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 = 1.3e-11
Ms = 700e3
d = 25e-9

p1 = (-30e-9, -30e-9, -15e-9)
p2 = (30e-9, 30e-9, 15e-9)
region = df.Region(p1=p1, p2=p2)
grains_mesh = df.Mesh(region=region, cell=((2*d)/5, (2*d)/5, (2*d)/5))
# 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]:
```
[(-2.5e-08, -2.5e-08, -9.999999999999999e-09),
 (-1.4999999999999995e-08, -2.5e-08, -9.999999999999999e-09),
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```

```
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```

```
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(1.5000000000000002e-08, 2.5000000000000005e-08, 1e-08),
(2.5000000000000005e-08, 2.5000000000000005e-08, 1e-08)]
```

In [4]:

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

Out[4]:

```
array([[-2.50000000e-08, -2.50000000e-08, -1.00000000e-08],
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```

```
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[ 2.50000000e-08,  2.50000000e-08,  1.00000000e-08]])
```

In [5]:

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

```
print(num_rows, num_cols)
print(Ngrains)
```

```
108 3
108
```

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]:

```
array([[ 1.62792386e-09, -2.87548830e-09,  8.01889410e-10],
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       [-1.54754475e-09,  3.45469132e-10,  3.93042119e-10],
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```

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       [-1.75243741e-09, -2.14048493e-09,  1.19936391e-09]])
```

In [7]:

```
#randomly displaced grains, averge size is close to 12nm
grain_centres = increament + grain_centres_originals
grain_centres
```

Out[7]:

```
array([[-2.33720761e-08, -2.78754883e-08, -9.19811059e-09],
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       [ 2.32475626e-08,  2.28595151e-08,  1.11993639e-08]])
```

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]:

```
array([[-0.88410039, -0.48678487,  0.02066357],
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       [ 0.77391018,  0.03357856,  0.25228734],
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```

```
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[ 0.38005277, -0.65681396,  0.38786135],
[-0.42946875, -0.88978816,  0.16444581],
[-0.40836255, -0.35436773,  0.93397878],
[-0.61013067, -0.30520699, -0.79197187],
[-0.1964363 , -0.81430471,  0.00968761],
[ 0.48518148, -0.98941898, -0.81967766],
```

```
       [-0.88763204,  0.76865133,  0.97117171],
       [ 0.04034937, -0.60316514,  0.86669663],
       [ 0.30919641,  0.58358349,  0.02243136],
       [ 0.57642378, -0.33040654, -0.77349373],
       [ 0.80962795, -0.99155217, -0.85299224],
       [-0.73541727,  0.88429984, -0.39414063],
       [-0.5733739 , -0.48867489, -0.80815987],
       [-0.19640423,  0.46205528,  0.29641987],
       [-0.49830884, -0.54512217, -0.00836768],
       [ 0.72952993,  0.26812751,  0.50898495],
       [-0.12575362, -0.19957582,  0.44583263],
       [-0.25526284,  0.10519606, -0.83907277],
       [ 0.18855113, -0.43815707,  0.48489517],
       [-0.40234561,  0.51507337, -0.54727972],
       [-0.99118471, -0.72043944, -0.4084726 ],
       [-0.60881237,  0.09776408, -0.58001566],
       [ 0.55698434, -0.03064019,  0.27868079],
       [-0.66460739,  0.84936521,  0.4346799 ],
       [-0.69037278,  0.44726721, -0.62718015],
       [ 0.65932913, -0.60671647,  0.92260134],
       [ 0.09519517, -0.5542728 , -0.57454662],
       [ 0.25597592,  0.26655226, -0.39344193],
       [ 0.6327355 , -0.16188657,  0.62771657],
       [-0.46956966,  0.96685094,  0.74461065],
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       [-0.9099089 , -0.97372091,  0.32362123],
       [-0.78497531, -0.38008472, -0.3841051 ],
       [-0.76505555,  0.89386284,  0.9547811 ],
       [ 0.80895851,  0.5923603 , -0.86914115],
       [ 0.43407725, -0.08817913, -0.69703257],
       [ 0.29344039, -0.94153086,  0.50704175],
       [ 0.77946589, -0.97923992, -0.34514431]])
```

In [9]:

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

Out[9]:

```
array([[ 0.11589961, -0.48678487,  0.02066357],
       [ 1.99051757, -0.70696864, -0.10097044],
       [ 1.20288075, -0.80545501, -0.42253024],
       [ 1.4415998 ,  0.10161213,  0.67715403],
       [ 1.1606627 , -0.63085653,  0.23100423],
       [ 1.77391018,  0.03357856,  0.25228734],
       [ 1.01011824,  0.81932515, -0.17339069],
       [ 1.07093743, -0.31471375, -0.74084645],
       [ 1.3256435 ,  0.87134   ,  0.22545836],
       [ 1.685477  , -0.56418313,  0.80634348],
       [ 0.01953995, -0.54837455, -0.73588975],
       [ 1.81508589,  0.82046127,  0.16211581],
       [ 0.17498611, -0.76624112,  0.54214251],
       [ 1.46559054, -0.82574329, -0.2850736 ],
       [ 1.54642324, -0.7370568 ,  0.07566487],
       [ 1.50944713, -0.45494765,  0.13303399],
       [ 0.95336994,  0.11324139, -0.11852589],
       [ 1.38747473,  0.43647436,  0.51276472],
       [ 0.07464402,  0.35767079, -0.0455584 ],
       [ 0.20034278,  0.22839247,  0.67582902],
       [ 1.46778808, -0.35686883, -0.86428938],
       [ 0.07466047,  0.11825061, -0.6782946 ],
       [ 0.53577637, -0.52857609, -0.96130508],
       [ 0.30337285, -0.93219497,  0.96366972],
       [ 0.72097062,  0.65092906, -0.17552518],
```

```
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[ 0.61821032, -0.72878046,  0.5018533 ],
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[ 1.67769318,  0.07470805, -0.49915213],
[ 0.11778802, -0.81610143, -0.65160011],
[ 0.8785087 ,  0.62186845,  0.82080425],
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[ 1.6133823 ,  0.85703871,  0.22787025],
[ 1.96400783,  0.42997591, -0.98268146],
[ 0.57629116,  0.68279732, -0.11364583],
[ 0.34609945, -0.77094578,  0.59576119],
[ 1.2978103 ,  0.003492  , -0.42871958],
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[ 1.5241336 ,  0.67977496, -0.79008518],
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[ 1.57642378, -0.33040654, -0.77349373],
[ 1.80962795, -0.99155217, -0.85299224],
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[ 0.87424638, -0.19957582,  0.44583263],
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```

```
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       [ 1.09519517, -0.5542728 , -0.57454662],
       [ 1.25597592,  0.26655226, -0.39344193],
       [ 1.6327355 , -0.16188657,  0.62771657],
       [ 0.53043034,  0.96685094,  0.74461065],
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       [ 0.0900911 , -0.97372091,  0.32362123],
       [ 0.21502469, -0.38008472, -0.3841051 ],
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       [ 1.80895851,  0.5923603 , -0.86914115],
       [ 1.43407725, -0.08817913, -0.69703257],
       [ 1.29344039, -0.94153086,  0.50704175],
       [ 1.77946589, -0.97923992, -0.34514431]])
```

In [10]:

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

Out[10]:

```
array([[ 0.23142037, -0.97197853,  0.04125959],
       [ 0.94125513, -0.33430394, -0.04774585],
       [ 0.79764038, -0.53410402, -0.28018337],
       [ 0.90328345,  0.06366854,  0.42429392],
       [ 0.8654722 , -0.47041125,  0.1722531 ],
       [ 0.98986366,  0.01873725,  0.14077943],
       [ 0.76982829,  0.62442163, -0.13214399],
       [ 0.79938398, -0.234913  , -0.55299289],
       [ 0.82733301,  0.54380257,  0.14070838],
       [ 0.86357251, -0.28906537,  0.41313887],
       [ 0.02128654, -0.59739115, -0.80166745],
       [ 0.90822721,  0.41053994,  0.08111902],
       [ 0.18326779, -0.80250552,  0.56780085],
       [ 0.85898581, -0.48396994, -0.16708226],
       [ 0.90183058, -0.42983081,  0.04412562],
       [ 0.9540657 , -0.28755558,  0.08408587],
       [ 0.98553744,  0.11706224, -0.12252505],
       [ 0.89964536,  0.2830121 ,  0.33247914],
       [ 0.2027235 ,  0.97138761, -0.12373072],
       [ 0.27037693,  0.308232  ,  0.91207968],
       [ 0.84339574, -0.20505798, -0.49662345],
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       [ 0.87764067,  0.19213994, -0.4391231 ],
       [ 0.63983433,  0.75808409, -0.12617667],
```

```
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[ 0.50959171, -0.30522553,  0.80445861],
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[ 0.66091431,  0.09335586, -0.7446321 ],
[ 0.87626897, -0.32303485,  0.3574929 ],
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[ 0.66903073, -0.24554467, -0.70150246],
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[ 0.36972425, -0.65353676, -0.66044961],
```

