

McStas Union components

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- University of Copenhagen



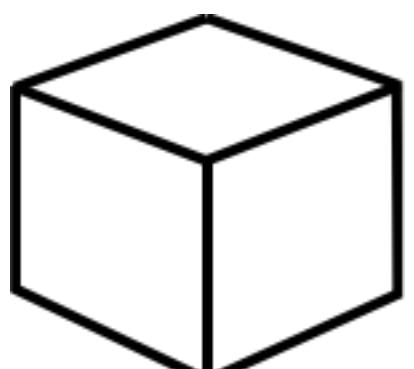
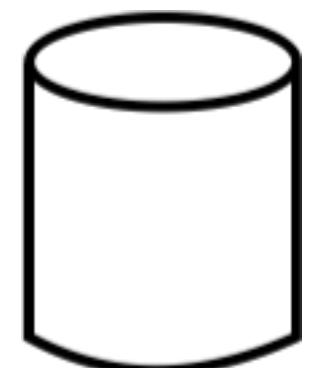
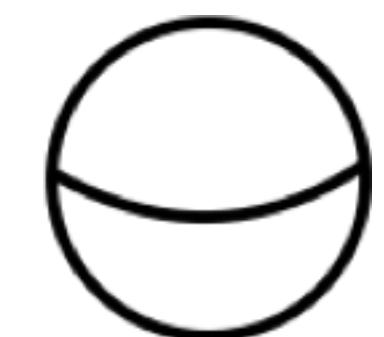
Background in McStas

- Sample holders with complicated geometry
- Many different materials
- Inside sample environment
- Co aligned crystals
- Twinned crystals



McStas Union components - Idea

Geometry



Physics

Aluminium

Incoherent

Powder Bragg

Nickel

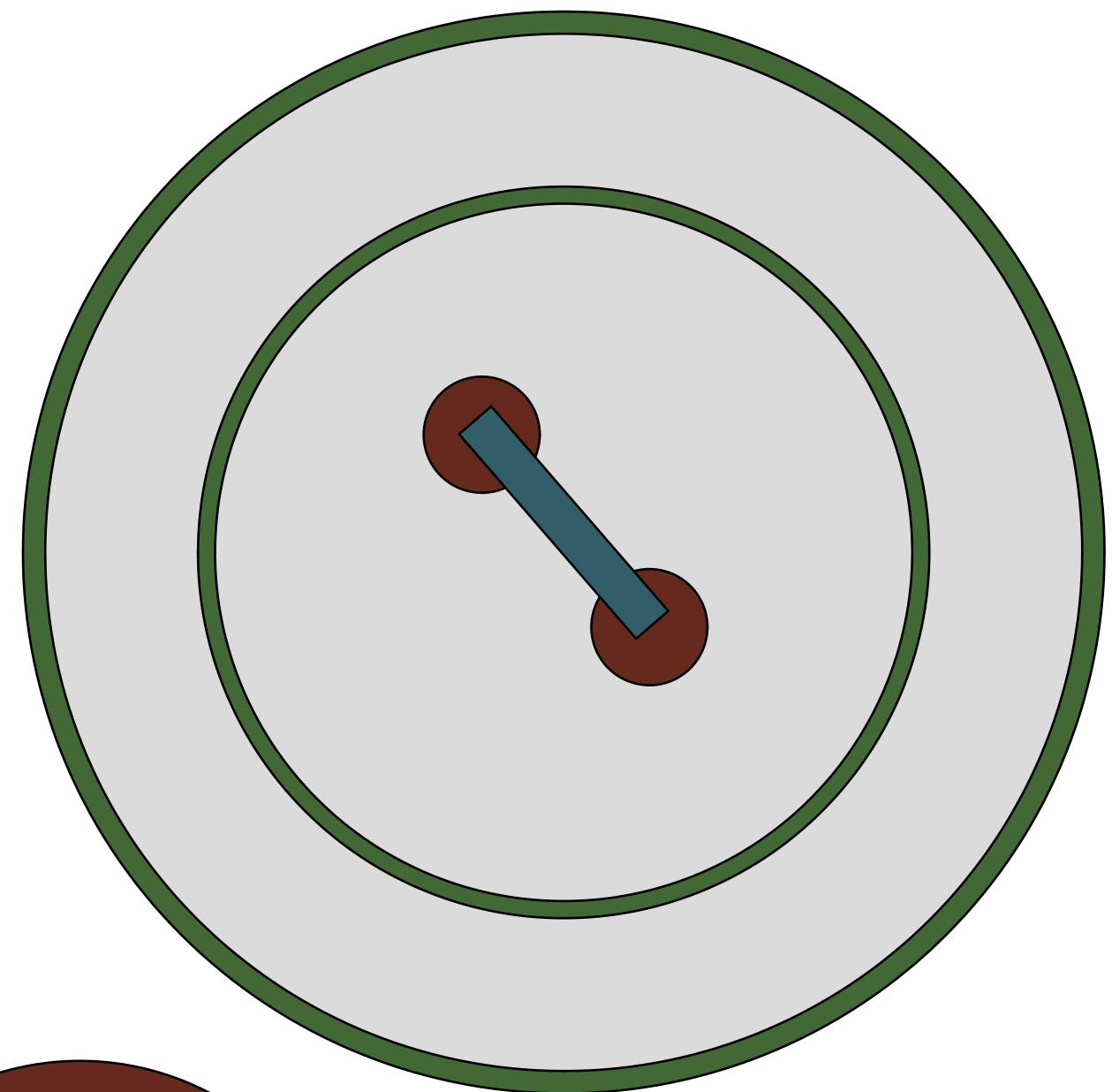
Incoherent

Single crystal Bragg

Excitation

McStas Union components - Priority

- Each geometry is assigned a material definition and a priority
- Priority decides which material is simulated in regions where several overlap
- This can be used to construct complex geometries with a range of materials



McStas Union components - Use

```
COMPONENT Al_incoherent = Incoherent_process(  
    sigma=4*0.0082,packing_factor=1,  
    unit_cell_volume=66.4)  
AT (0,0,0) ABSOLUTE
```

sigma in [barns]
unit_cell_volume in [\AA^3]

```
COMPONENT Al_powder = Powder_process(  
    reflections="Al.laz")  
AT (0,0,0) ABSOLUTE
```

```
COMPONENT Al = Union_make_material(  
    my_absorption=100*4*0.231/66.4,  
    process_string="Al_incoherent,Al_powder")  
AT (0,0,0) ABSOLUTE
```

my [1/m] = cross section per unit cell / unit cell volume



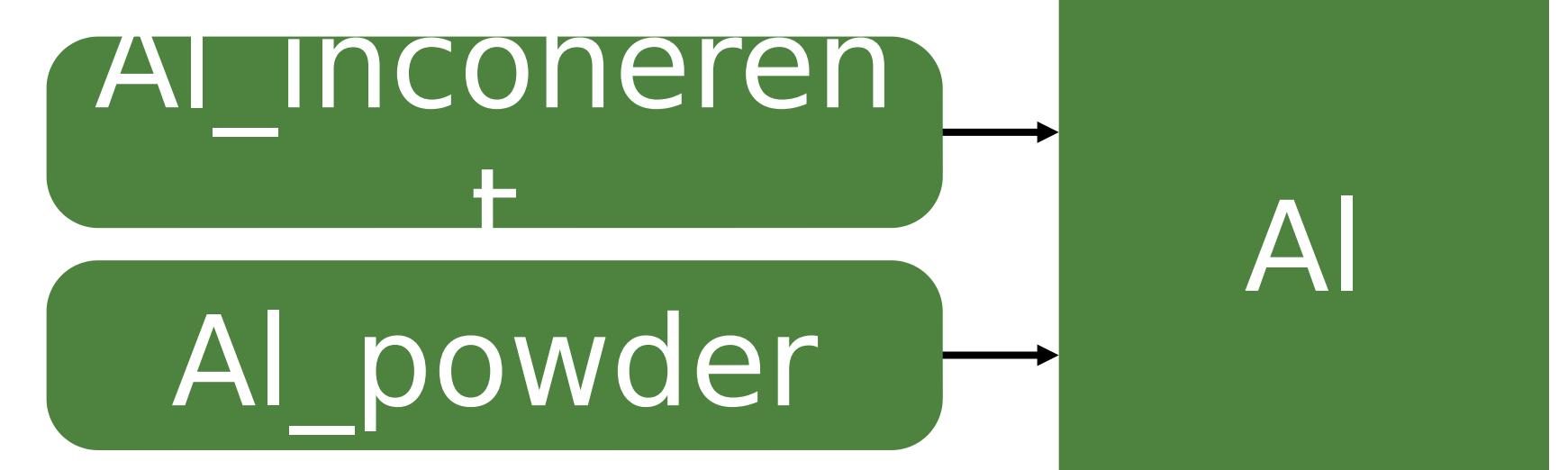
McStas Union components - Use

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```

sigma in [barns]
unit_cell_volume in [\AA^3]



my [1/m] = cross section per unit cell / unit cell volume



McStas Union components - Use

```
COMPONENT cryostat_shell = Union_cylinder(  
    radius_input=0.15,height_input=0.4,  
    priority_input=10,material_string="Al")
```

```
AT (0,0,0) RELATIVE target
```

```
ROTATED (0,0,0) RELATIVE target
```

Uses our Al definition!

```
COMPONENT cryostat_vacuum = Union_cylinder(  
    radius_input=0.147,height_input=0.4,  
    priority_input=11,material_string="Vacuum")
```

```
AT (0,0,0) RELATIVE target
```

```
ROTATED (0,0,0) RELATIVE target
```

Uses default material definition

Does not do any simulation what so ever



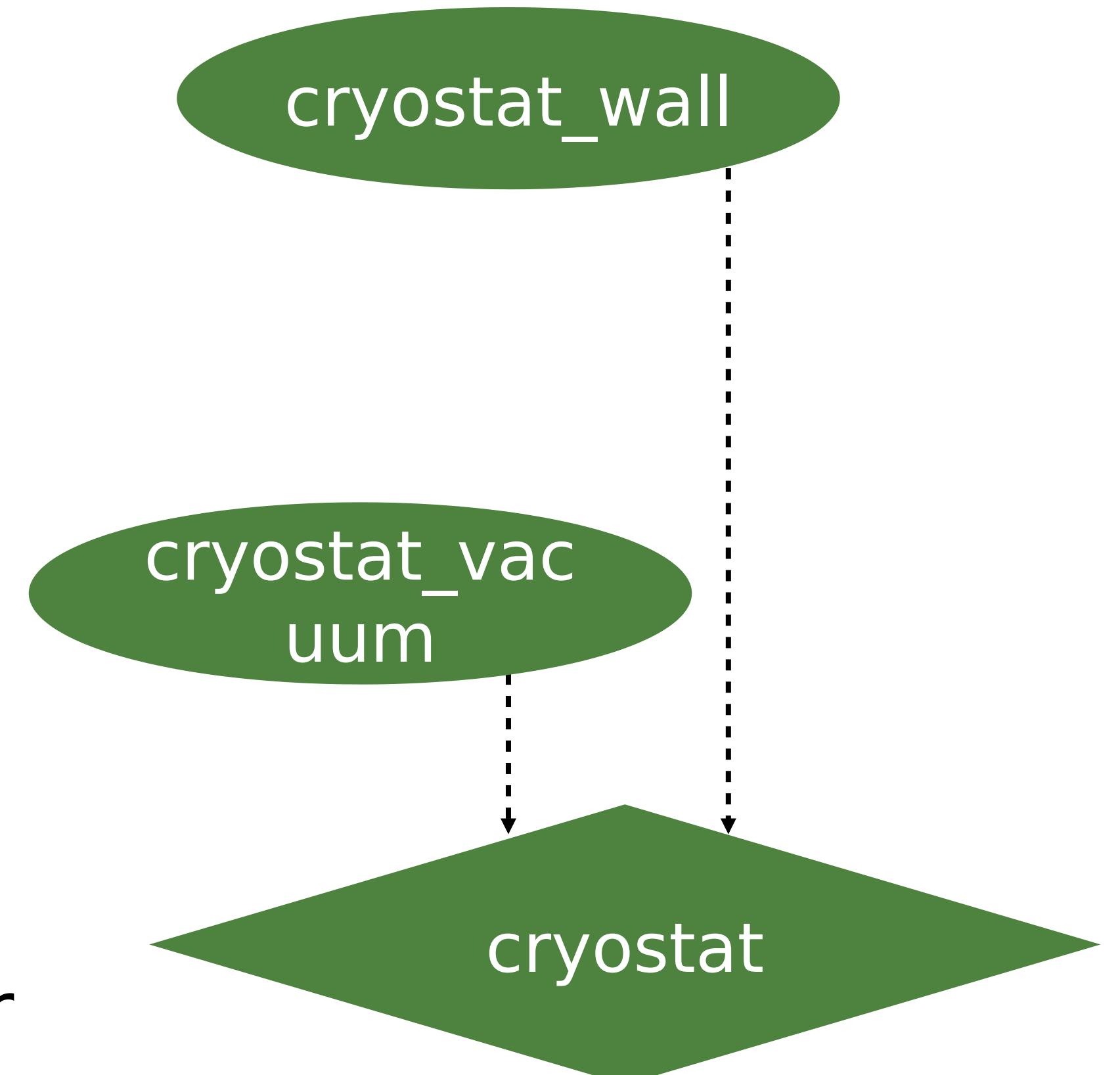
McStas Union components - Use

```
COMPONENT cryostat_shell = Union_cylinder(  
    radius_input=0.15,height_input=0.4,  
    priority_input=10,material_string="Al")  
AT (0,0,0) RELATIVE target  
ROTATED (0,0,0) RELATIVE target
```

