In [1]:

```
import discretisedfield as df
import micromagneticmodel as mm
import oommfc as mc
import math
import numpy as np
import matplotlib.pyplot as plt
%env OOMMFTCL=E:\oommf/oommf.tcl
```

```
env: OOMMFTCL=E:\oommf/oommf.tcl
```

In [2]:

```
from scipy.spatial import cKDTree
import numpy as np

A = 10e-10
Ms = 700e3
d = 30e-9

p1 = (-36e-9, -36e-9, -15e-9)
p2 = (36e-9, 36e-9, 15e-9)
region = df.Region(p1=p1, p2=p2)
grains_mesh = df.Mesh(region=region, cell=((2*d)/5, (2*d)/5, (d)/6))
# grains with size of # x= 2*d/5, y = (2*d)/5, z = (2*d)/5
```

In [3]:

```
all_grains_centres = list(grains_mesh)  # This extracts cell centre points of grains
all_grains_centres
```

Out[3]:

```
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```

In [4]:

```
grain_centres_originals = np.array(all_grains_centres)
grain_centres_originals
```

Out[4]:

```
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```

In [5]:

```
#number of grains
num_rows,num_cols = grain_centres_originals.shape
Ngrains = num_rows
print(num_rows, num_cols)
print(Ngrains)
```

```
216 3
216
```

In [6]:

```
# we will displace the grain centers randomly to make noncubic grains
np.random.seed(10)
increament = np.random.uniform(-3e-9, 3e-9, size=(Ngrains,3))
increament
```

Out[6]:

```
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In [7]:

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grain_centres
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Out[7]:
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```

In [8]:

```
# Create positions to be grain centres, and create a cKDTree to
# perform Voronoi Tesselation
voronoi_kdtree = cKDTree(grain_centres)


# Generate random anisotropy axes
axes = np.random.uniform(-1, 1, (Ngrains, 3))
axes
```

Out[8]:

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```

In [9]:

```
# Weight them towards +z - assume grains oriented along field cooled direction
axes[:, 0] += 1.0
axes
```

Out[9]:
```
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```

In [10]:

```
# Normalise
axes /= np.linalg.norm(axes, axis=1)[:, np.newaxis]
axes
```

Out[10]:

```
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       [ 0.4924237 , -0.13394174, -0.85998751]])
```

In [11]:

```python
Ku = 200
# Generate a normal distribution of anisotropy strengths:
strengths = np.random.normal(Ku, Ku*0.2, Ngrains)
strengths
```

Out[11]:

```
array([199.68683138, 214.61064965, 183.99888069, 245.30101949,
       196.0553483 , 191.55911227, 136.790491  , 162.81343104,
       176.08385563, 142.68117347, 181.32165727, 164.23420921,
```

```
        67.29323791, 235.81118334, 247.9851759 , 215.26418407,
       203.60691456, 198.50205522, 106.67303877, 197.32201663,
       141.87563589, 161.14083712, 144.09646869, 203.43568348,
       306.02759524, 180.60320941, 254.80396905, 218.1880466 ,
       263.14213107, 247.84720282, 126.43301685, 244.37525267,
       221.92710053, 153.93118017, 216.38861585, 142.88049958,
       207.83573288, 246.32810093, 209.57411725, 151.71450788,
       188.0987921 , 213.92581781, 232.73147324, 208.02002786,
       185.37841729, 177.83343918, 219.26819357, 265.38010698,
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       259.78150441, 197.01521348, 243.74106516, 187.58042045,
       194.20101932, 257.65903504, 149.05339615, 209.60829707,
       177.14039176, 211.61689026, 204.87769841, 292.702283  ,
       214.10451829, 151.4759896 , 183.78650502, 228.67153505,
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       155.76278789, 177.15240483, 203.47493074, 128.80812684,
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       176.50948697, 260.478154  , 230.19645523, 147.48175575,
       202.19109608, 178.60772017, 232.25563975, 229.98192578,
       255.17352519, 181.13621546, 188.98771939, 209.5526897 ,
       214.02098771, 174.1337488 , 228.59350969, 197.07488642,
       101.51109684, 103.55073713, 160.16212151, 261.11560699,
       236.48038548, 213.41327831, 183.77493625, 195.5647055 ,
       222.40641506, 184.90727673, 251.78916024, 260.37491834,
       244.13325031, 176.31925115, 194.6479831 , 197.60916481,
       211.72249504, 143.56674292, 250.17030964, 164.38893684,
       206.84054176, 202.35021521, 191.69361585, 246.54343181,
       214.76864045, 236.19095685, 230.49249392, 172.73770084,
       255.11293842, 247.38219164, 160.71746901, 189.98156723,
       187.21316136, 212.89570027, 218.71647976, 292.96194982,
       167.04189135, 187.91522062, 249.4373394 , 247.62776691,
       170.00415881, 232.60888093, 185.48474323, 225.72913656,
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       286.61049956, 155.04346036, 122.1793456 , 195.07955779,
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       262.79710025, 203.14115261, 201.5566807 , 142.73463635,
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       214.01772025, 297.92019215, 168.64898674, 230.60989231,
       228.23840177, 228.9194733 , 270.33891698, 177.87562637,
       175.75883694, 207.61890458, 225.62808322, 149.71188911,
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       201.99169461, 240.83927712, 122.55186849, 182.8645536 ,
       145.16654836, 191.69089547, 234.9990571 , 176.92118729,
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       196.89553216, 126.18694535, 219.94156267, 190.71193488,
       142.8932122 , 164.78849095, 128.95982345, 282.34109438,
       136.82990652, 276.56402917, 186.03407502, 204.24566886,
       213.24403286, 240.47623362, 131.3273767 , 206.73727876])
```