```
       [ 0.17680513,  0.67266765,  0.71851108],
       [ 0.86448922,  0.28308504, -0.41535677],
       [ 0.89801747, -0.05521767, -0.43648097],
       [ 0.7707028 , -0.56101578,  0.30212331],
       [ 0.86372332, -0.47530687, -0.16752734]])
```

In [11]:

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

Out[11]:

```
array([166.89959948, 166.86115132, 180.29970146, 169.93518236,
       136.46476736, 181.25077147, 142.7552613 , 149.46012546,
       150.39005471, 157.87536106, 154.71209049, 163.56215777,
       189.59040458, 232.58618078, 146.10634109, 242.38113304,
       220.98162943, 221.33956086, 189.85767928, 207.68489172,
       222.51687171, 225.09803874, 186.40205512, 229.48715924,
       248.11611689, 238.82238107, 228.15514883, 175.80049128,
       200.18842178, 205.8813576 , 181.49843531, 208.74235328,
       206.75014435, 198.00011287, 194.00375418, 198.58687751,
       201.34466138, 185.33696039, 183.03154317, 197.966014  ,
       155.04983188, 125.70567337, 191.33900273, 152.83181991,
       265.79044527, 228.93716786, 249.92597184, 229.30903081,
       187.15909048, 220.03579868, 220.79769245, 144.88496683,
       231.38842583, 164.14769332, 152.86648272, 229.64749622,
       177.08602674, 161.55978628, 247.51671978, 129.35339998,
       169.18353371, 244.96967662, 306.86740356, 202.57782   ,
       236.53937255, 160.1197516 , 283.00194678, 176.39253877,
        87.35995131, 204.38177705, 205.70677174, 168.63857757,
       210.3044294 , 252.51690988, 146.03898523, 220.00547404,
       160.61653408, 259.43917656, 222.8277382 , 179.48499231,
       211.03129692, 184.42873832, 225.9411766 , 199.02285844,
       252.33948618, 306.50309895, 213.70905595, 234.90520662,
       215.09588022, 179.73362476, 219.32064519, 239.07624123,
       233.87365145, 206.26607028, 193.81912901, 273.20588601,
       237.16445182, 255.30149947, 173.90954566, 256.91413381,
       141.64622495, 219.10595777, 201.17603176, 206.47251145,
       183.56305593, 237.23342539, 221.53074593, 207.80771184])
```

In [12]:

```
# 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)
```

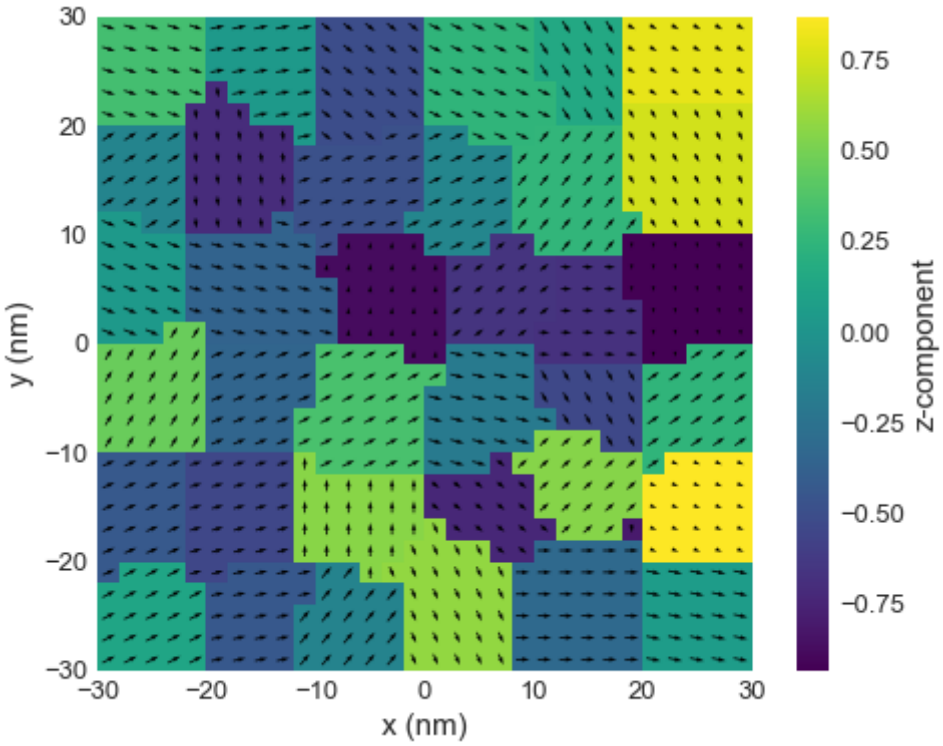
In [25]:
```
#after difining the grains with random anisotropy and desired size,
#now lets us decrease the cell size for micromagnetic calculations and make mesh

