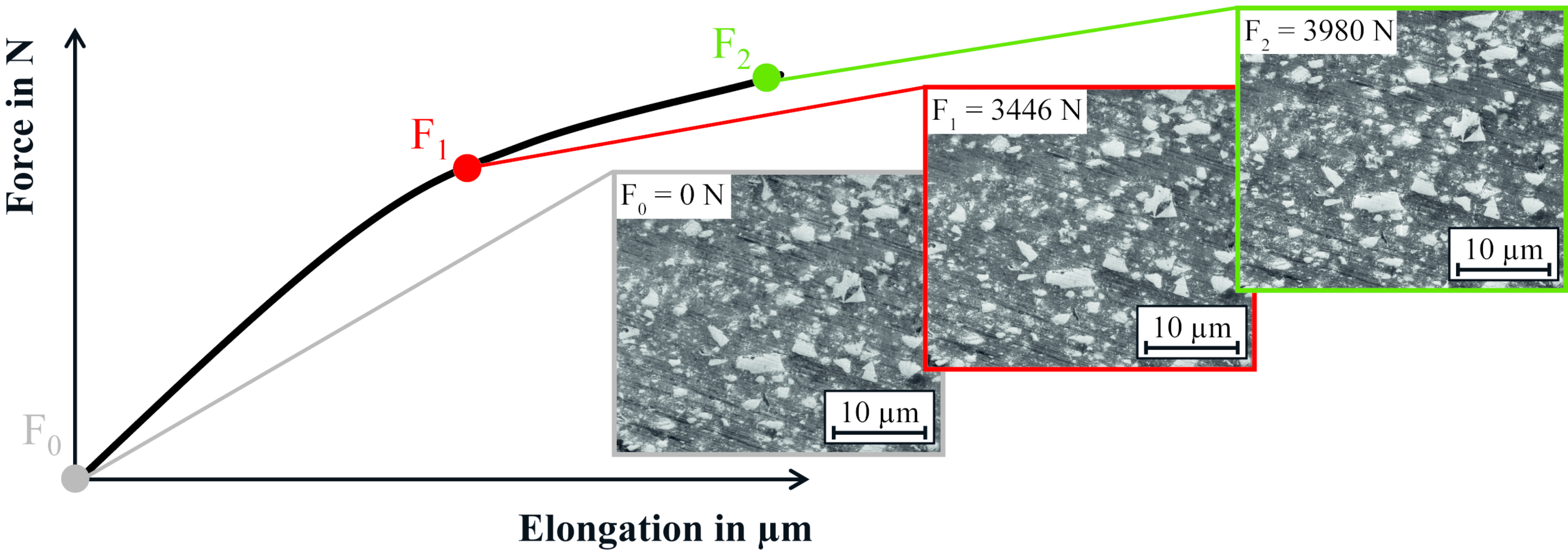




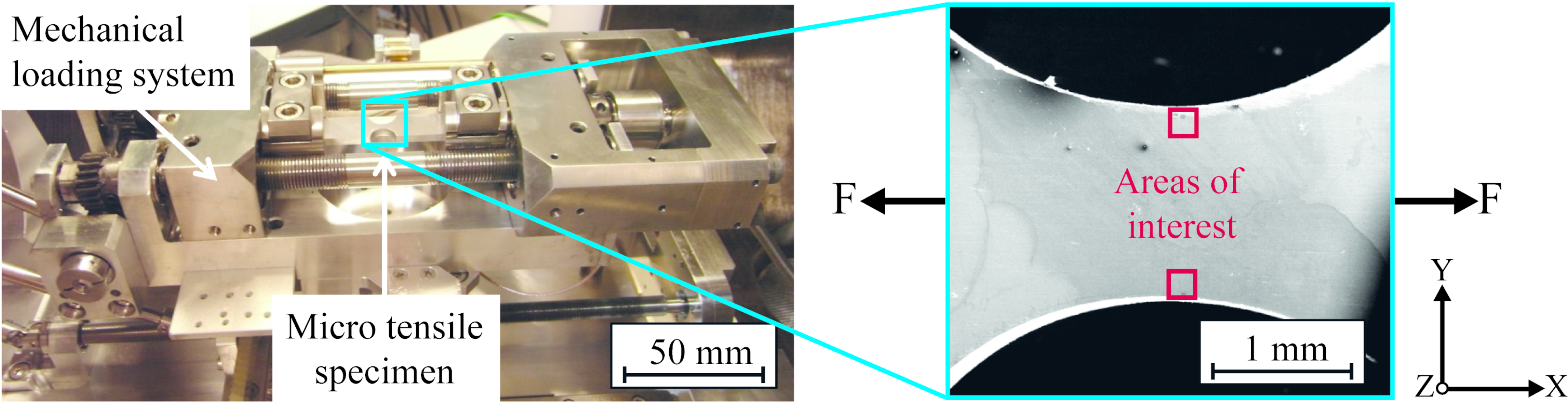


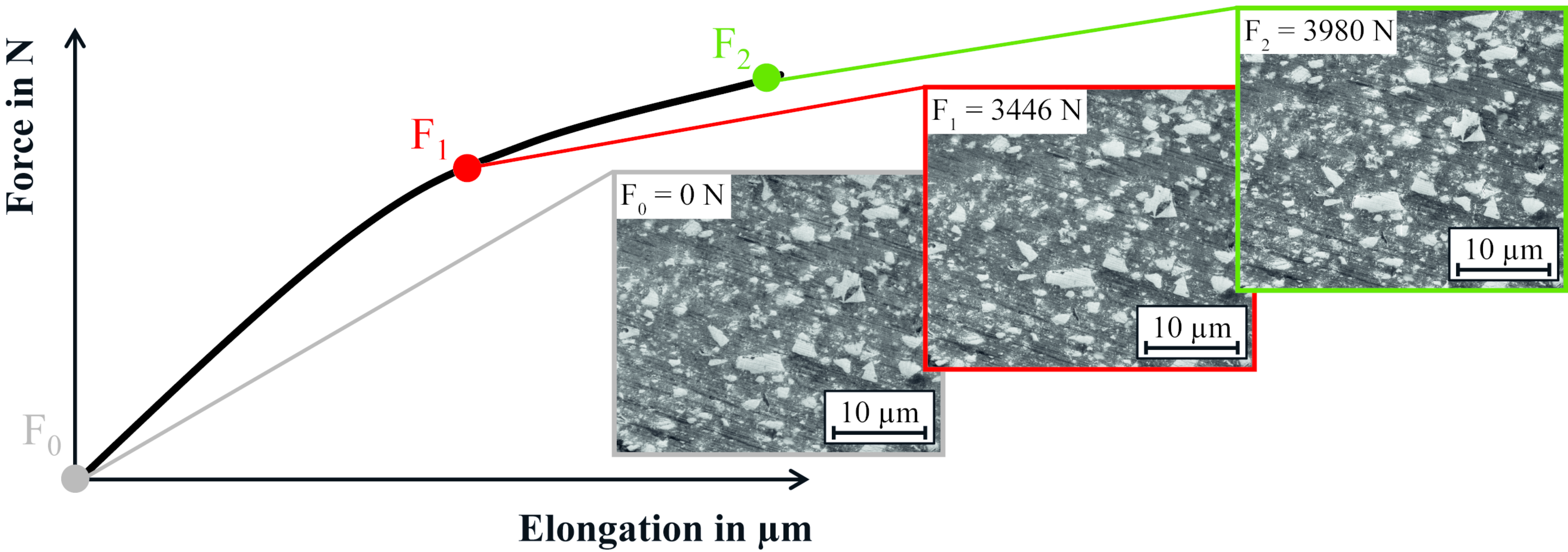


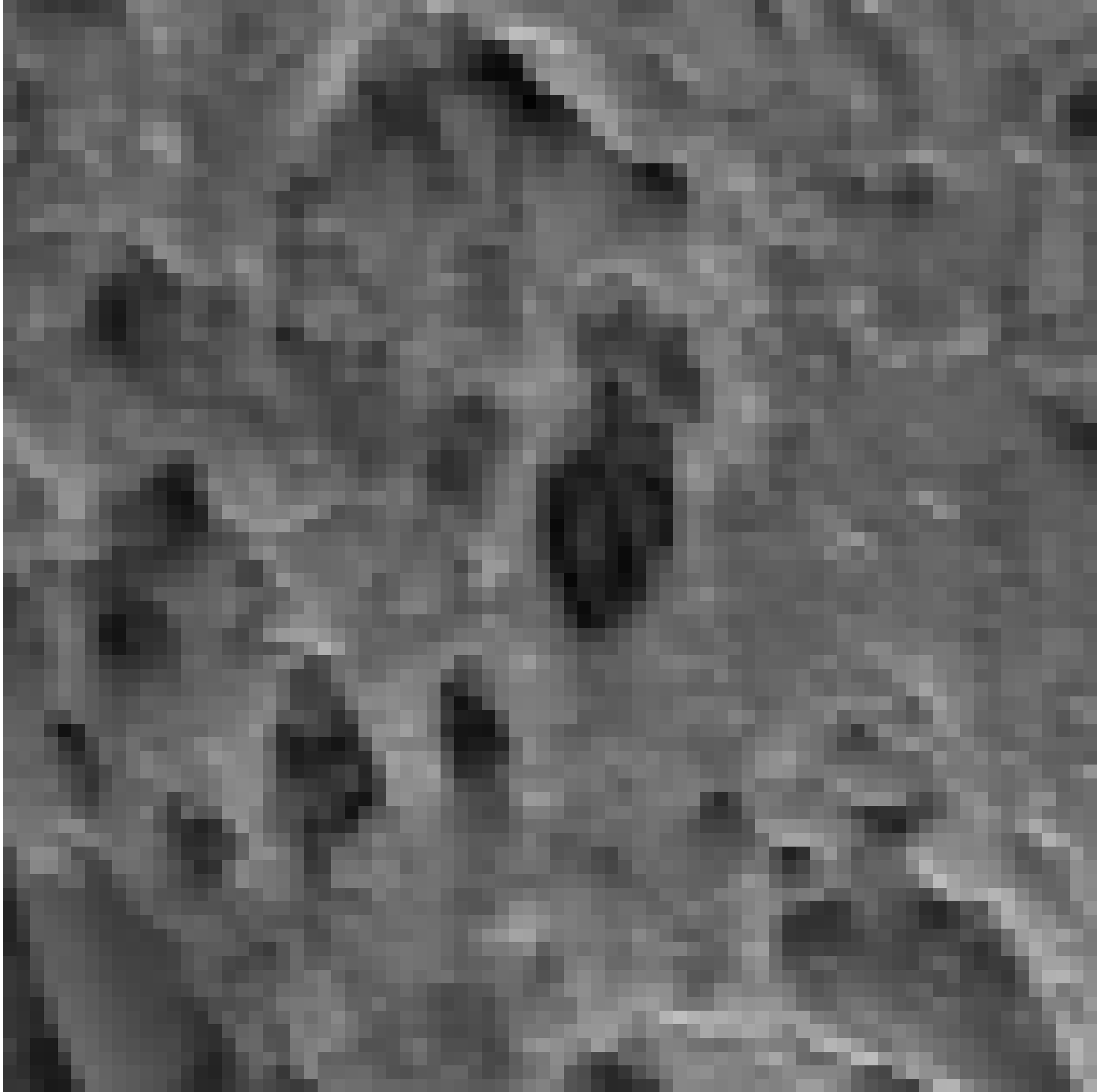
Mechanical loading system
Micro tensile specimen
50 mm
F
Areas of interest
1 mm
F
Y
Z
X