In [12]:

```python
# We then use the cKDTree in two functions. We get the x, y position
# of each micromagnetic cell, and query the tree for the region that
# the cell sits in. The functions then return the axis and strength
# at that region index.

def K_axis(pos):
    x, y, z = pos
    _, test_point_regions = voronoi_kdtree.query(np.array([[x, y, z]]), k=1)
    region = test_point_regions[0]
    return axes[region]
```

```
def K_mag(pos):
    x, y, z = pos
    _, test_point_regions = voronoi_kdtree.query(np.array([[x, y, z]]), k=1)
    region = test_point_regions[0]
    return strengths[region]

#def A_fun(pos): # not complete yet. need a proper function
   # x, y, z = pos
    #if x, y ,z # within grain:
     #   return 1e-12
    #else: # at the boundries or between grains
     #   return 0.5e-15


#A = df.Field(mesh, dim=1, value=A_fun)
```

In [13]:

```
#after difining the grains with random anisotropy and desired size,
#now lets us decrease the cell size for micromagnetic calculations and make mesh

mesh = df.Mesh(region=region, cell=(2e-9, 2e-9, 3e-9))  # 2nm cell size
```

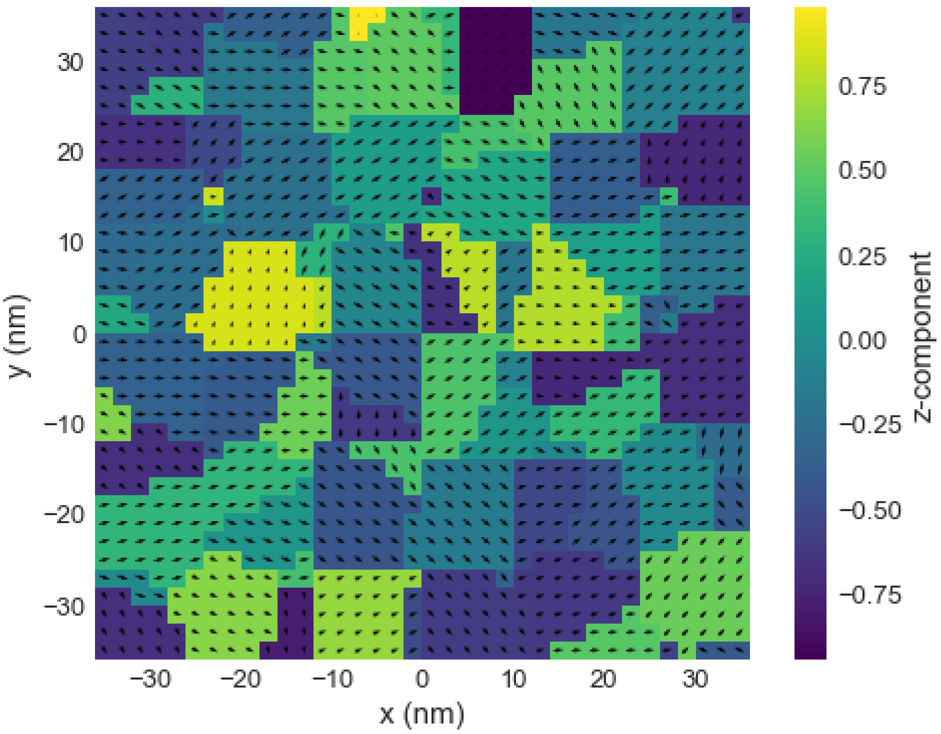
In [14]:

```
K  = df.Field(mesh, dim=3, value=K_mag)
u  = df.Field(mesh, dim=3, value=K_axis)

# uniaxial anisotropy axis
system = mm.System(name='grain1')
system.energy = mm.UniaxialAnisotropy(K=K, u=u)
```