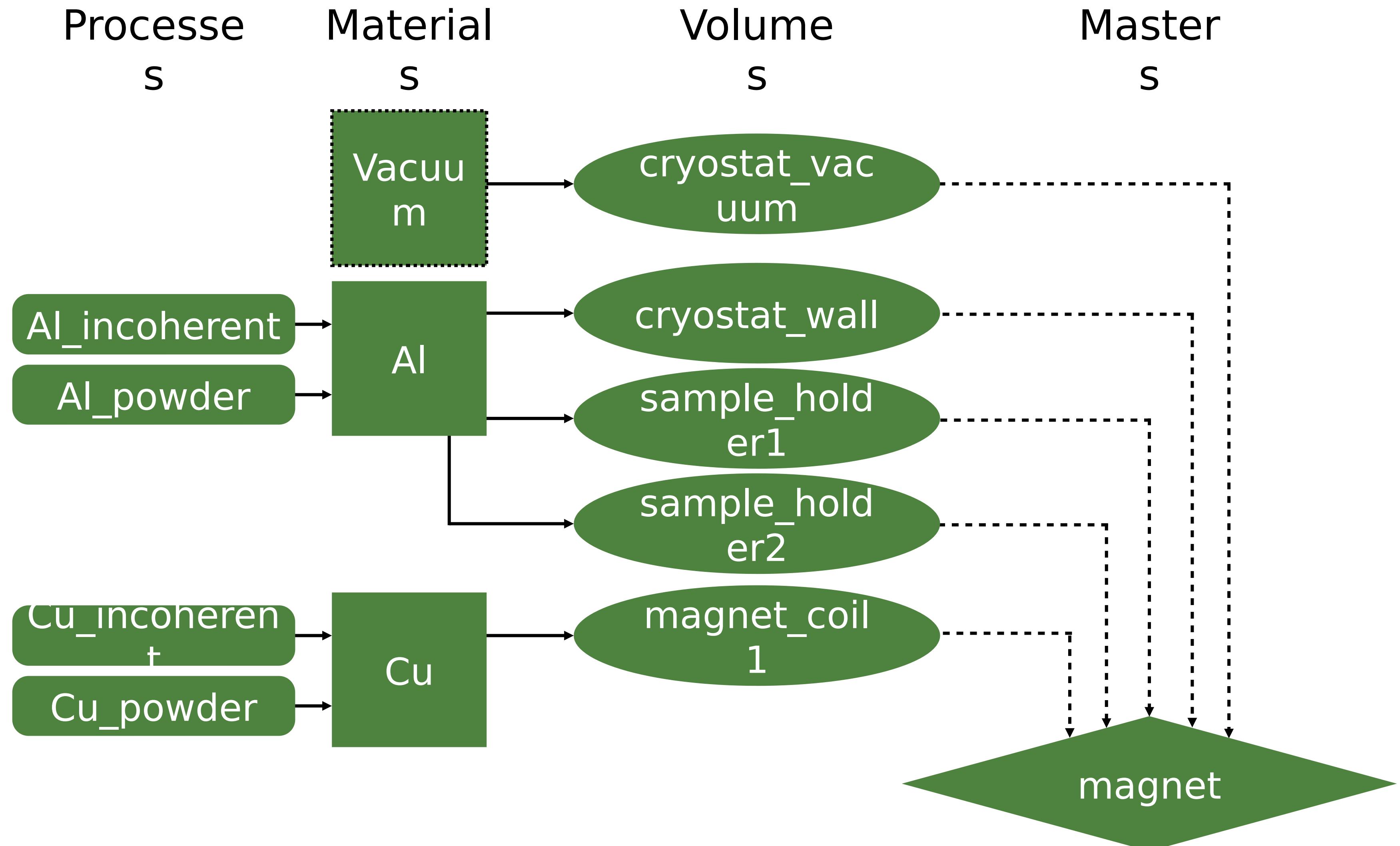
```
COMPONENT cryostat_vacuum = Union_cylinder(  
    radius_input=0.147,height_input=0.4,  
    priority_input=11,material_string="Vacuum")  
AT (0,0,0) RELATIVE target  
ROTATED (0,0,0) RELATIVE target
```

```
COMPONENT cryostat = Union_master()  
AT (0,0,0) RELATIVE target  
ROTATED (0,0,0) RELATIVE target
```