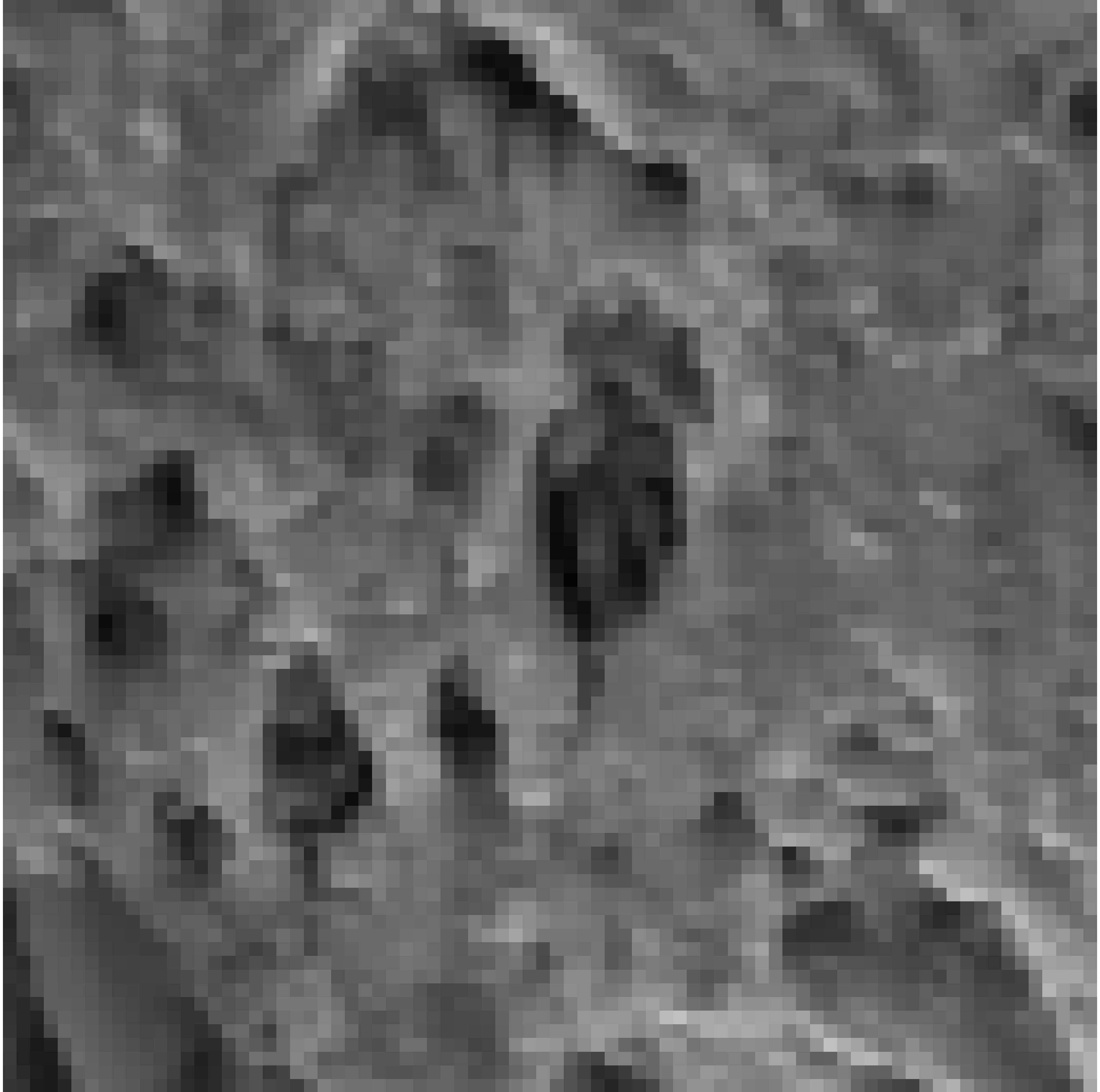


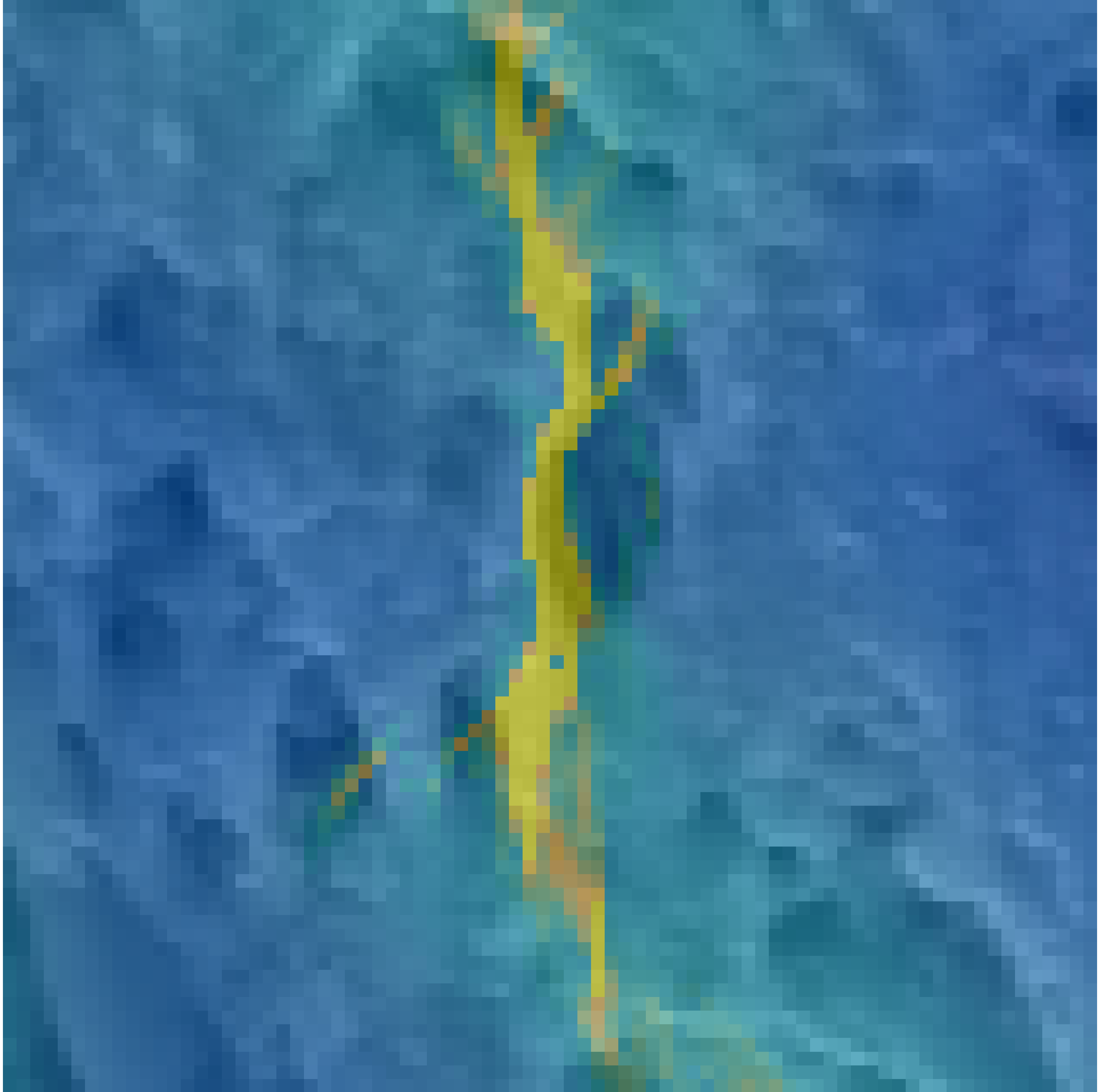
Force in N
Elongation in µm
F0
F1
F2
F0 = 0 N
F1 = 3446 N
F2 = 3980 N
10 µm
10 µm
10 µm