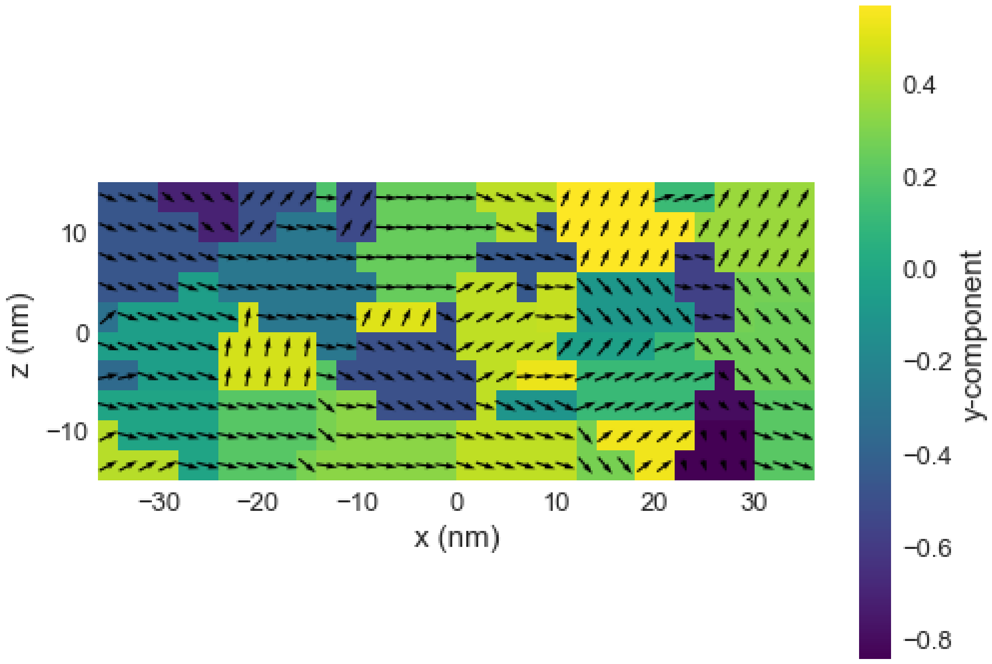
In [15]:

```
u.plane('z').mpl()
```

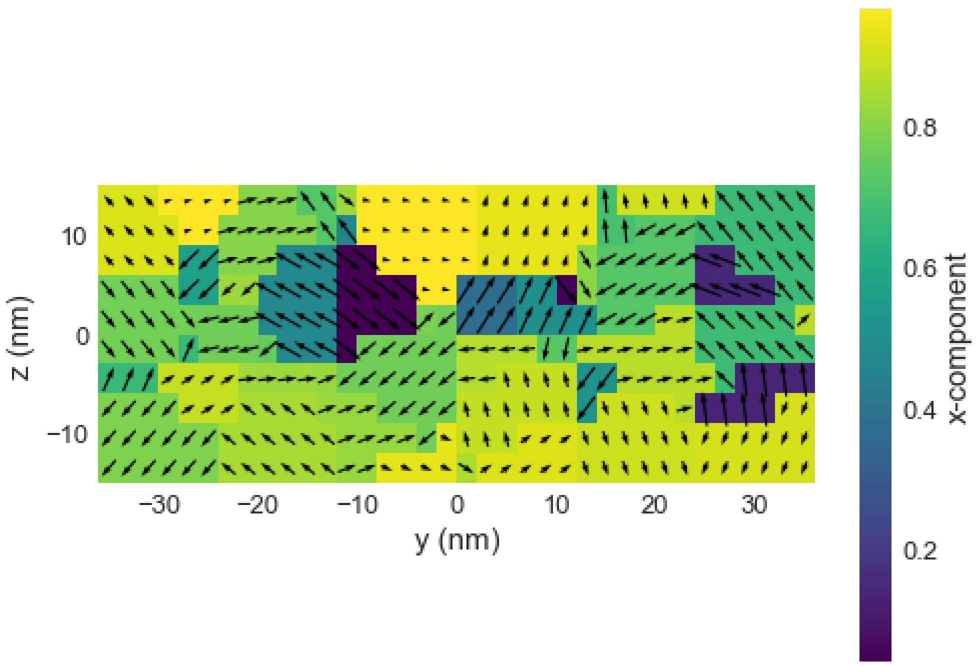


In [16]:

```
u.plane('y').mpl()
```



In [17]:
```
u.plane('x').mpl()
```



In [18]:
```
#gamma0 = 0  # gyromagnetic ratio (m/As)
gamma0 = 2.211e5  # gyromagnetic ratio (m/As)
alpha = 0.0133  # Gilbert damping
system.dynamics = mm.Precession(gamma0=gamma0) + mm.Damping(alpha=alpha)


system.energy = mm.Exchange(A=A) +  mm.UniaxialAnisotropy(K=K, u=u) + mm.Demag()
system.m = df.Field(mesh, dim=3, value=(1, 0, 0), norm=Ms)
Hmin = (-0.008/mm.consts.mu0, 0, 0)
Hmax = (0.008/mm.consts.mu0, 0, 0)
n = 61
```

In [19]:
```
hd = mc.HysteresisDriver()
hd.drive(system, Hmin=Hmin, Hmax=Hmax, n=n)
```

```
Running OOMMF (TclOOMMFRunner) [2022/02/22 09:36]... (130857.3 s)