The Union_master
does the simulation



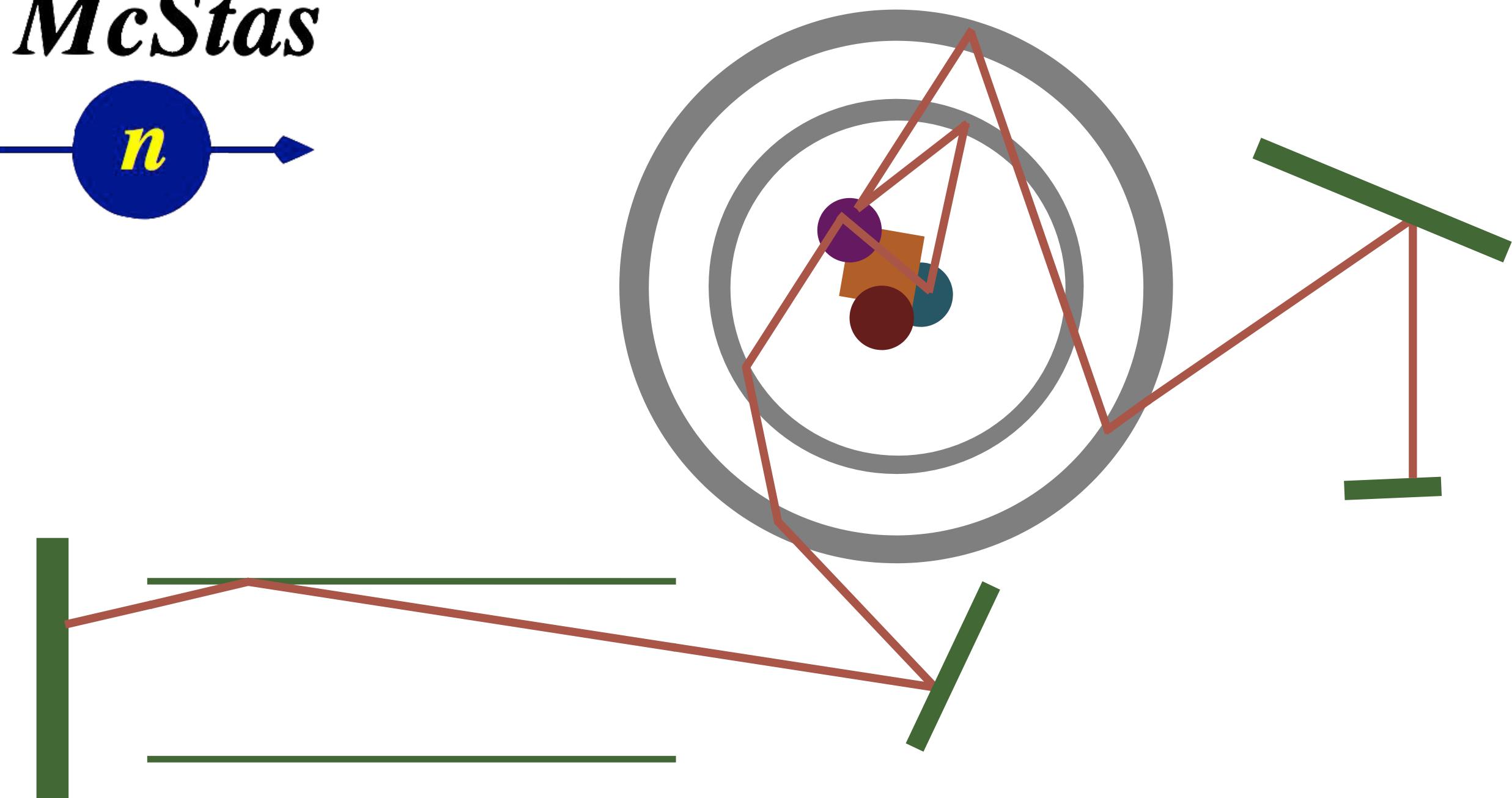
McStas Union components - Use



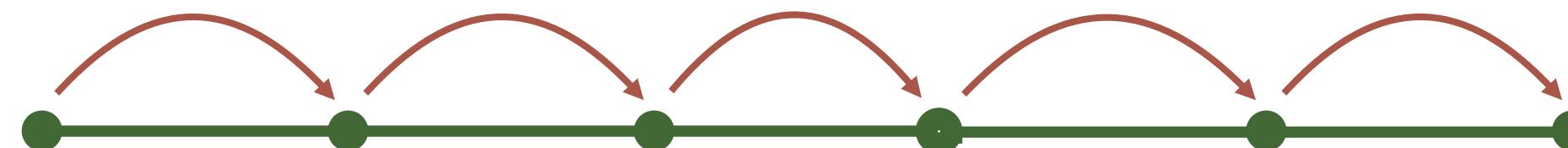
Union in instrument file

- Only the Union_master component affects the McStas simulation

McStas
 n

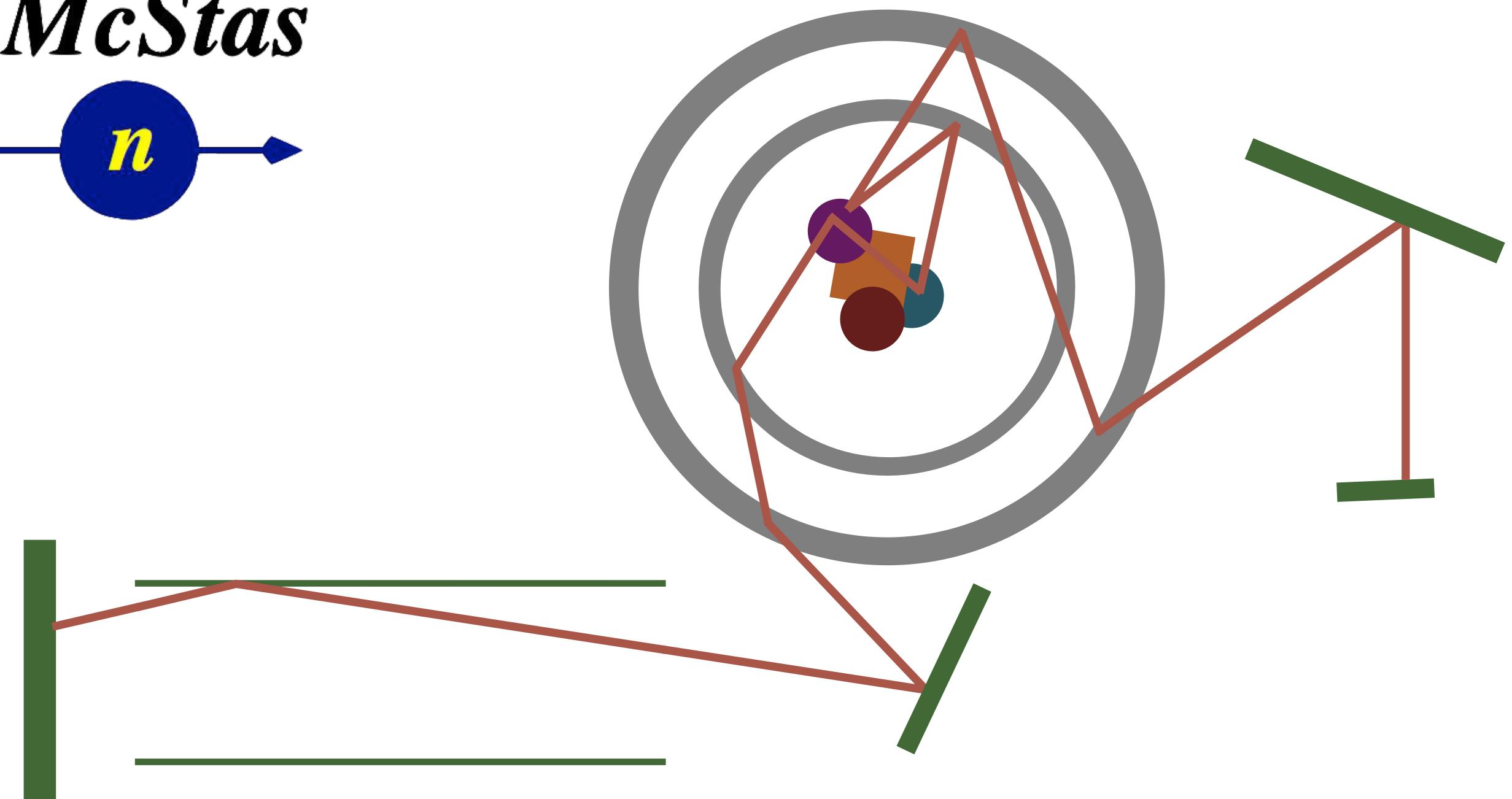


Simulated 3D space
Instrument file

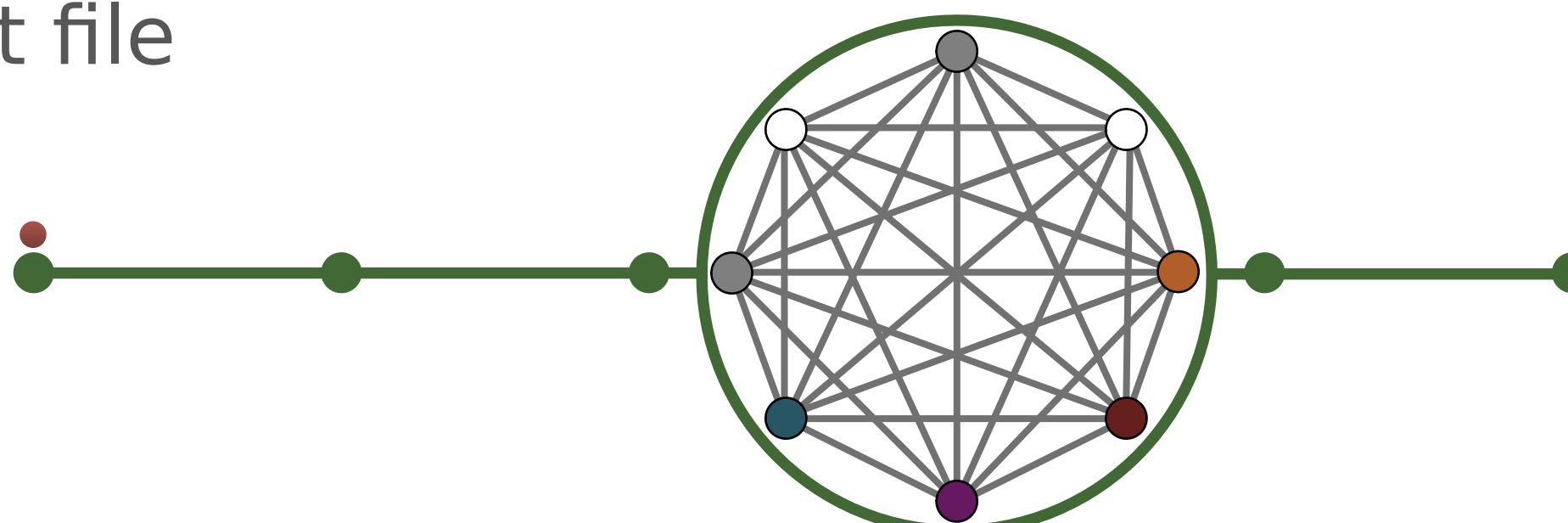


Union in instrument file

- Only the Union_master component affects the McStas simulation
- The Union_master component uses a network for propagation

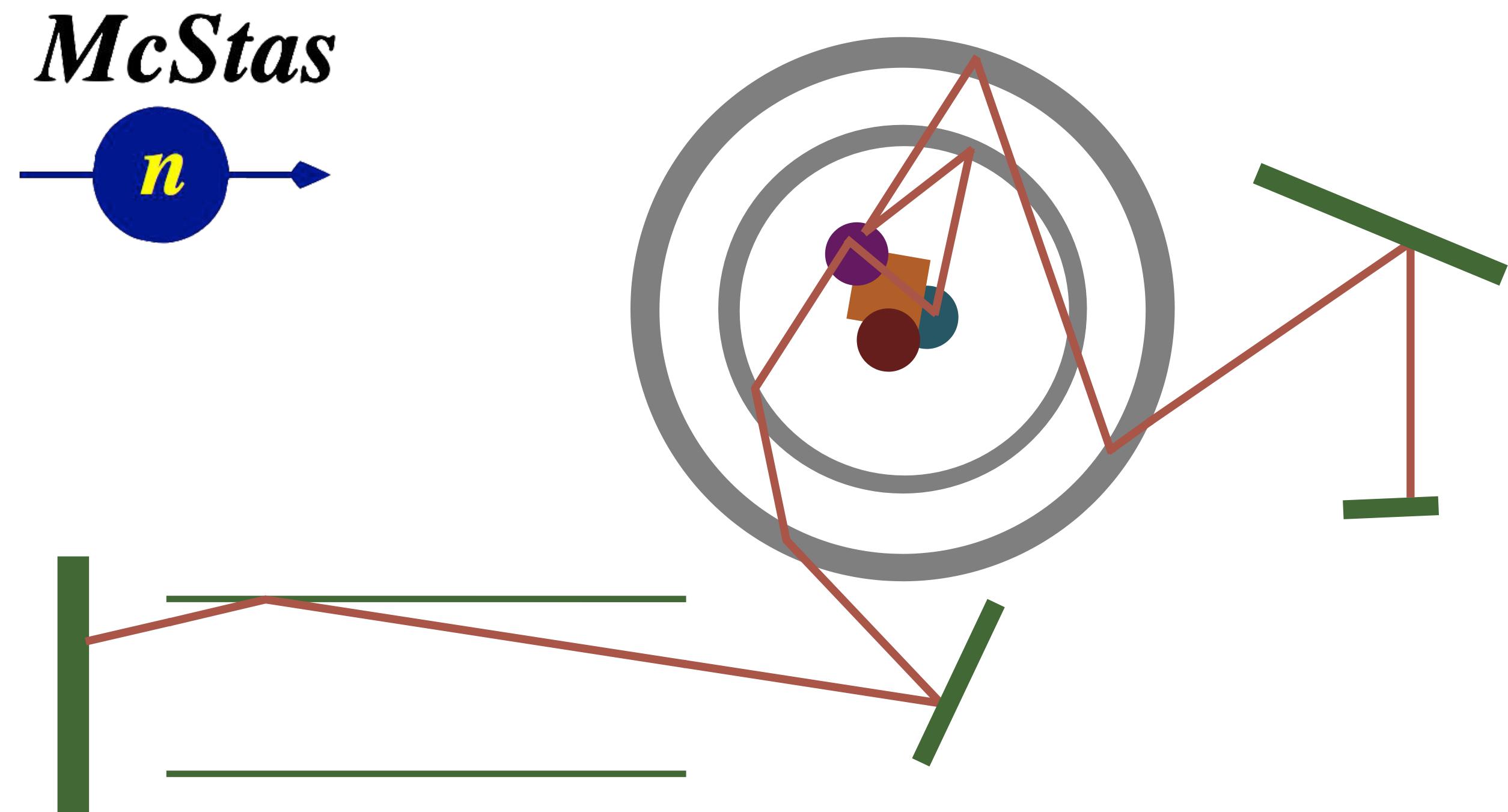


Simulated 3D space
Instrument file

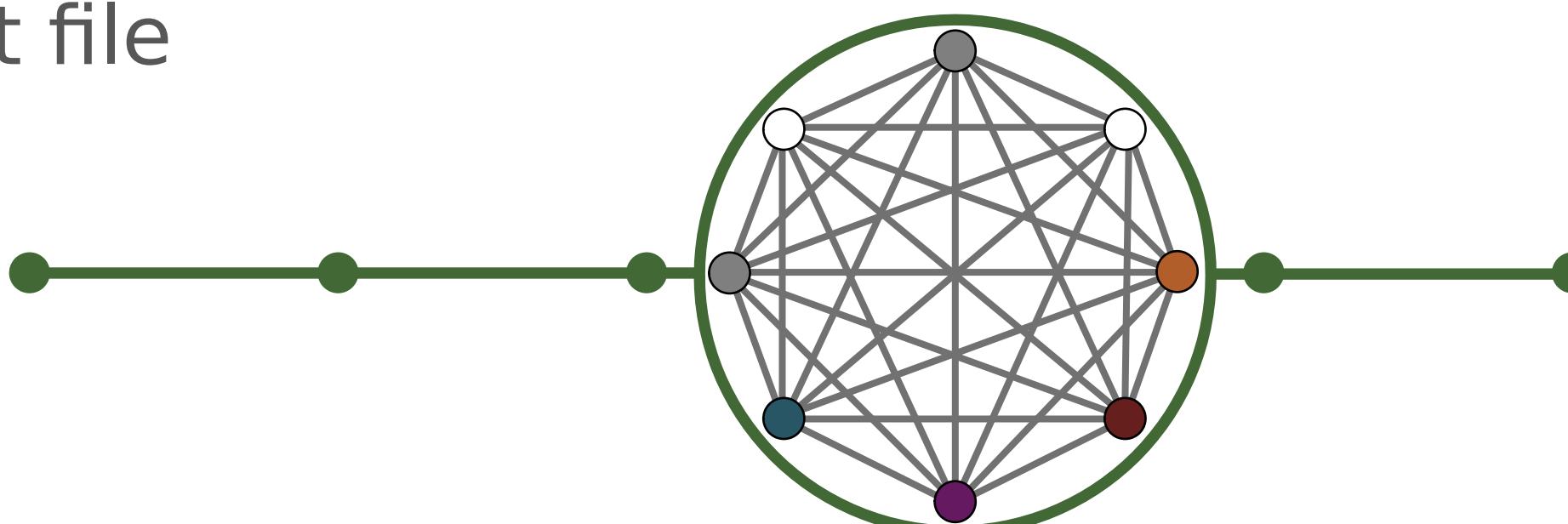


Union in instrument file

- Only the Union_master component affects the McStas simulation
- The Union_master component uses a network for propagation
- Analysis prior to simulation reduces the network complexity