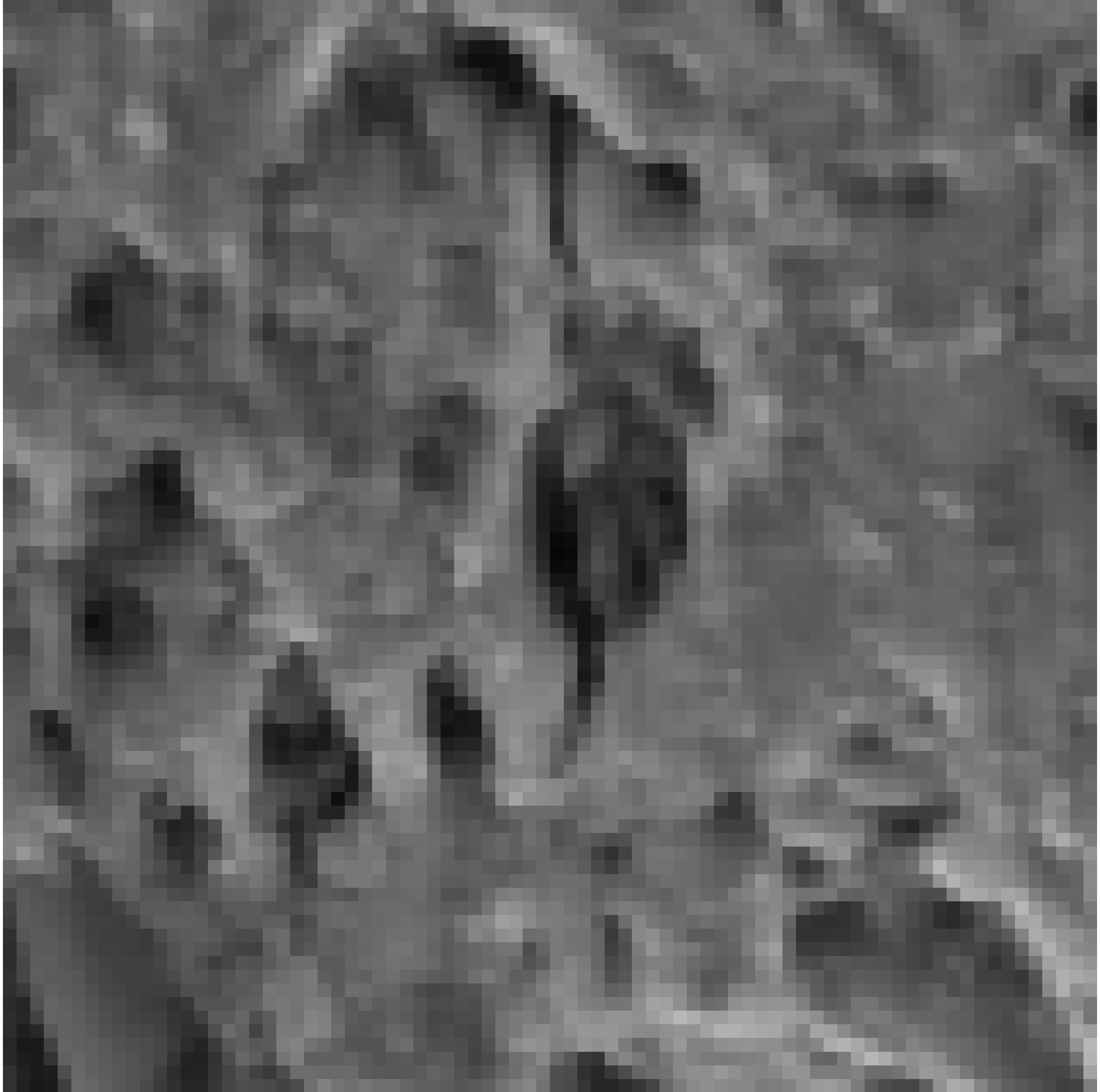

Mechanical
loading system
Micro tensile
specimen
50 mm
Areas of
interest
1 mm
F
F
Y
Z
X

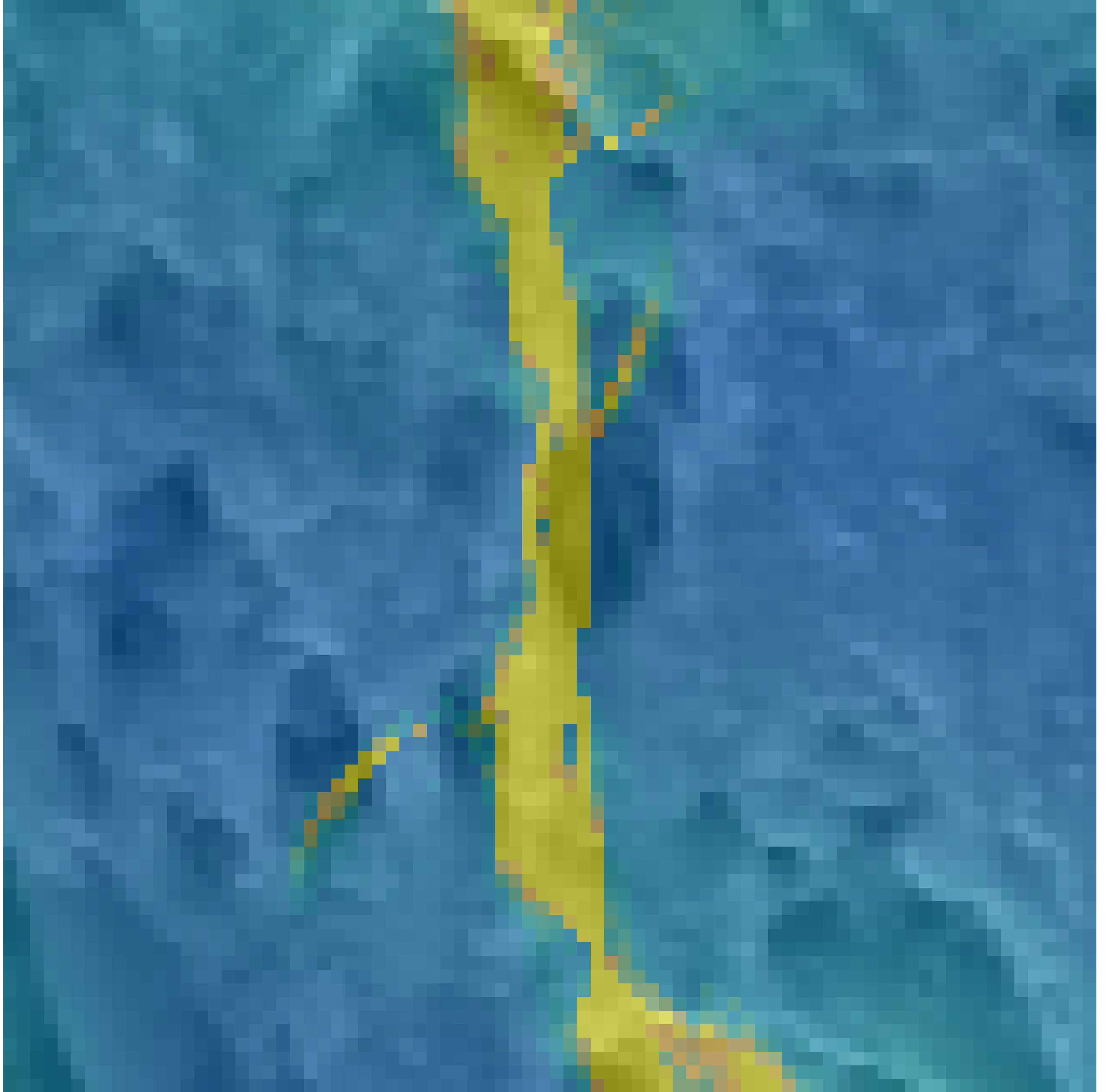

Force in N
Elongation in µm
F0
F1
F2
F0 = 0 N
F1 = 3446 N
F2 = 3980 N
10 µm
10 µm
10 µm