```

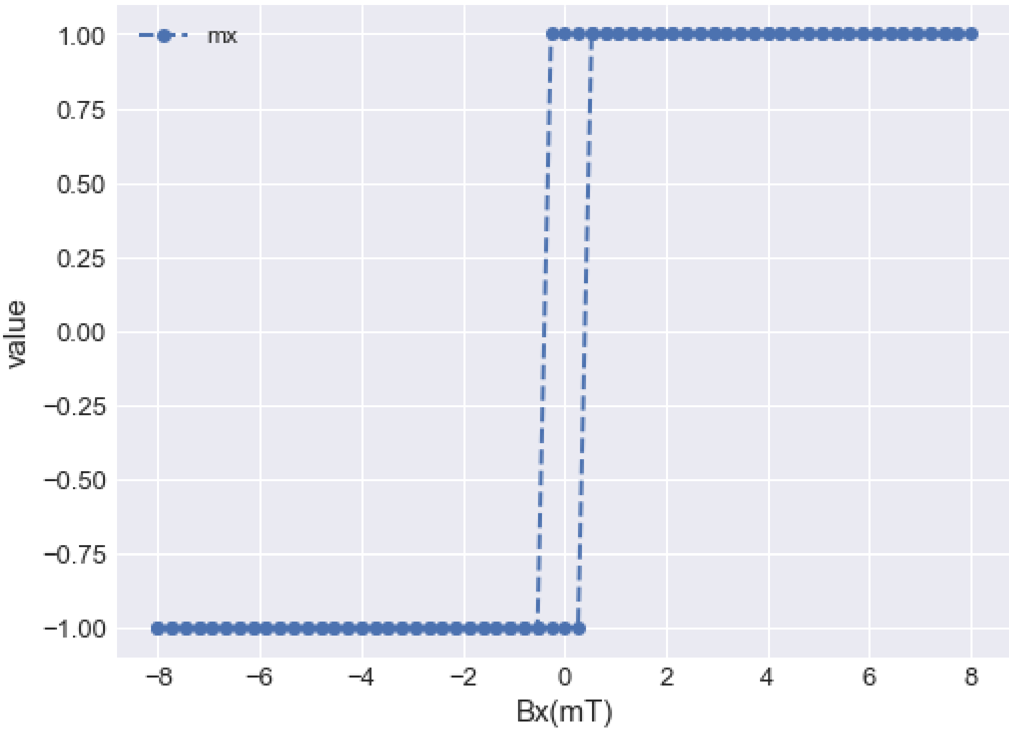
In [21]:
```
system.table.data.head()
```

Out[21]:

	max_mxHxm	E	delta_E	bracket_count	line_min_count	conjugate_cycle_count	cy
0	0.098848	1.017477e-17	0.000000e+00	33544.0	17545.0	221.0	
1	0.098850	1.020380e-17	1.540744e-33	37666.0	19733.0	247.0	
2	0.096601	1.023283e-17	0.000000e+00	41542.0	21813.0	273.0	
3	0.097041	1.026186e-17	0.000000e+00	45354.0	23827.0	297.0	
4	0.095044	1.029089e-17	0.000000e+00	49777.0	26148.0	324.0	

5 rows × 26 columns

In [22]:
```
system.table.mpl(x='Bx', y=['mx'], marker='o', linewidth=2, linestyle='dashed')
```



In [23]:
```
pd1=system.table.data
pd1.to_excel (r'E:\ubermag-tests\results\24_02_12grain.xlsx', index = False, header=
```

In [ ]:
```
```