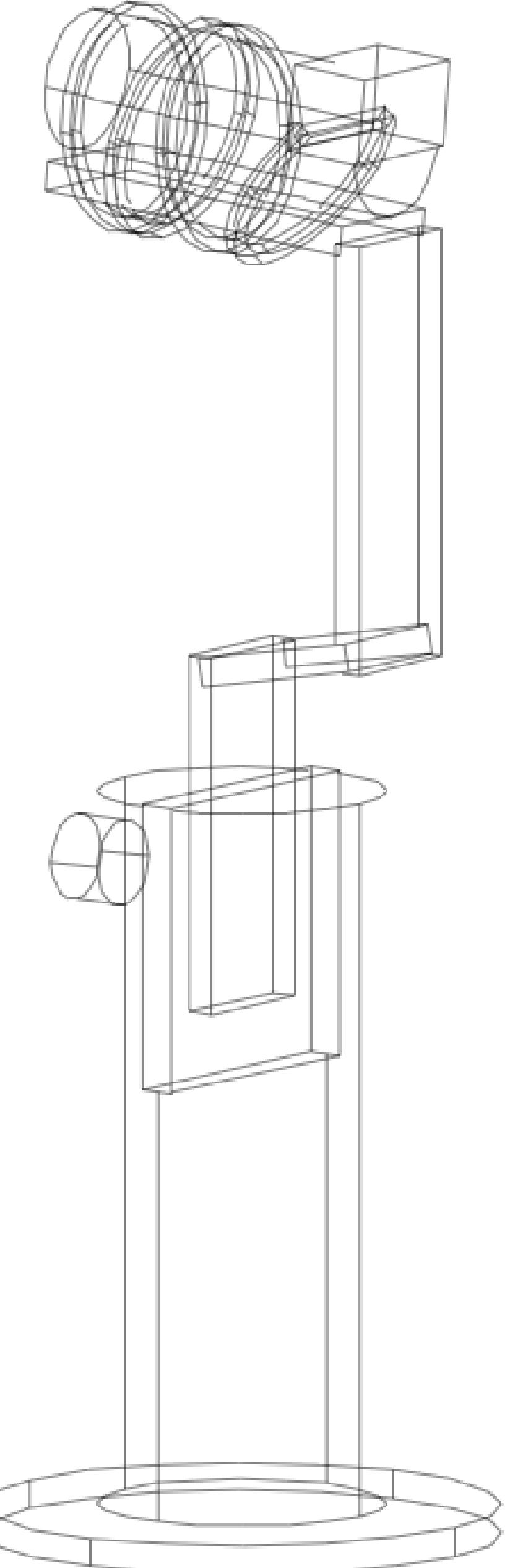


Simulated 3D space
Instrument file



McStas Union components

- Replicated from picture
- Easily assembled using Union components in McStas
- Material definitions made for sample / Aluminium
- Al absorption exaggerated

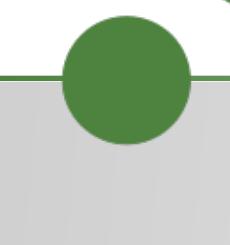
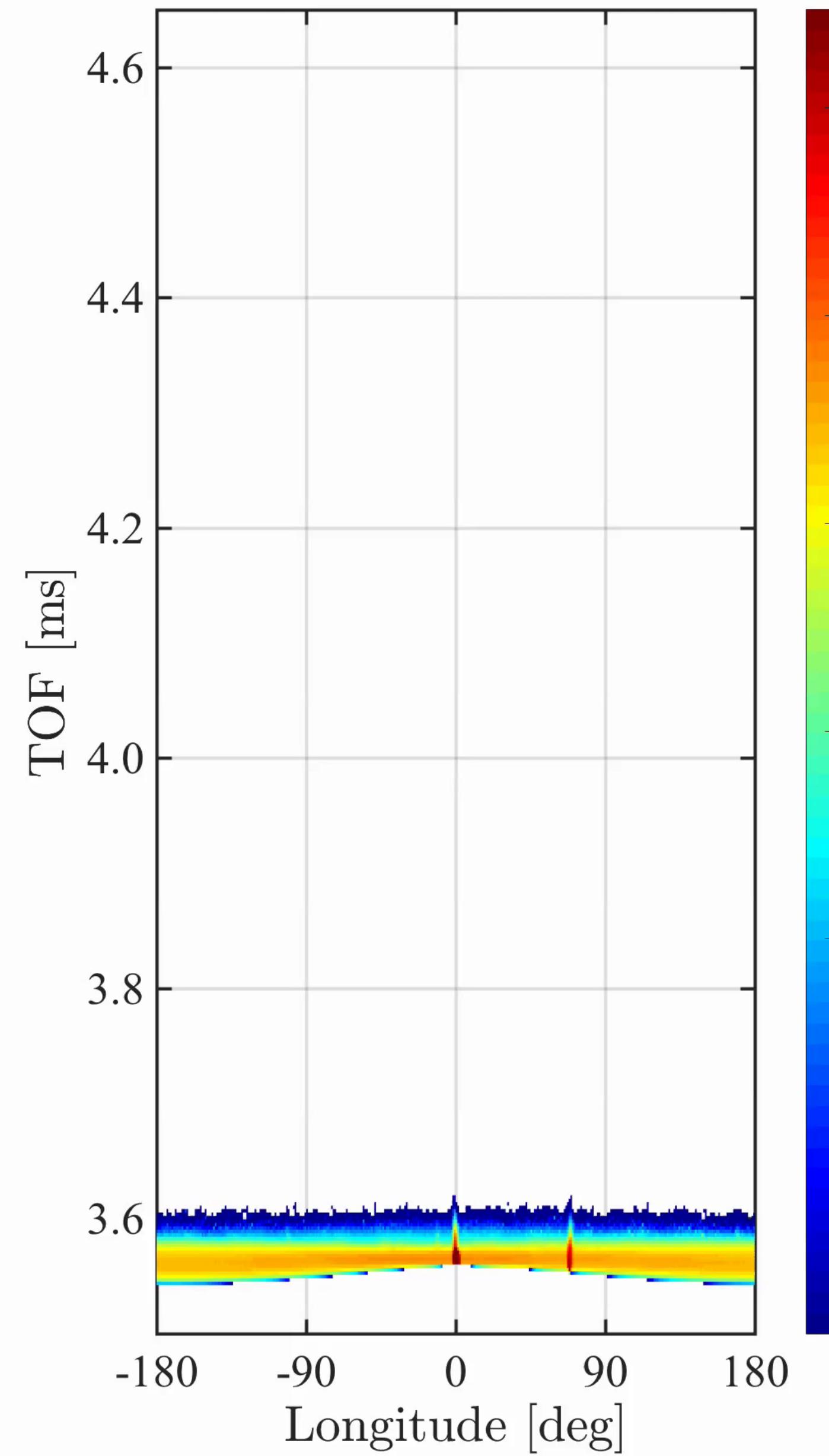
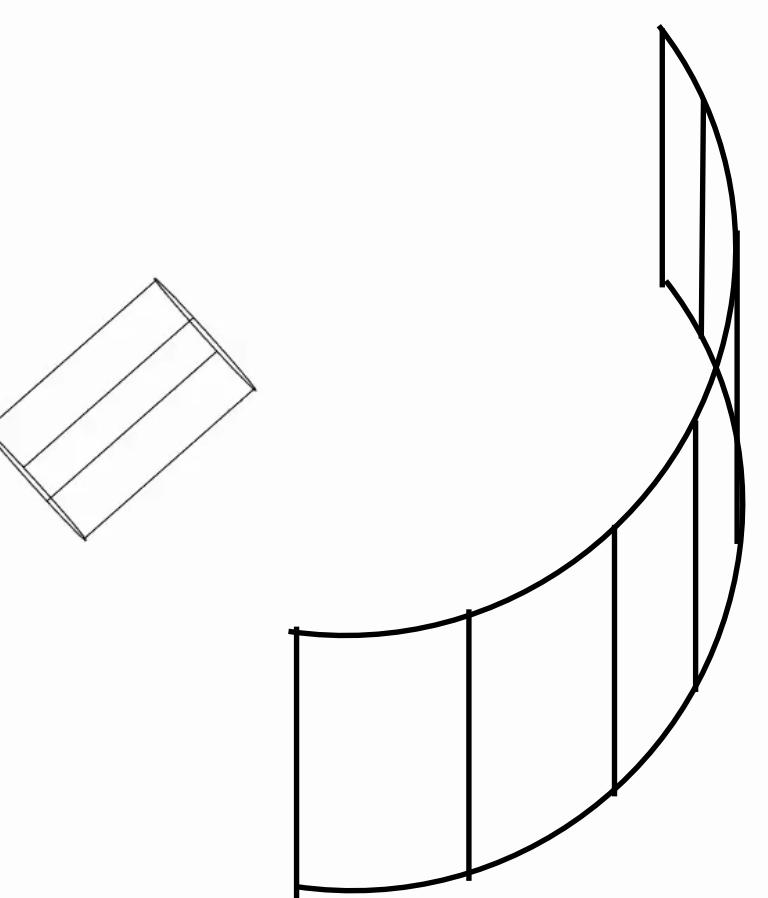