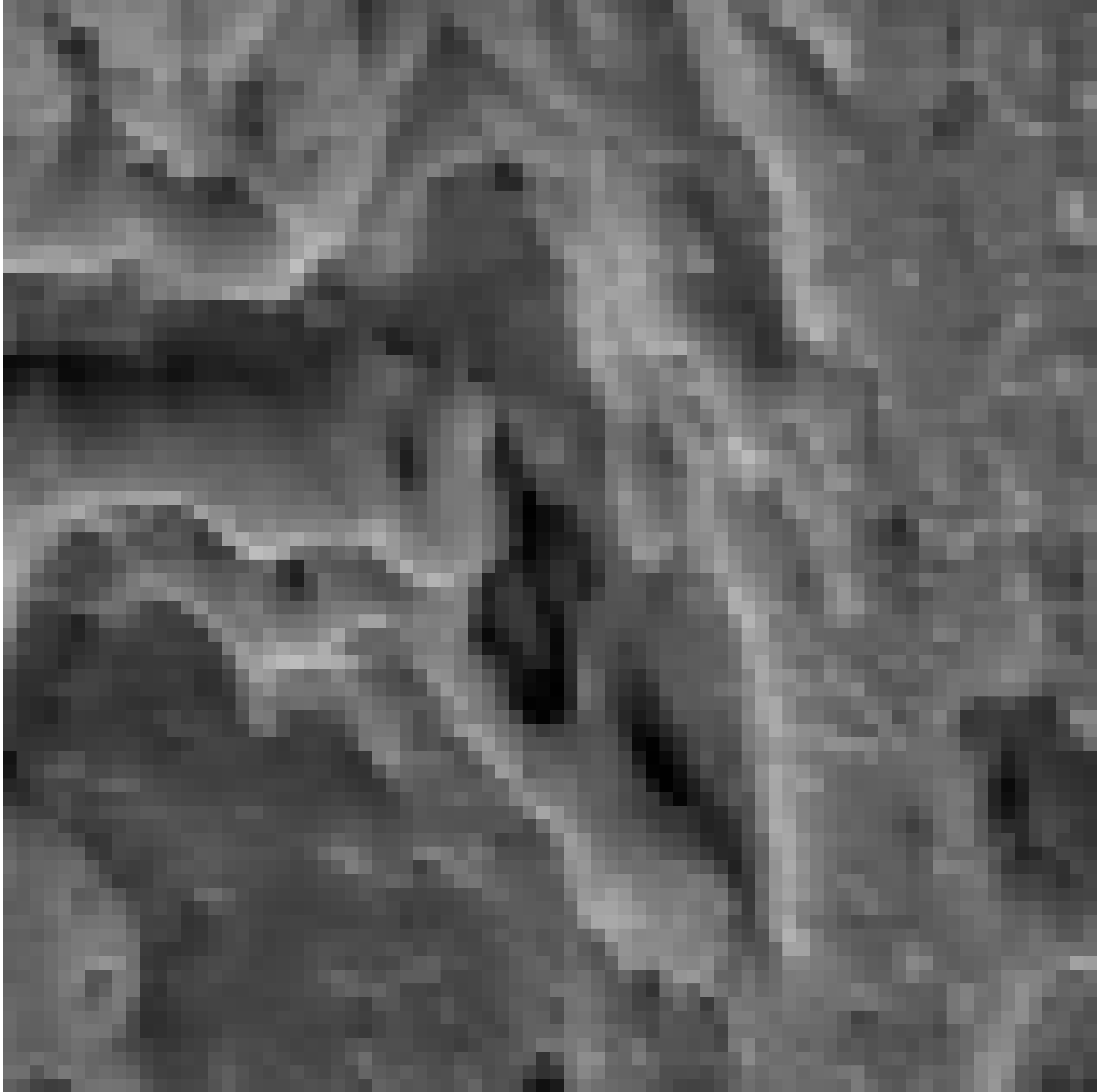


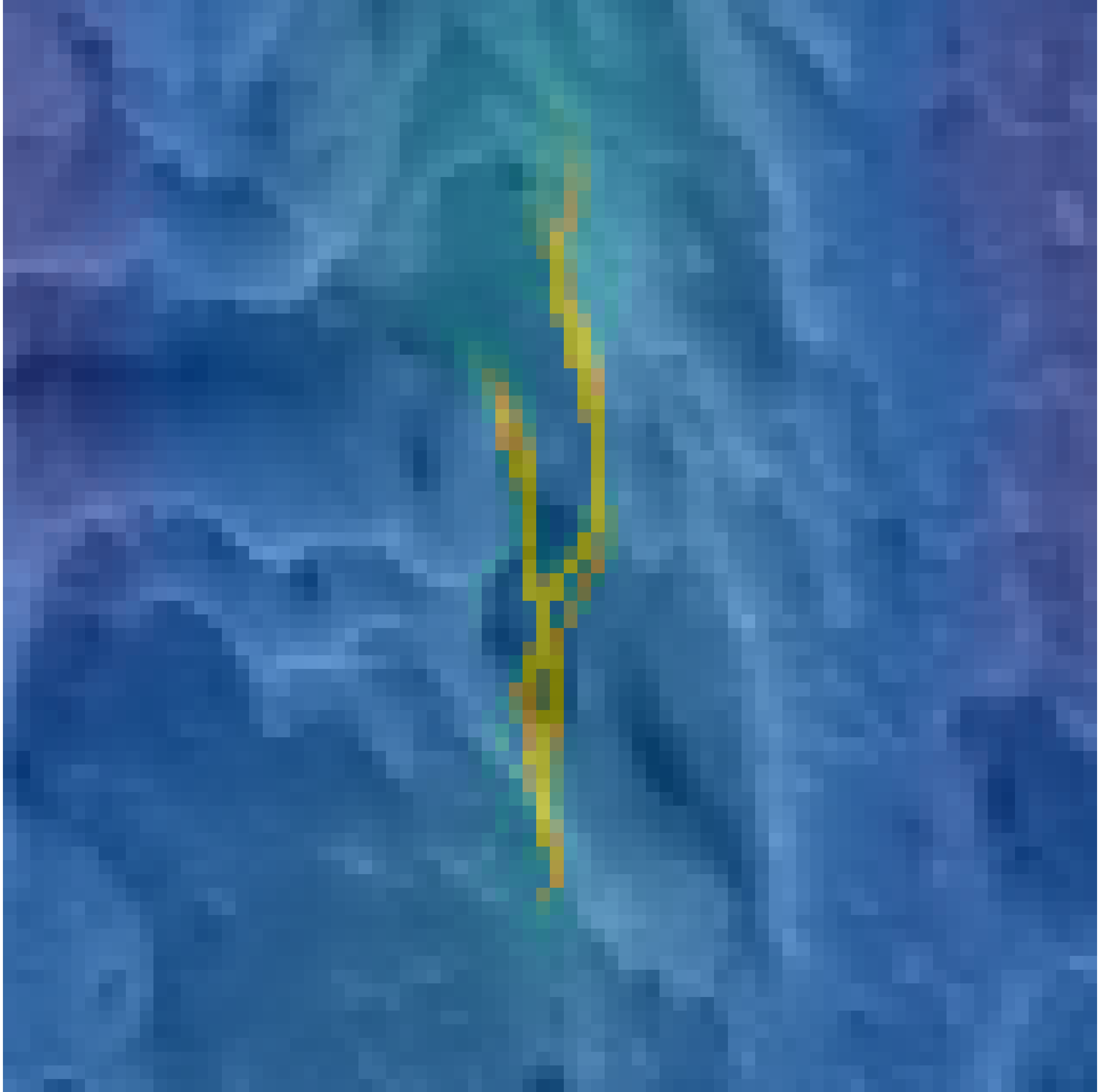


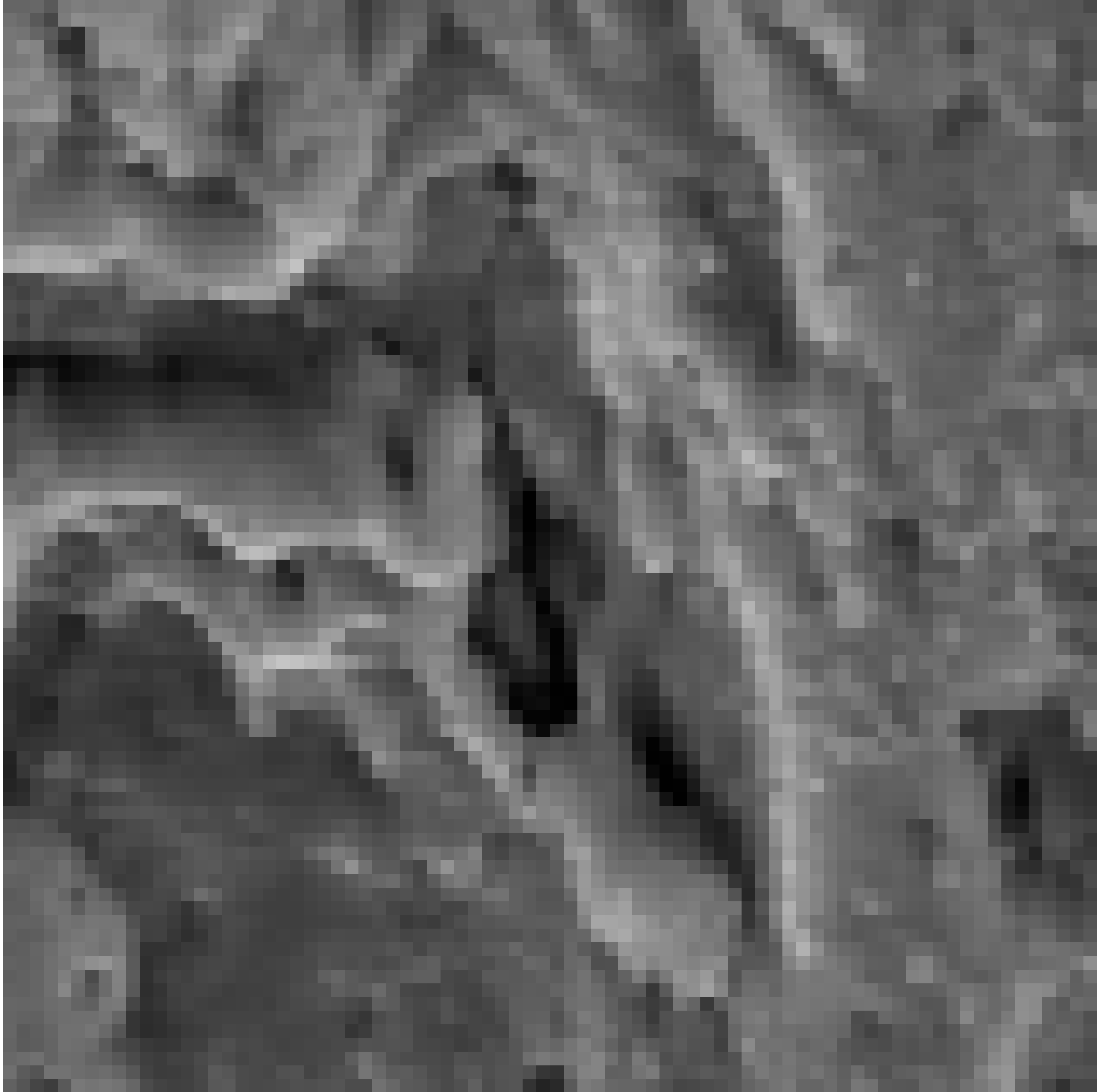


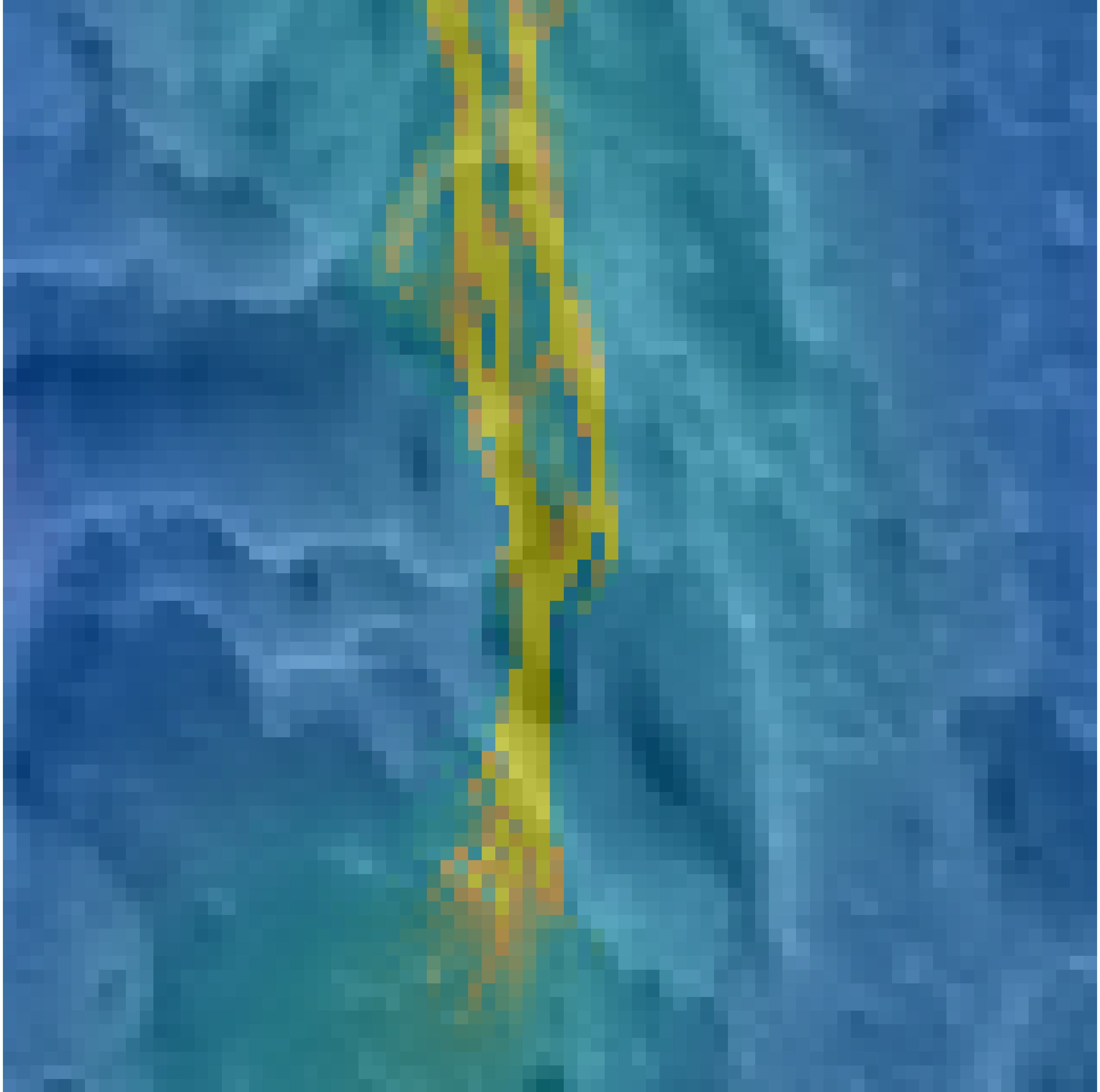