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

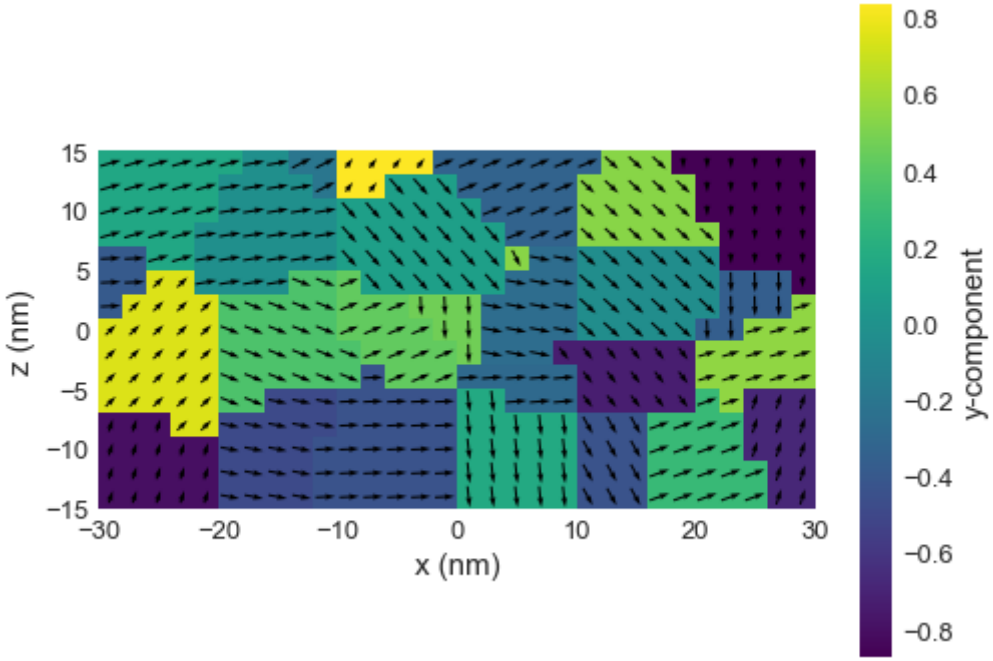
In [26]:
```
K = df.Field(mesh, dim=3, value=K_mag)
u = df.Field(mesh, dim=3, value=K_axis)

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

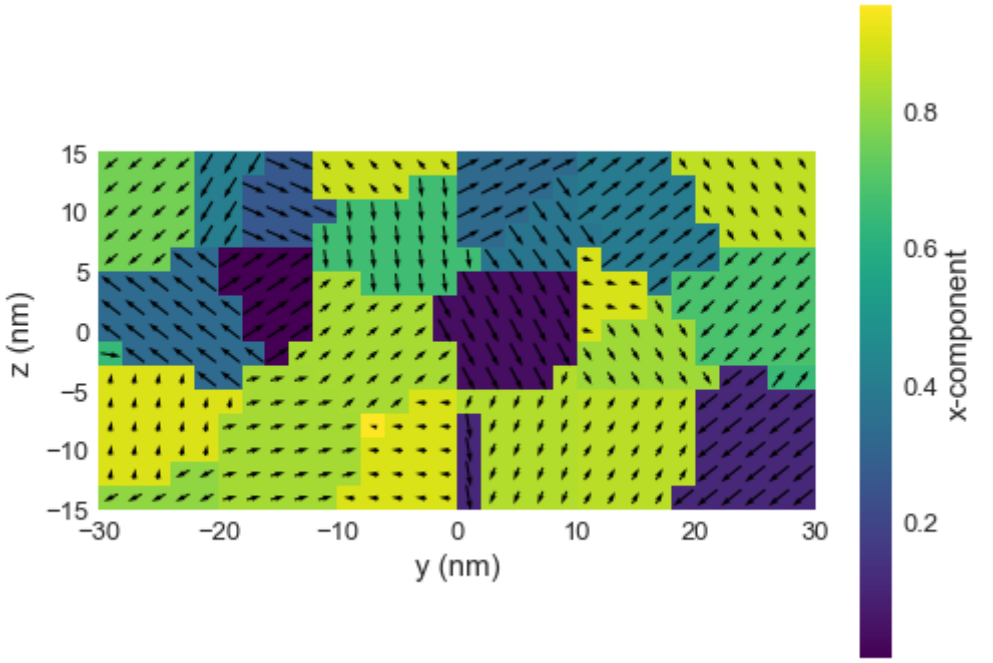
In [27]:
```
u.plane('z').mpl()
```



In [28]:
```
u.plane('y').mpl()
```



In [29]:
```
u.plane('x').mpl()
```



In [34]:
```
#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 = (-0.05/mm.consts.mu0, 0, 0)
Hmax = (0.05/mm.consts.mu0, 0, 0)
n = 61
```

In [35]:
```
hd = mc.HysteresisDriver()
hd.drive(system, Hmin=Hmin, Hmax=Hmax, n=n)
```