$\log(I)$

Building a sample



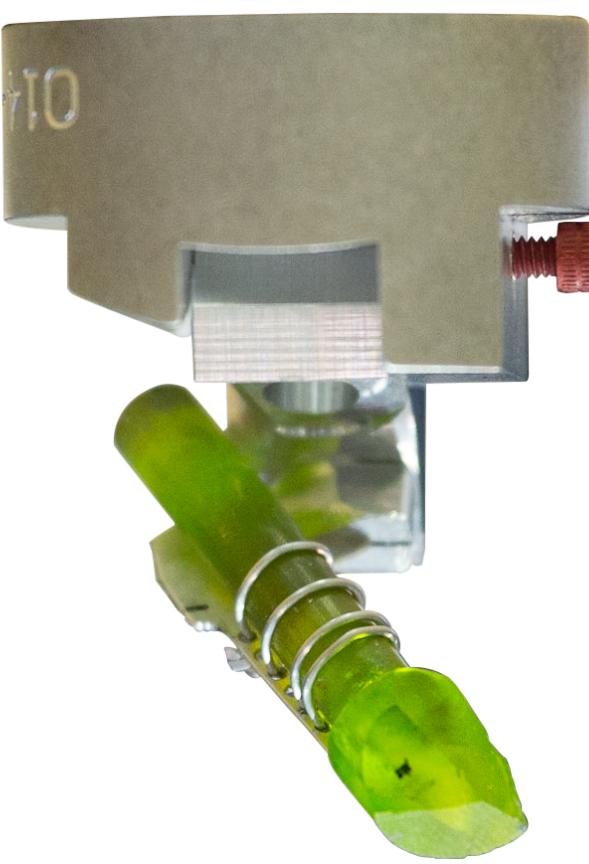
5 meV
beam



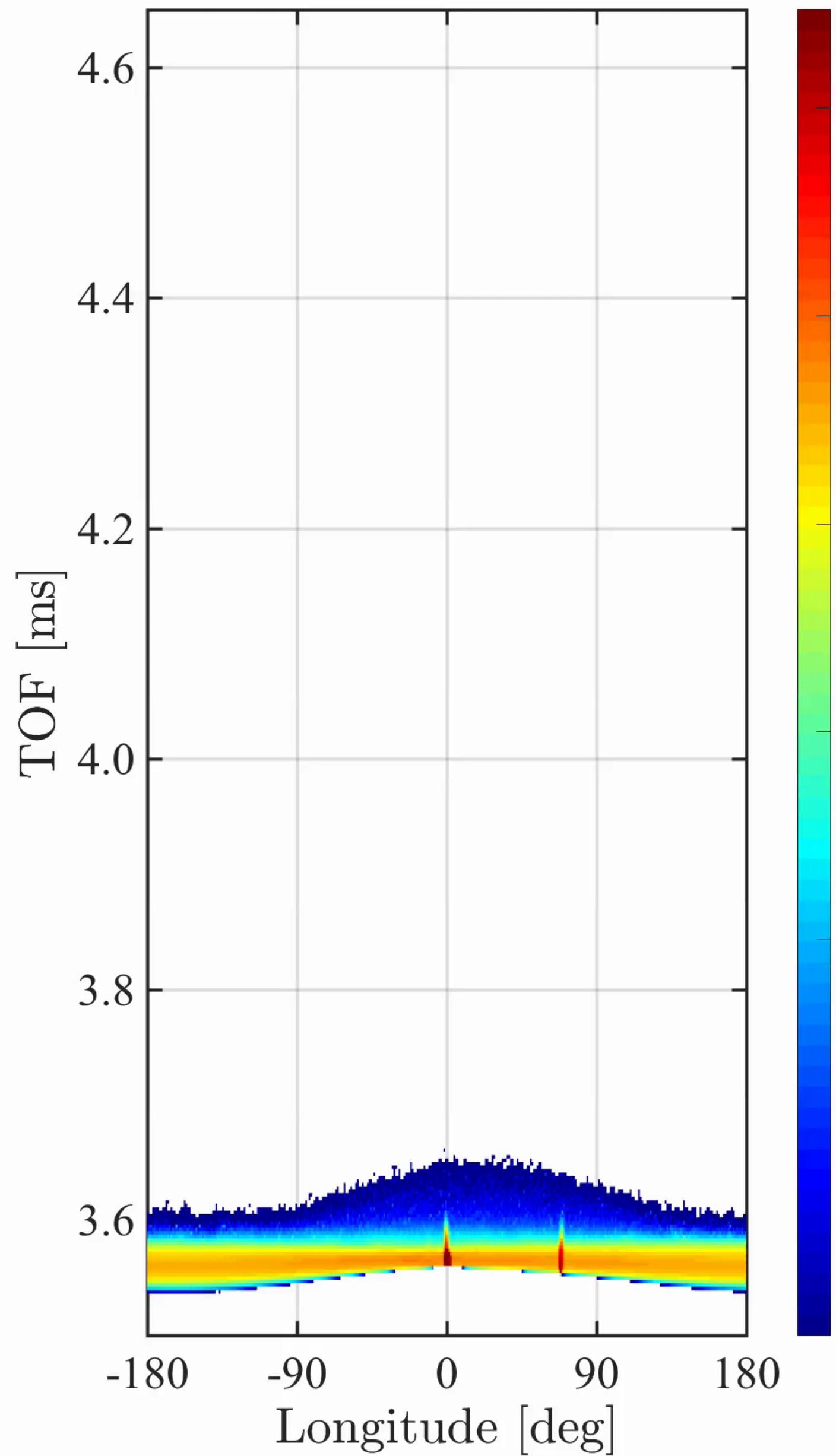
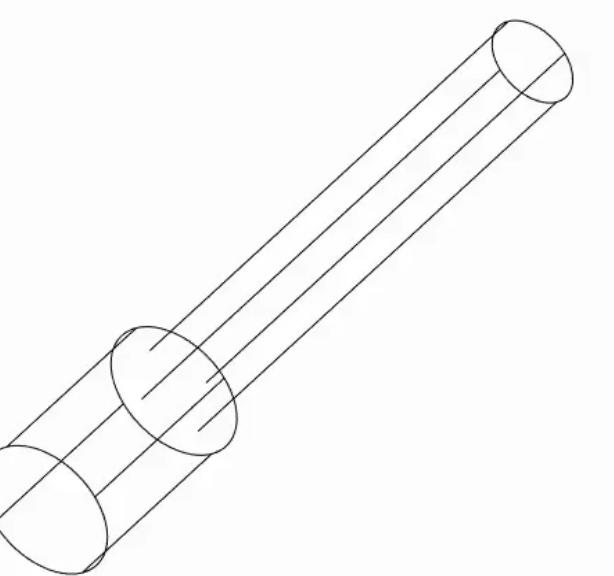
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Building a sample

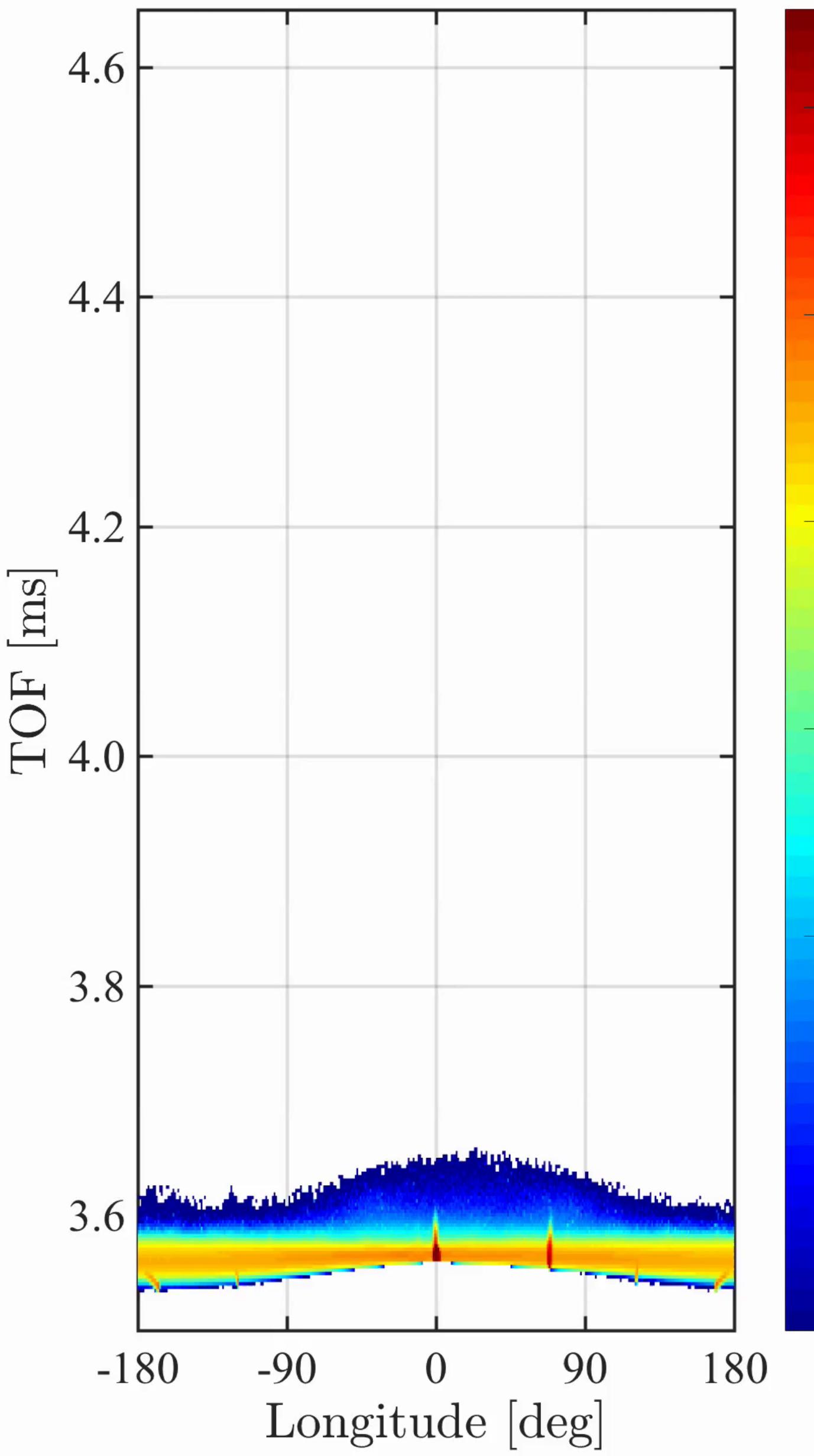
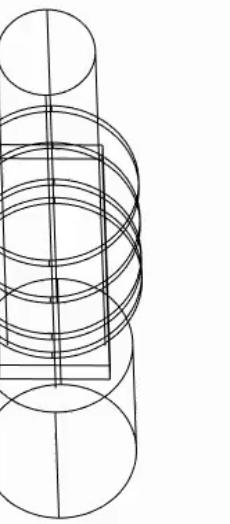