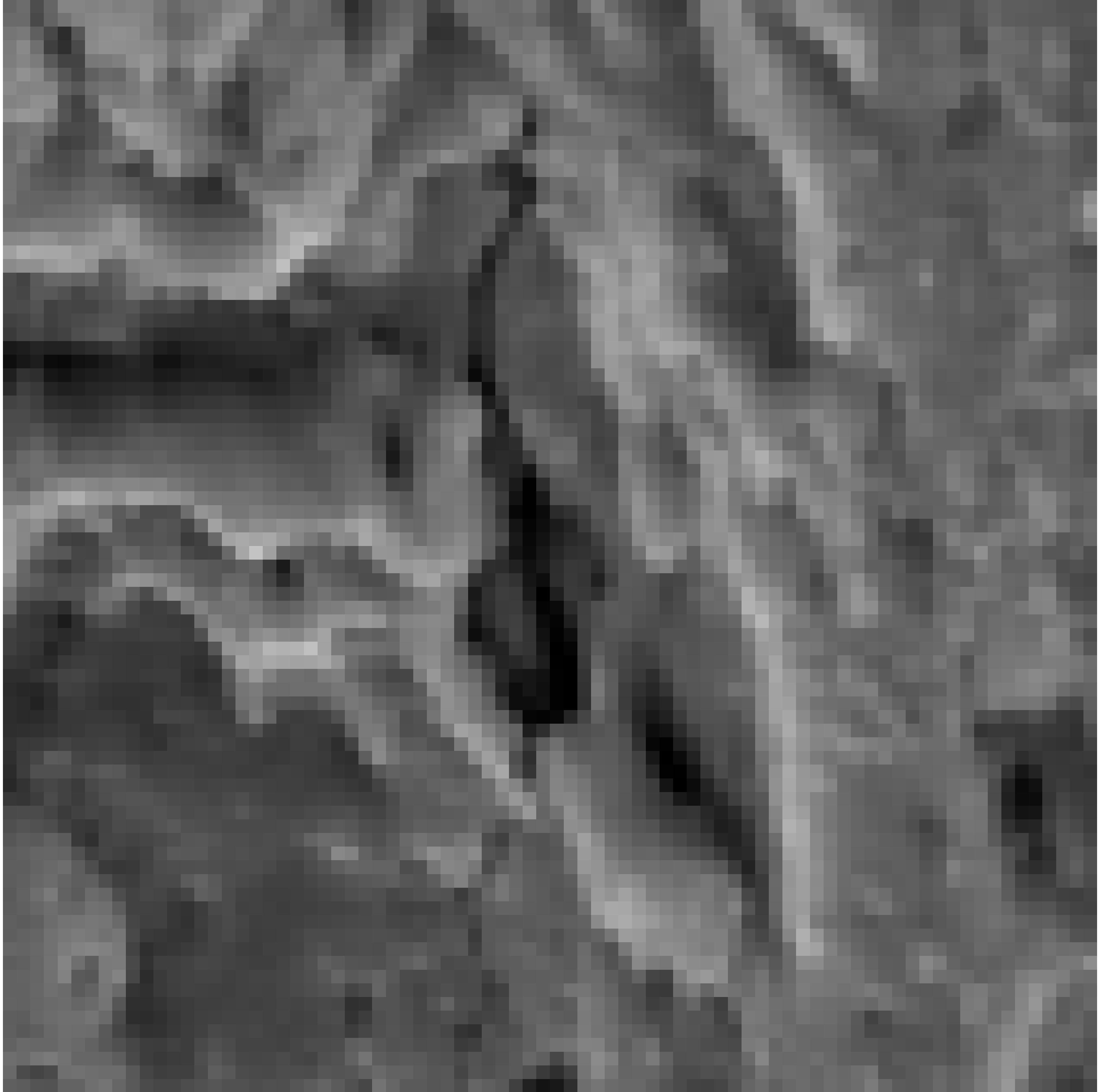


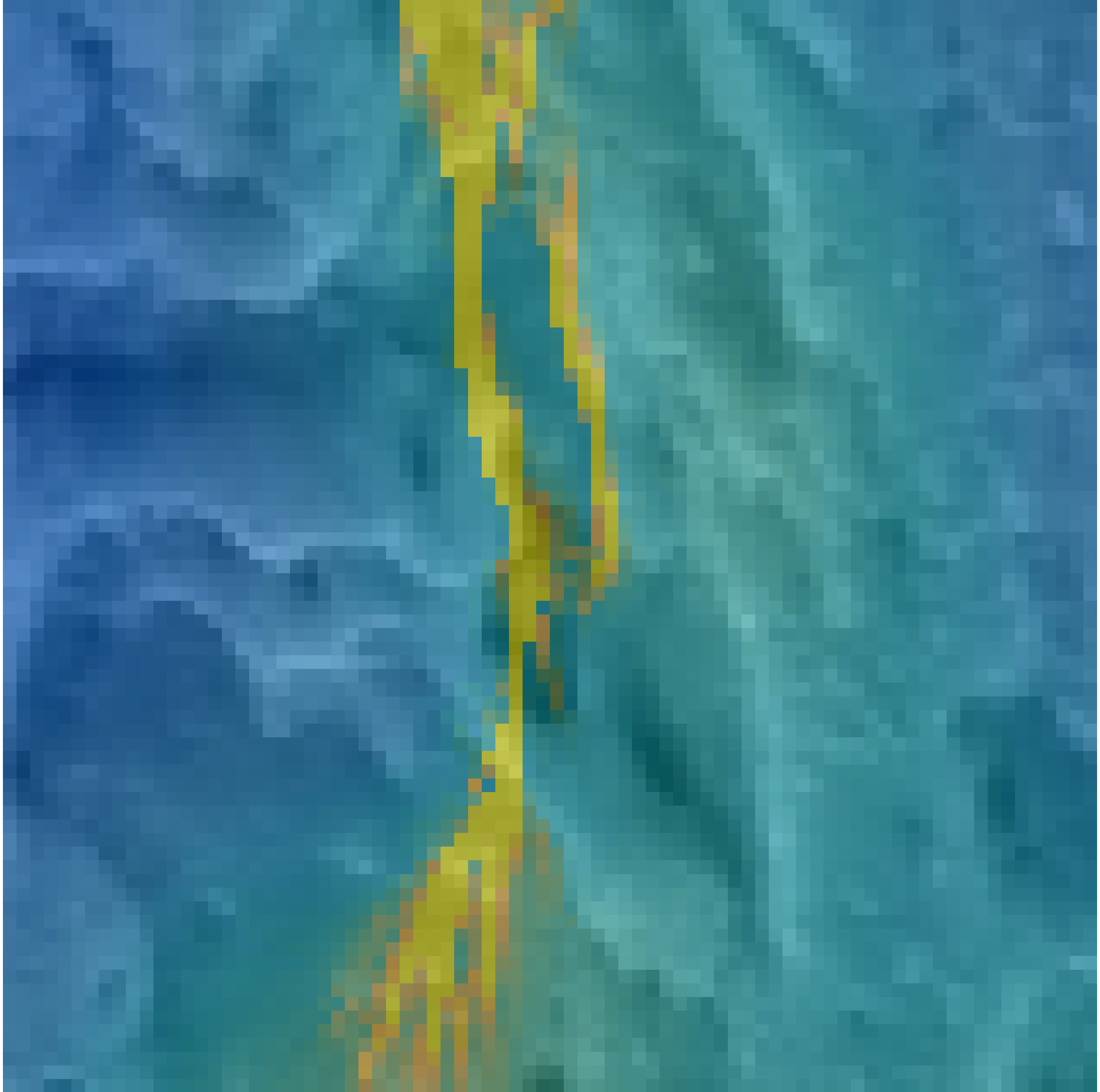












(a)

(b)

(c)

(d)

(e)

(f)