```
Running OOMMF (TclOOMMFRunner) [2022/02/16 12:28]... (214.2 s)
```

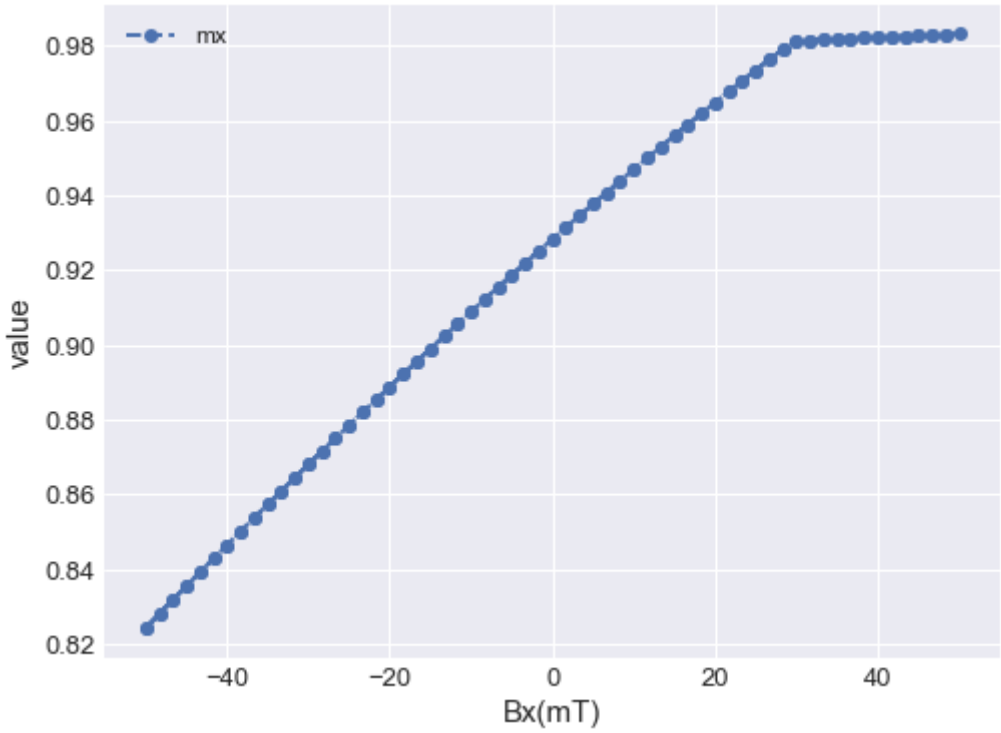
In [36]:
```
system.table.data.head()
```

Out[36]:

	max_mxHxm	E	delta_E	bracket_count	line_min_count	conjugate_cycle_count	cy
0	0.096708	1.097604e-17	0.000000e+00	1999.0	1960.0	3.0	
1	0.095154	1.087194e-17	0.000000e+00	2173.0	2129.0	4.0	
2	0.097503	1.076738e-17	0.000000e+00	2347.0	2297.0	5.0	
3	0.083629	1.066235e-17	0.000000e+00	2522.0	2464.0	6.0	
4	0.096340	1.055685e-17	-1.540744e-33	2696.0	2629.0	7.0	

5 rows × 26 columns

In [37]:
```
system.table.mpl(x='Bx', y=['mx'], marker='o', linewidth=2, linestyle='dashed')
```



In [138…
```
pd1=system.table.data
pd1.to_excel (r'E:\ubermag-tests\results\11_02_1727.xlsx', index = False, header=Tru
```

In [ ]:
```
```