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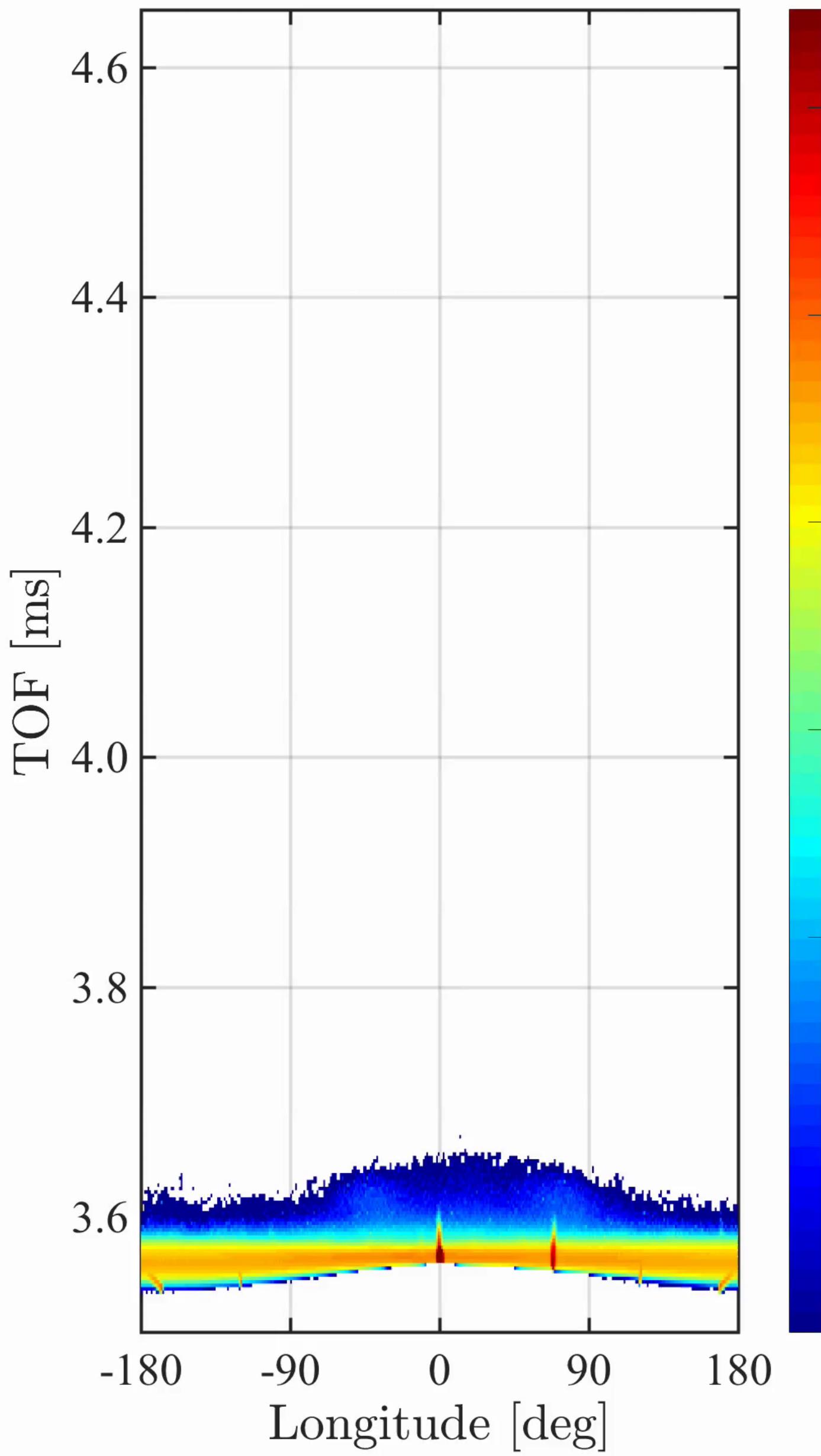
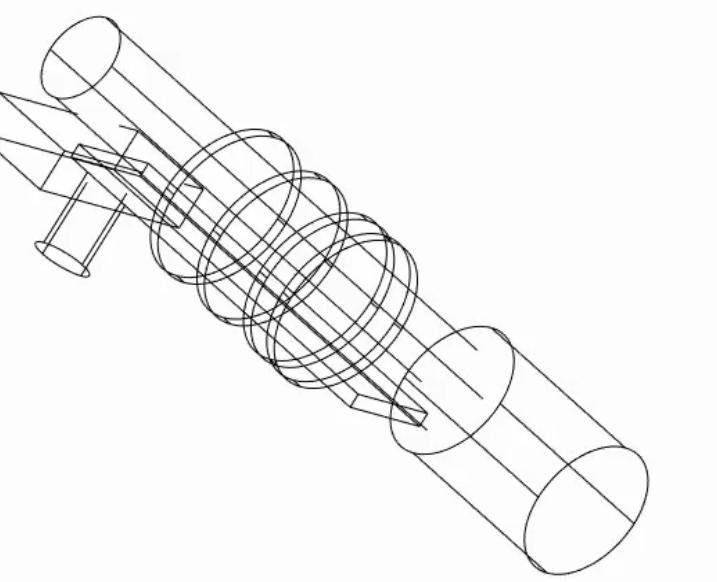
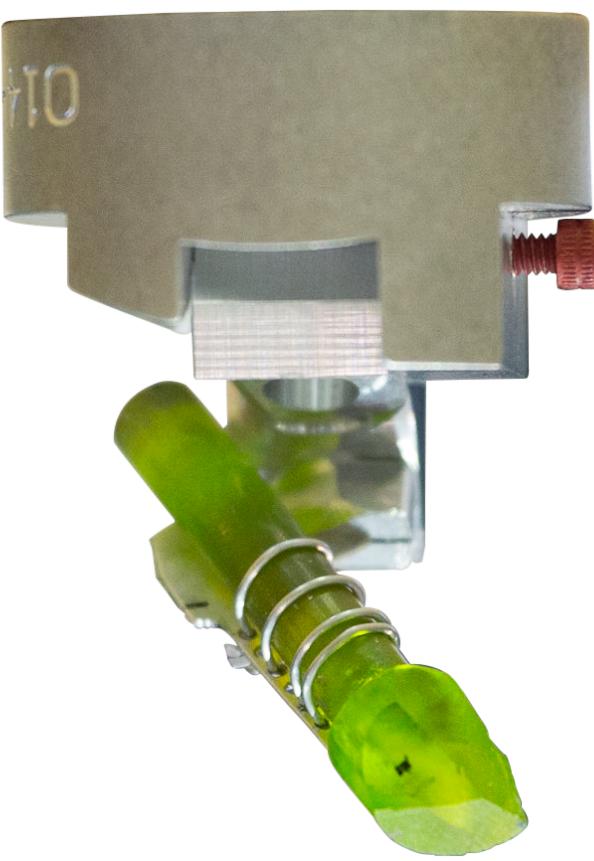
Building a sample



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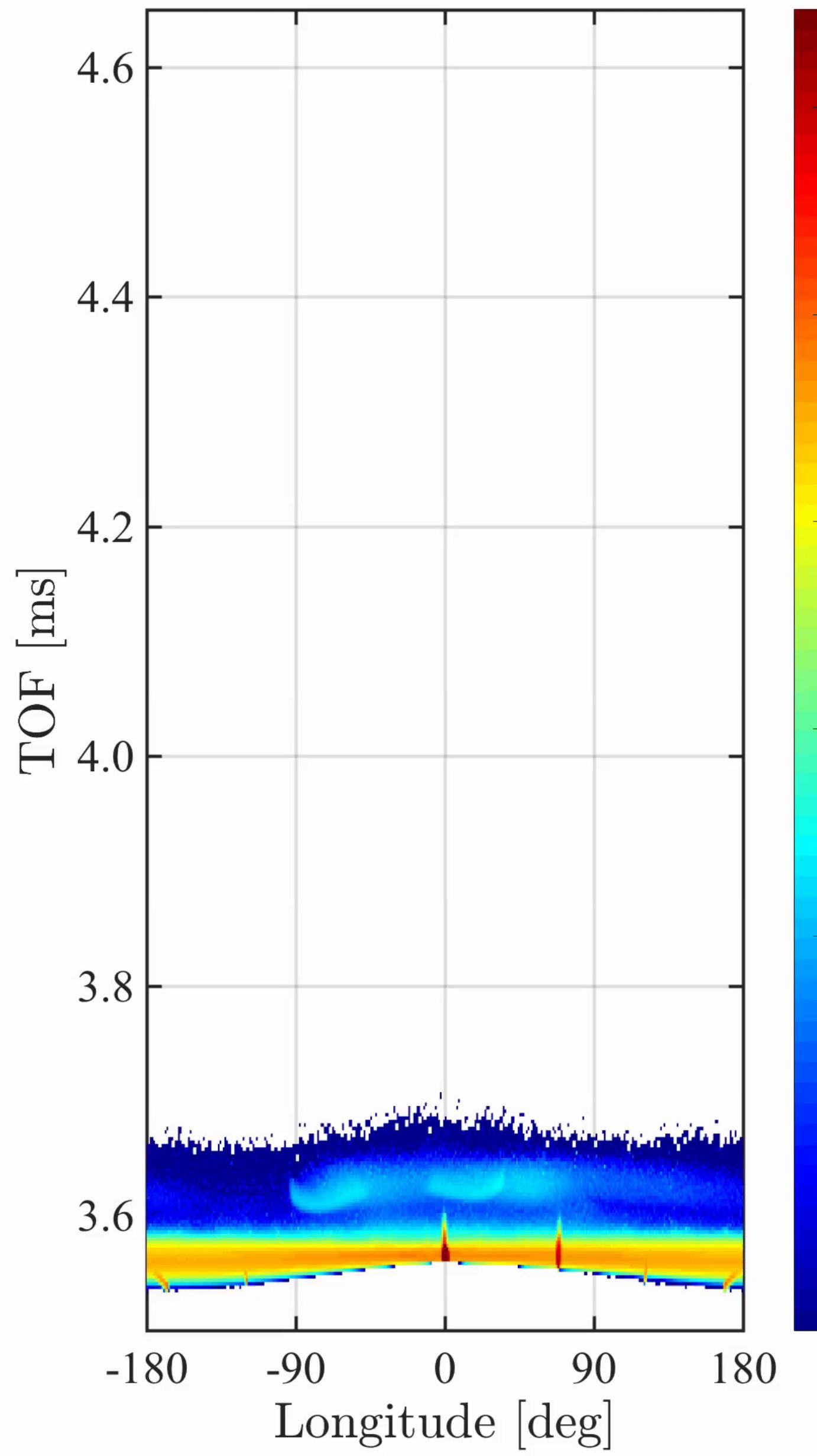
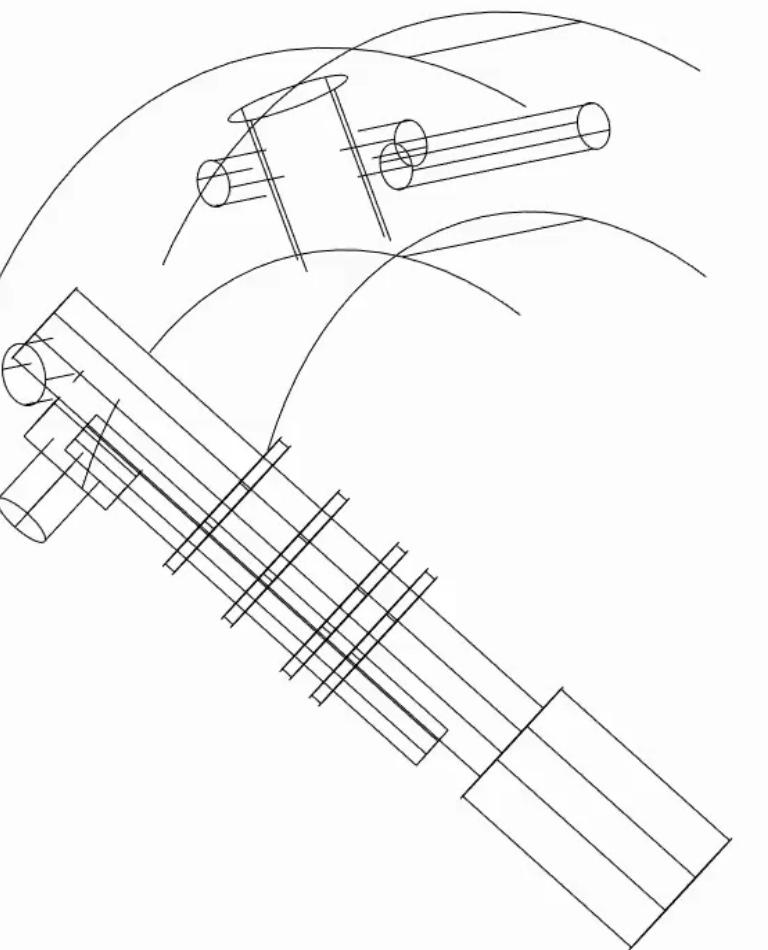
Building a sample



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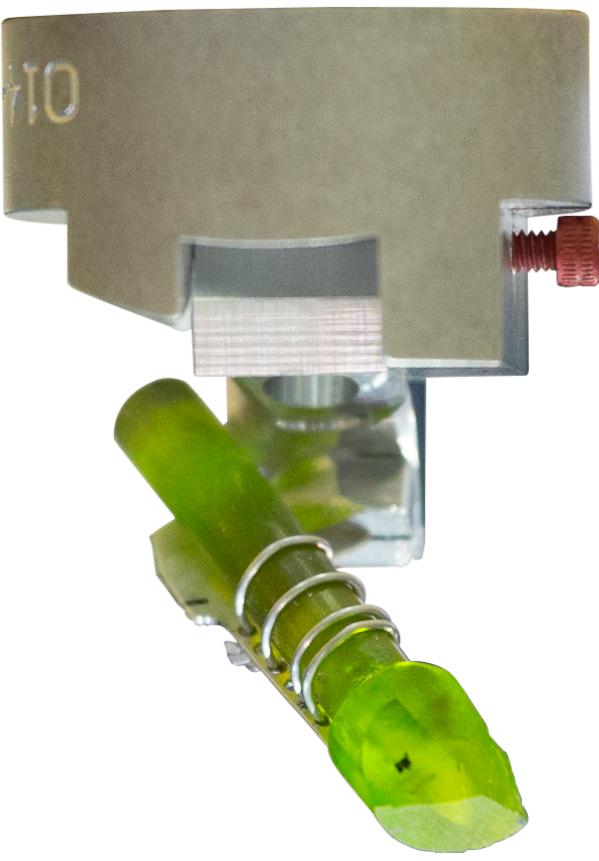
Building a sample