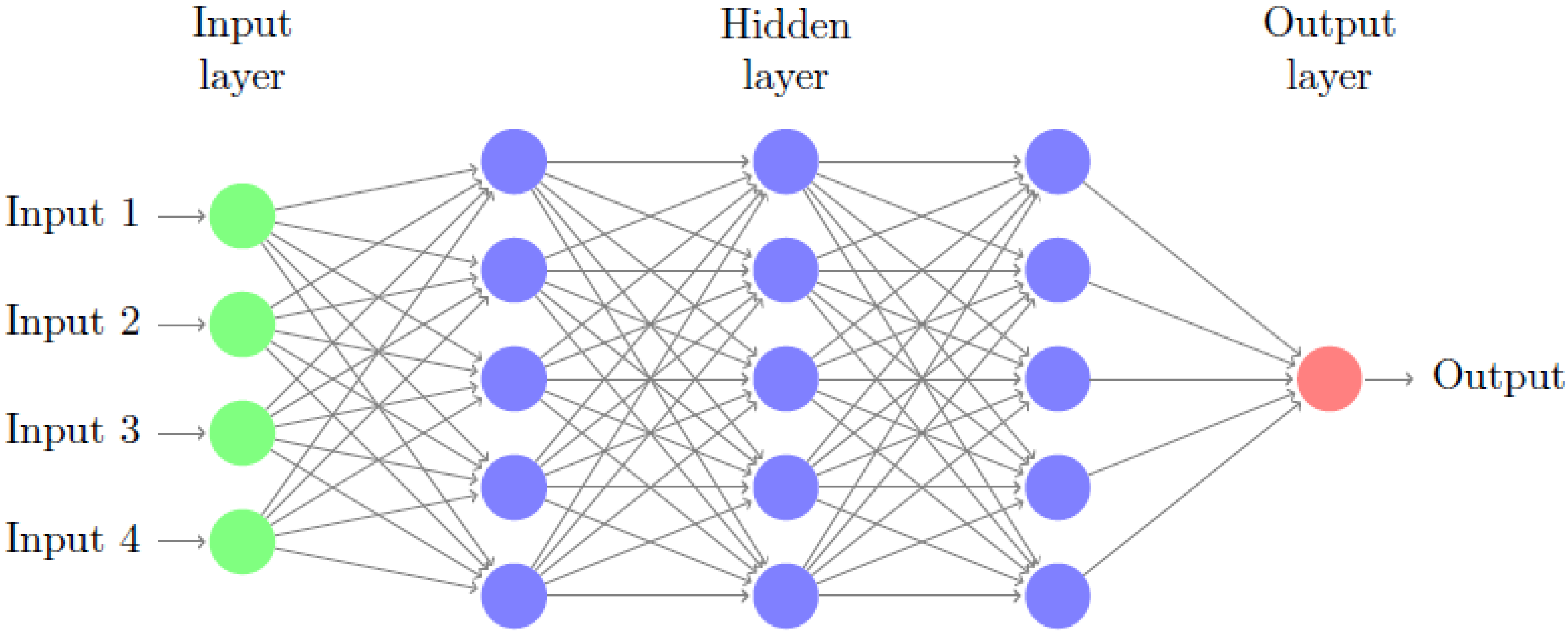
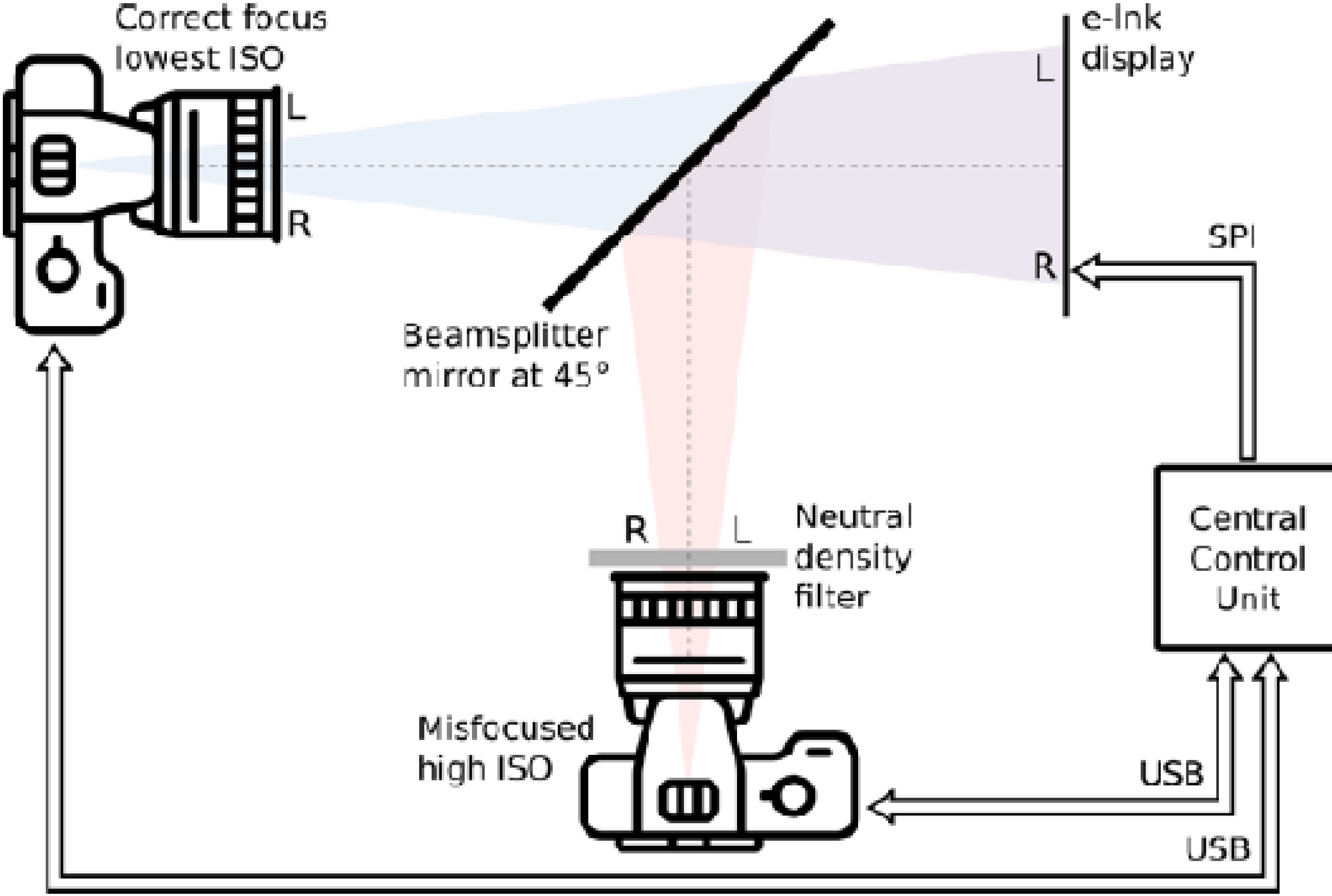
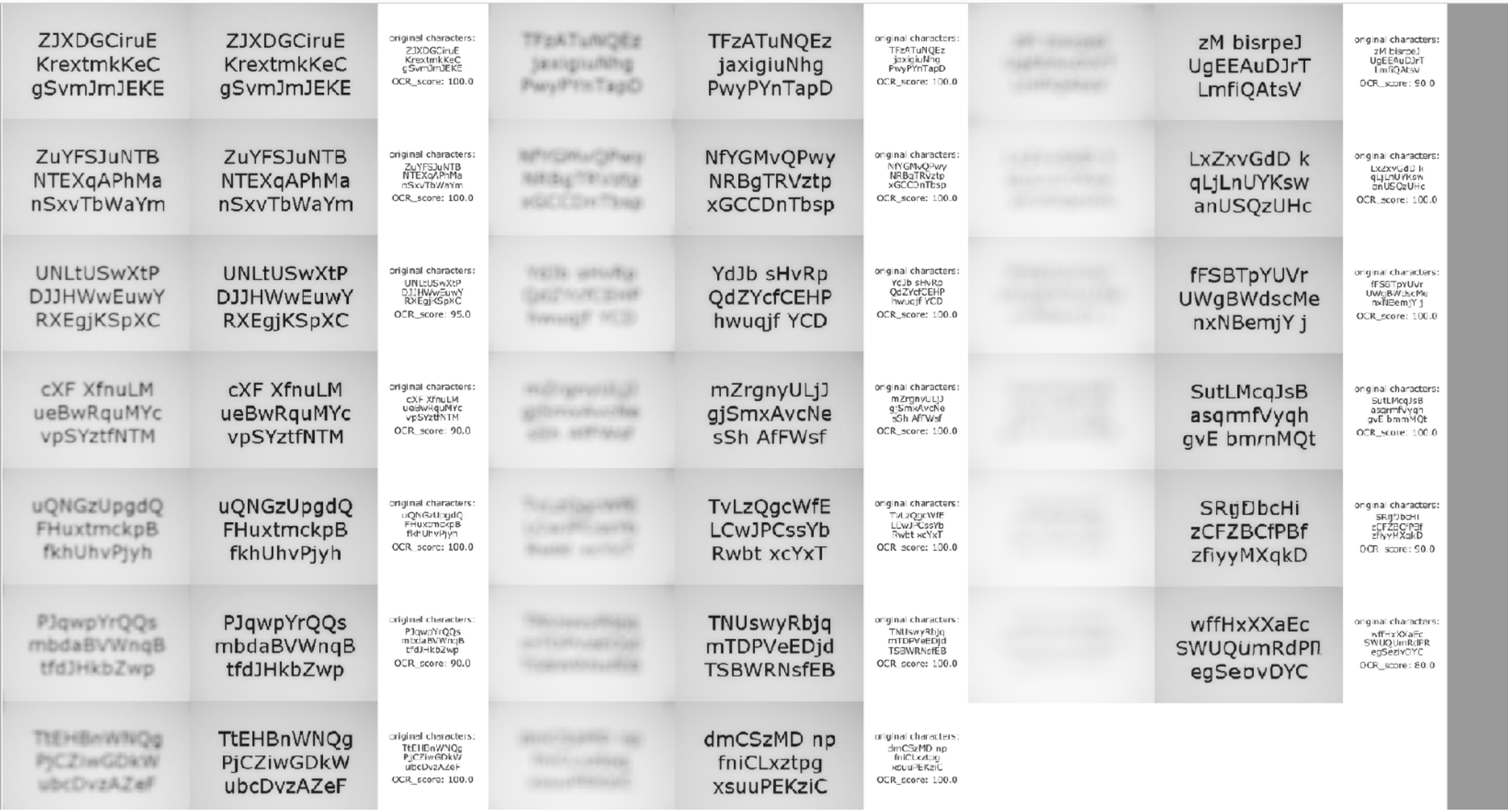
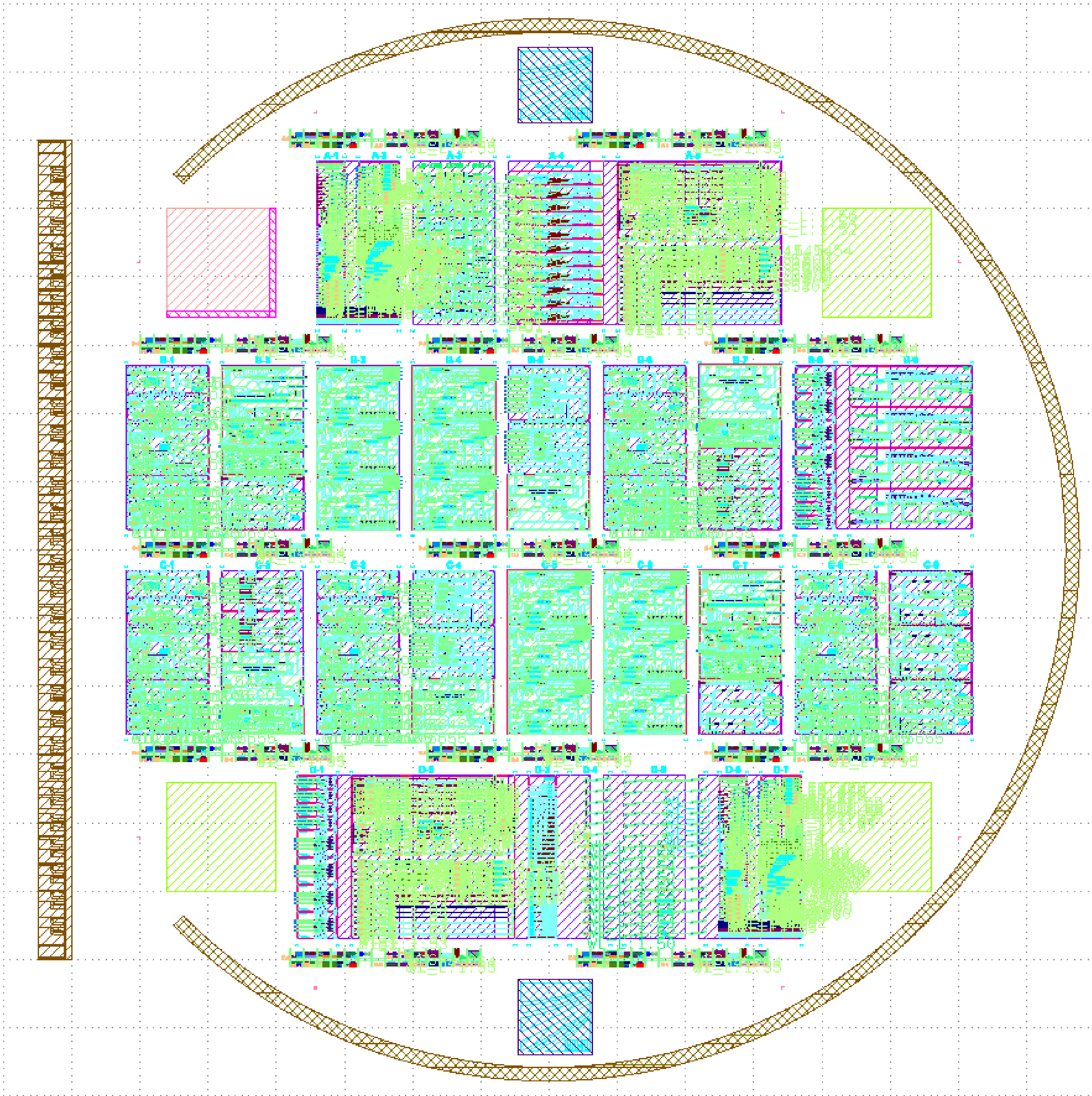