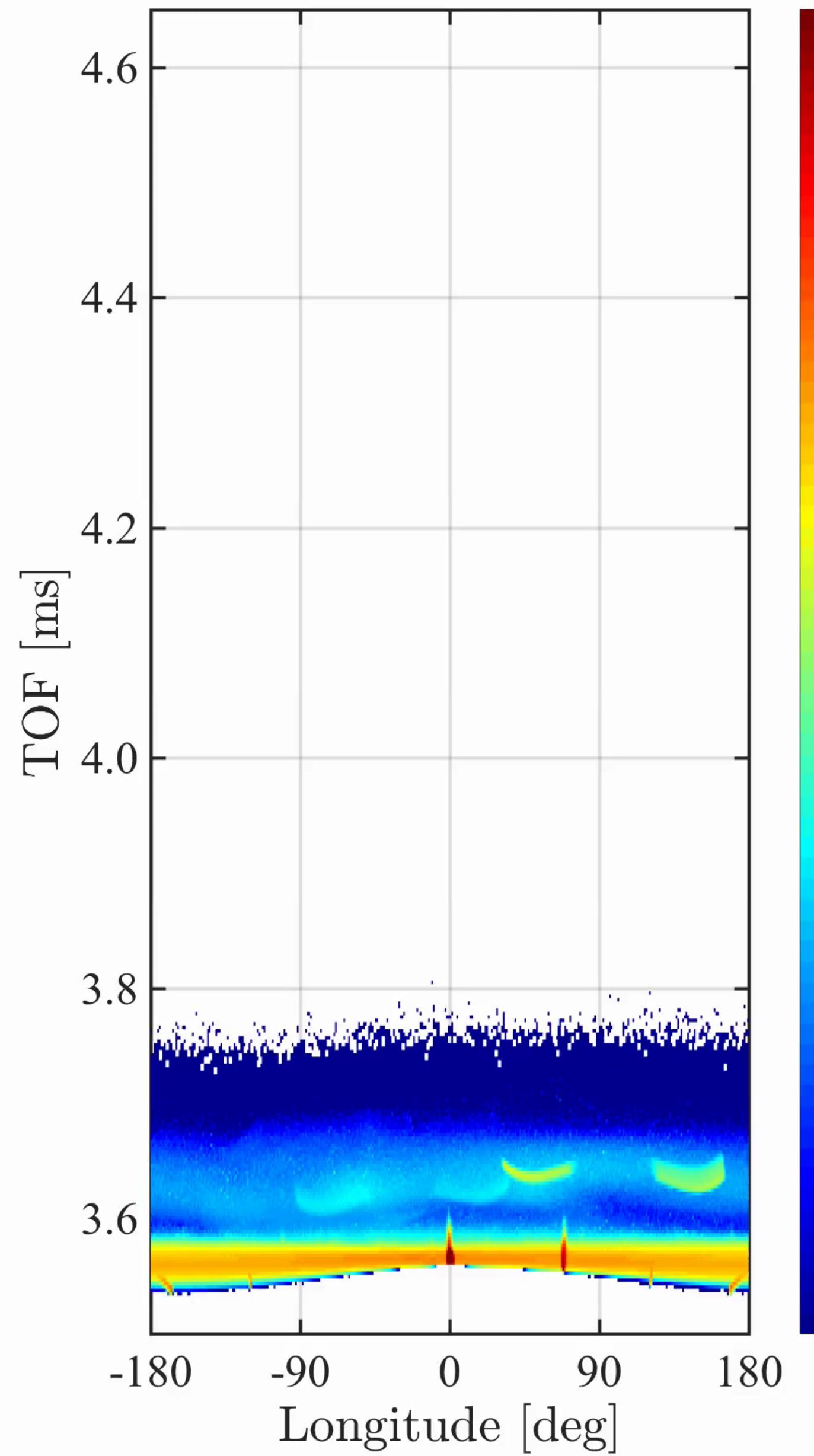
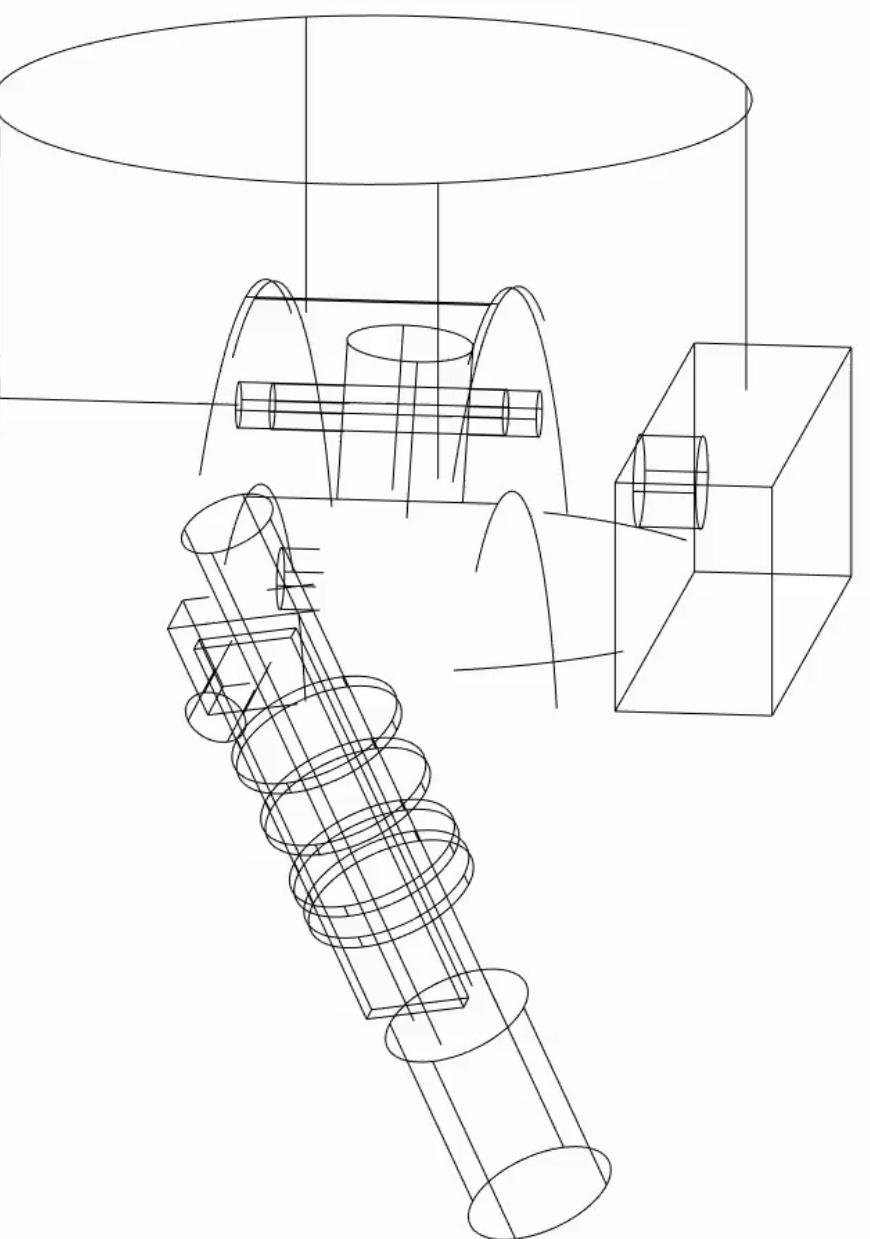
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Building a sample

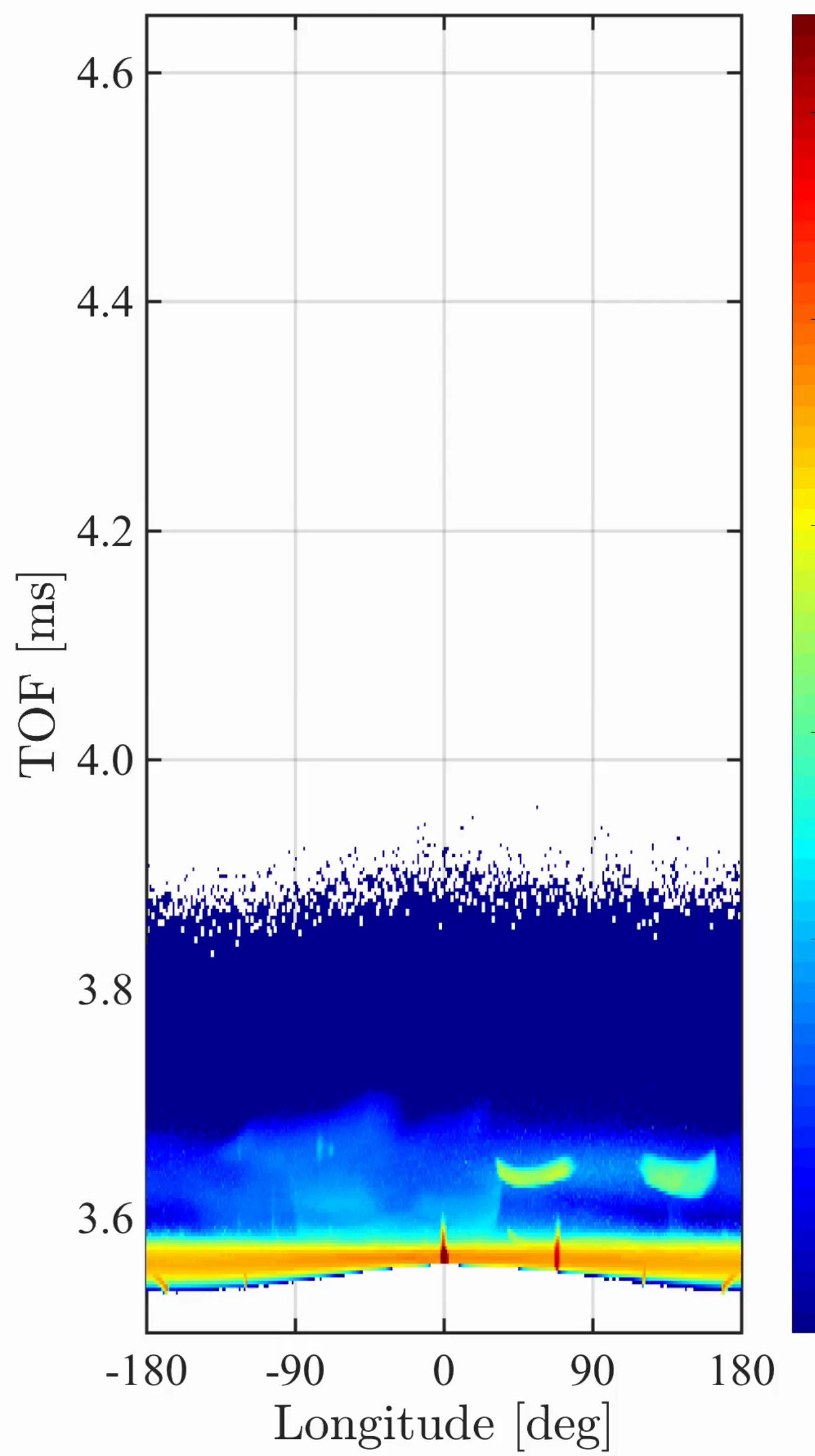
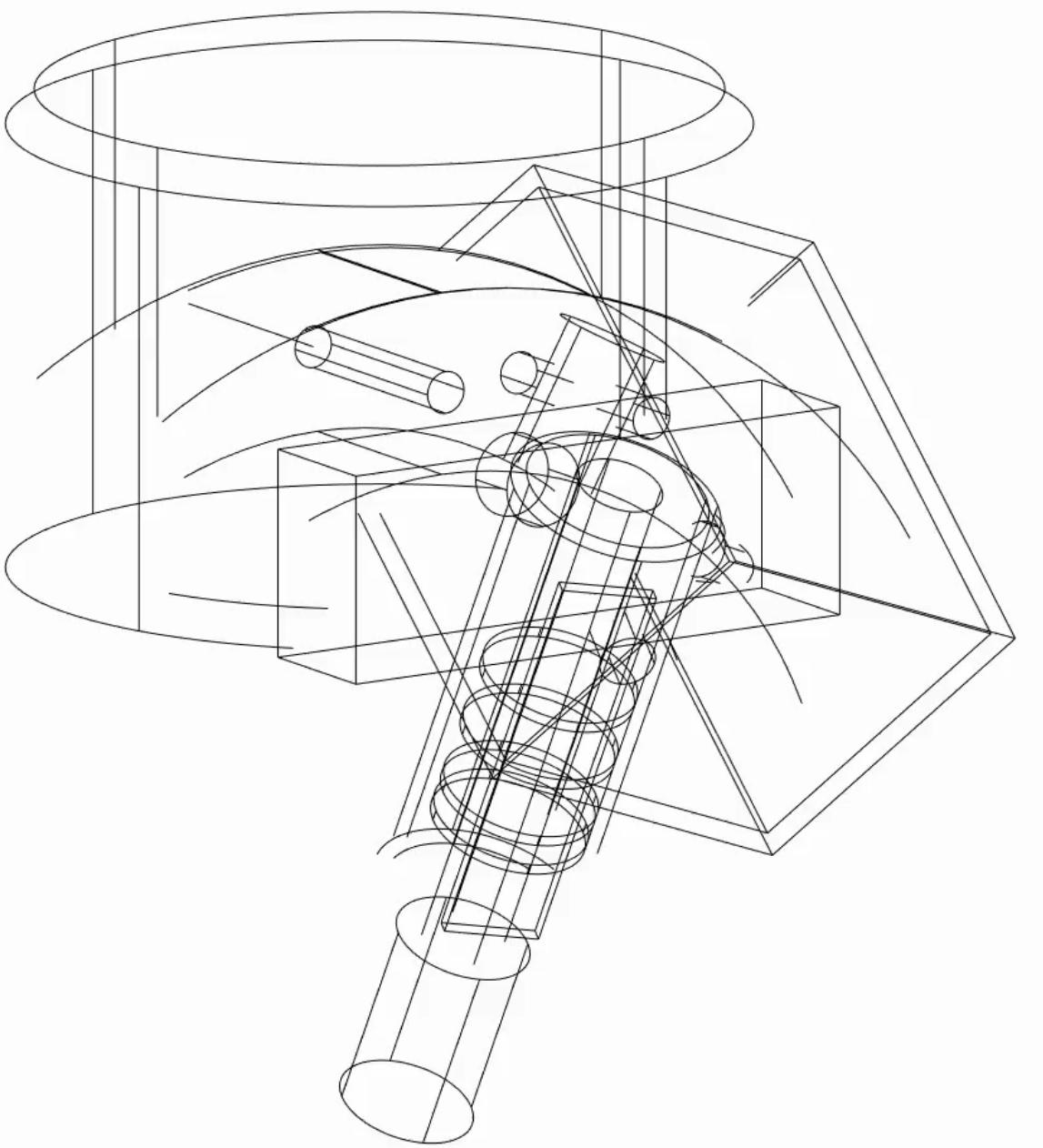