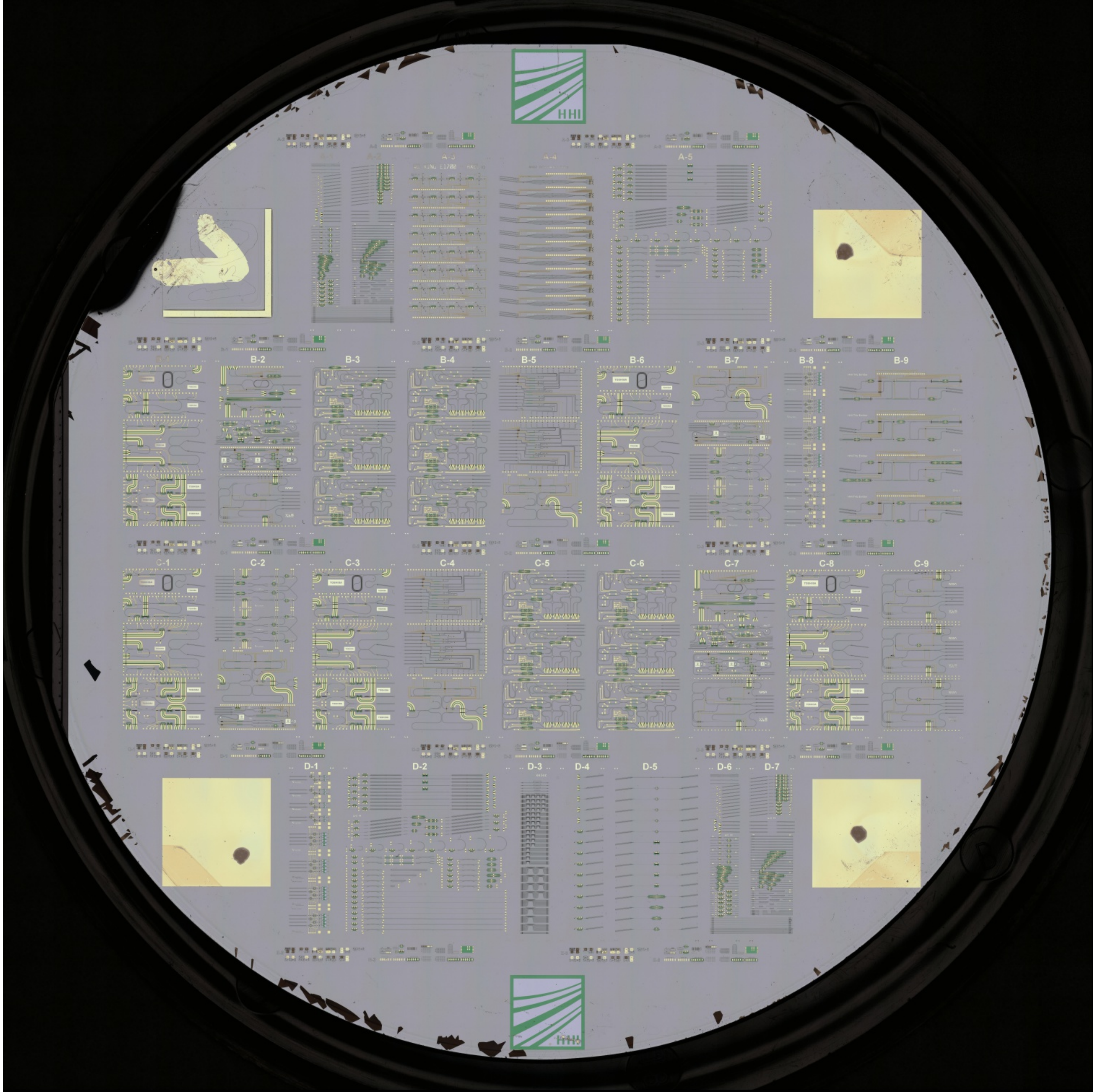

Figure 1: Model of a NN with three hidden layers, i.e., $d = 4$, $K = 4$, $n_1 = n_2 = n_3 = 5, n_4 = 1$.

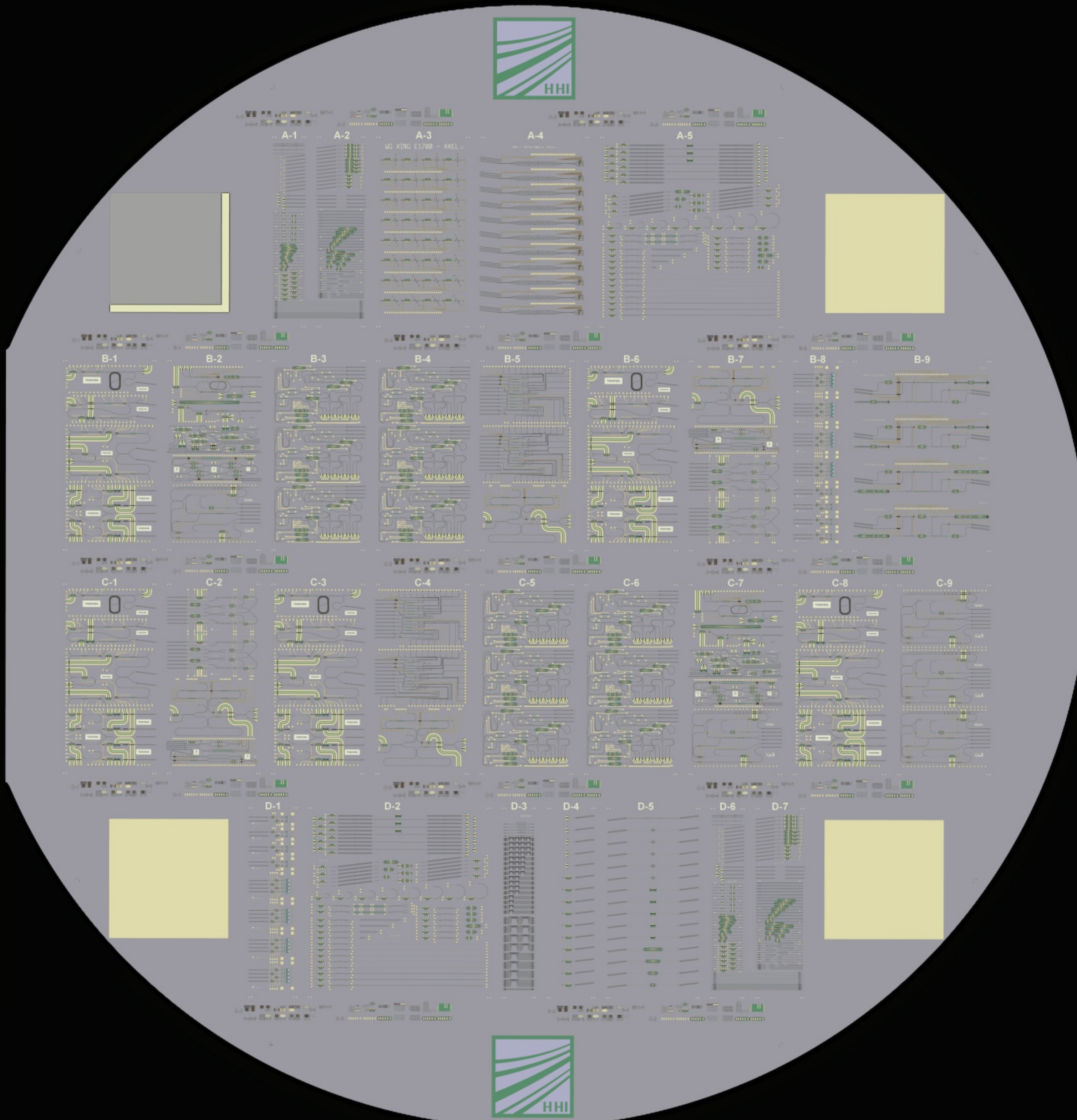


Correct focus
lowest ISO
L
R
Beamsplitter
mirror at 45°
e-Ink
display
L
R
SPI
R
L
Neutral
density
filter
Central
Control
Unit
Misfocused
high ISO
USB
USB


ZJXDGCiruE
KrextmkKeC
gSvmJmJEKE
ZJXDGCiruE
KrextmkKeC
gSvmJmJEKE
original characters:
ZJXDGCiruE
KrextmkKeC
gSvmJmJEKE
OCR_score: 100.0
TFzATuNQEz
jaxigiuNhg
PwyPYnTapD
original characters:
TFzATuNQEz
jaxigiuNhg
PwyPYnTapD
OCR_score: 100.0
zM bisrpeJ
UgEEAuDJrT
LmfiQAtsV
original characters:
zM bisrpeJ
UgEEAuDJrT
LmfiQAtsV
OCR_score: 90.0
ZuYFSJuNTB
NTEXqAPhMa
nSxvTbWaYm
ZuYFSJuNTB
NTEXqAPhMa
nSxvTbWaYm
original characters:
ZuYFSJuNTB
NTEXqAPhMa
nSxvTbWaYm
OCR_score: 100.0
NfYGMvQPwy
NRBgTRVztp
xGCCDnTbsp
original characters:
NfYGMvQPwy
NRBgTRVztp
xGCCDnTbsp
OCR_score: 100.0
LxZxvGdD k
qLjLnUYKsw
anUSQzUHc
original characters:
LxZxvGdD k
qLjLnUYKsw
anUSQzUHc
OCR_score: 100.0
UNLtUSwXtP
DJJHWwEuwY
RXEgjKSpXC
UNLtUSwXtP
DJJHWwEuwY
RXEgjKSpXC
original characters:
UNLtUSwXtP
DJJHWwEuwY
RXEgjKSpXC
OCR_score: 95.0
YdJb sHvRp
QdZYcfCEHP
hwuqjf YCD
original characters:
YdJb sHvRp
QdZYcfCEHP
hwuqjf YCD
OCR_score: 100.0
fFSBTpYUVr
UWgBWdscMe
nxNBemjY j
original characters:
fFSBTpYUVr
UWgBWdscMe
nxNBemjY j
OCR_score: 100.0
cXF XfnuLM
ueBwRquMYc
vpSYztfNTM
cXF XfnuLM
ueBwRquMYc
vpSYztfNTM
original characters:
cXF XfnuLM
ueBwRquMYc
vpSYztfNTM
OCR_score: 90.0
mZrgnyULjJ
gjSmxAvcNe
sSh AfFWsf
original characters:
mZrgnyULjJ
gjSmxAvcNe
sSh AfFWsf
OCR_score: 100.0
SutLMcqJsB
asqmfVyqh
gvE bmMQt
original characters:
SutLMcqJsB
asqmfVyqh
gvE bmMQt
OCR_score: 100.0
uQNGzUpgdQ
FHuxtmckpB
fkhUhvPjyh
uQNGzUpgdQ
FHuxtmckpB
fkhUhvPjyh
original characters:
uQNGzUpgdQ
FHuxtmckpB
fkhUhvPjyh
OCR_score: 100.0
TvLzQgcWfE
LCwJPCssYb
Rwbt xcYxT
original characters:
TvLzQgcWfE
LCwJPCssYb
Rwbt xcYxT
OCR_score: 100.0
SRgDbcHi
zCFZBCfPBf
zfiyyMXqkD
original characters:
SRgJDbcHi
zCFZBCfPBf
zfiyyMXqkD
OCR_score: 90.0
PJqwpYrQQs
mbdaBVWnqB
tfdJHkbZwp
PJqwpYrQQs
mbdaBVWnqB
tfdJHkbZwp
original characters:
PJqwpYrQQs
mbdaBVWnqB
tfdJHkbZwp
OCR_score: 90.0
TNUswyRbjq
mTDPVeEDjd
TSBWRNsfEB
original characters:
TNUswyRbjq
mTDPVeEDjd
TSBWRNsfEB
OCR_score: 100.0
wffHxXXaEc
SWUQUmRdPR
egSeovDYC
original characters:
wffHxXXaEc
SWUQUmRdPR
egSezvDYC
OCR_score: 80.0
TtEHBnWNQg
PjCZiwGDkW
ubcDvzAZeF
TtEHBnWNQg
PjCZiwGDkW
ubcDvzAZeF
original characters:
TtEHBnWNQg
PjCZiwGDkW
ubcDvzAZeF
OCR_score: 100.0
dmCSzMD np
fniCLxztpg
xsuuPEKziC
original characters:
dmCSzMD np
fniCLxztpg
xsuuPEKziC
OCR_score: 100.0




HHI
A-3
A-4
A-5
B-2
B-3
B-4
B-5
B-6
B-7
B-8
B-9
C-1
C-2
C-3
C-4
C-5
C-6
C-7
C-8
C-9
D-1
D-2
D-3
D-4
D-5
D-6
D-7
HHI


HHI
A-1
A-2
A-3
WG XING E1700 - AXEL
A-4
A-5
B-1
B-2
B-3
B-4
B-5
B-6
B-7
B-8
B-9
C-1
C-2
C-3
C-4
C-5
C-6
C-7
C-8
C-9
D-1
D-2
D-3
D-4
D-5
D-6
D-7
HHI