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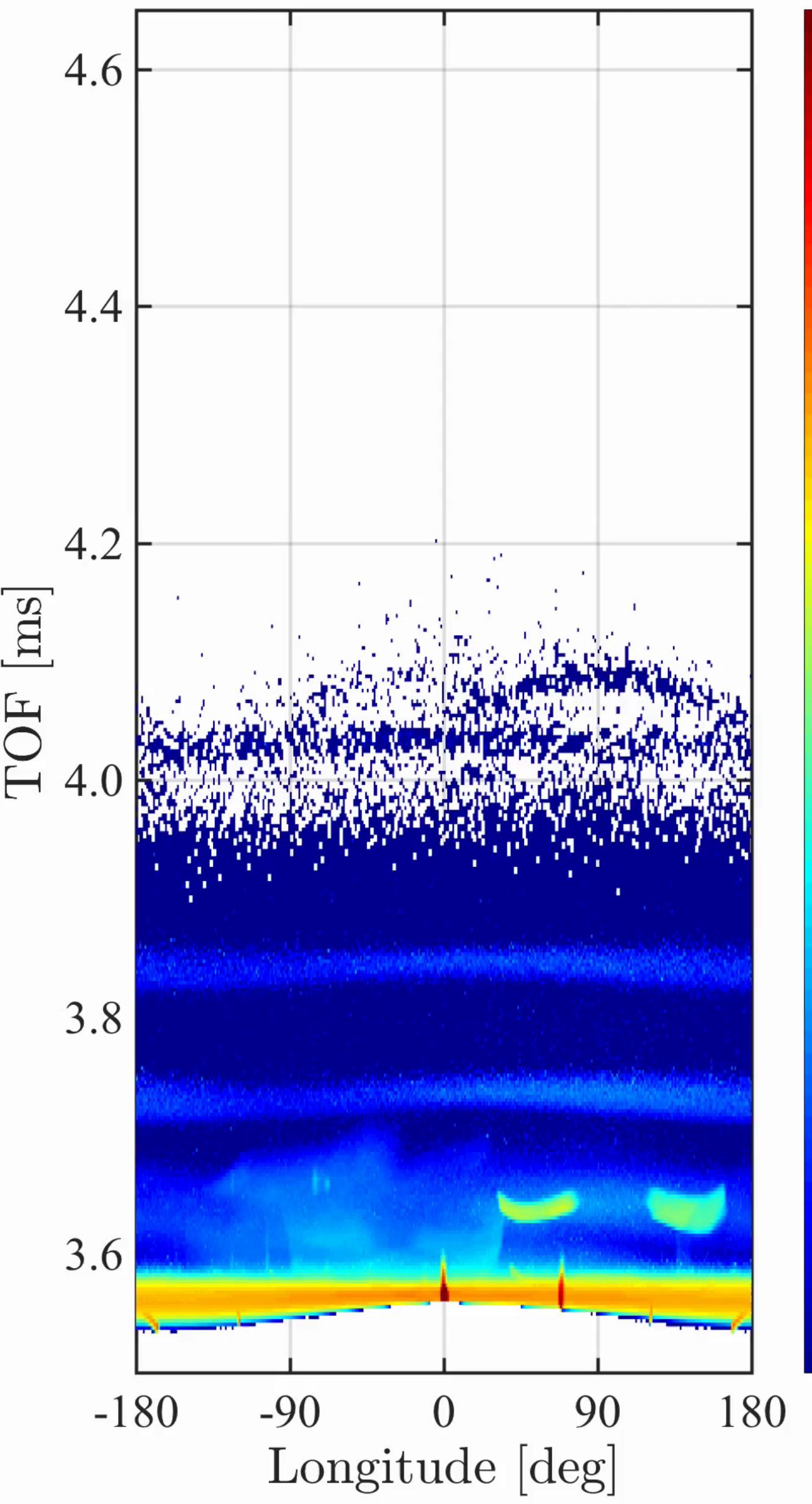
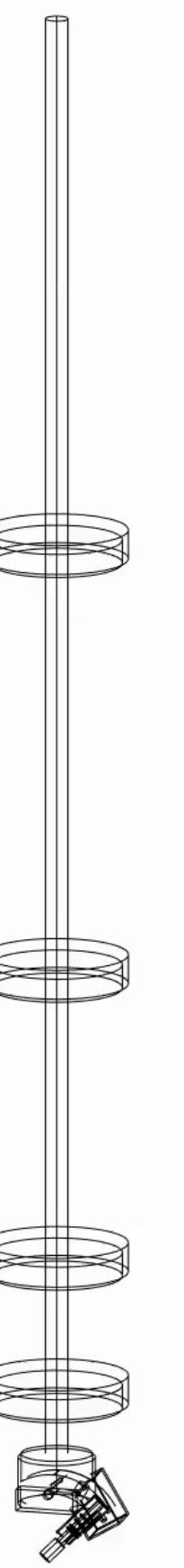
Building a sample



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$\log(I)$

Building a sample



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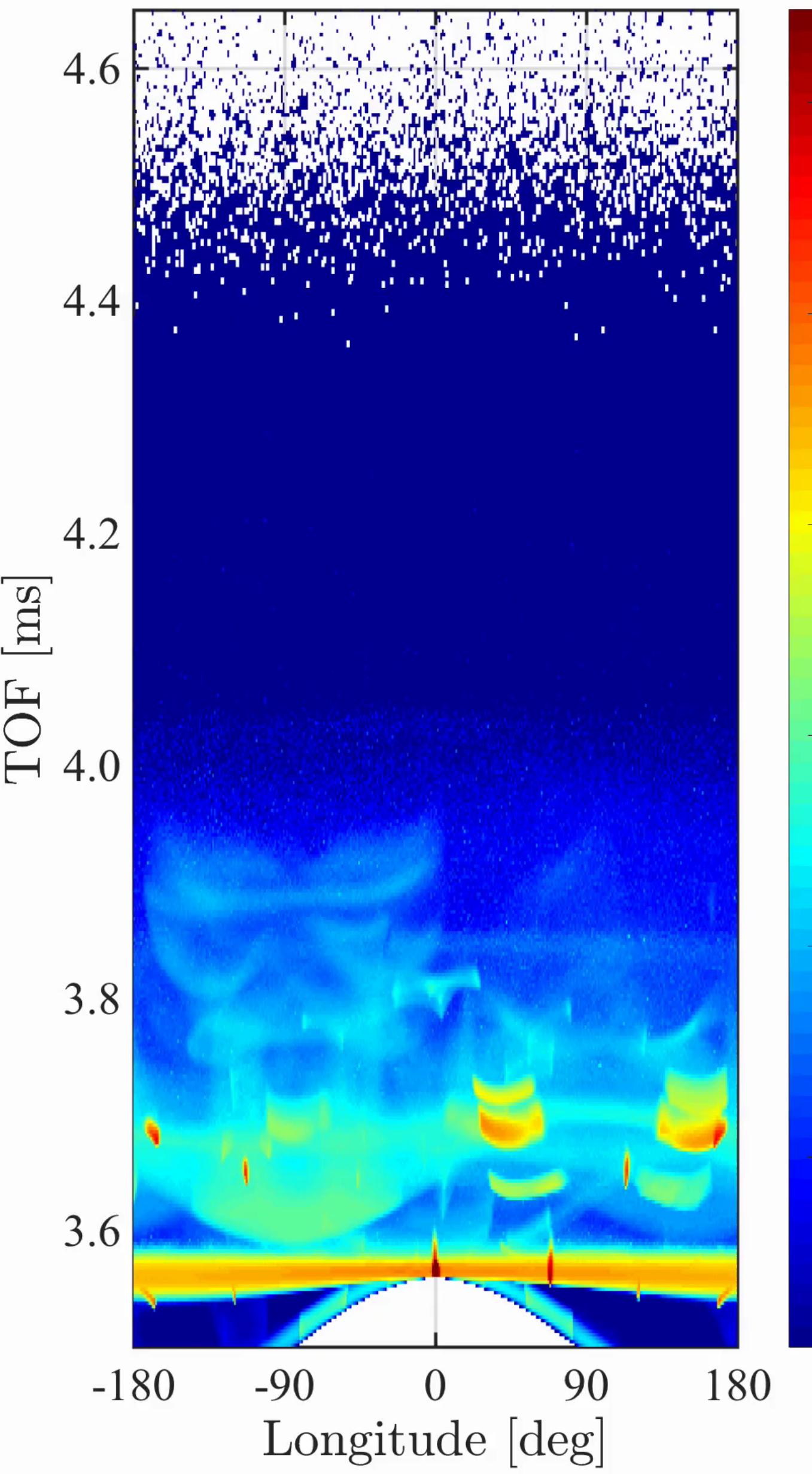
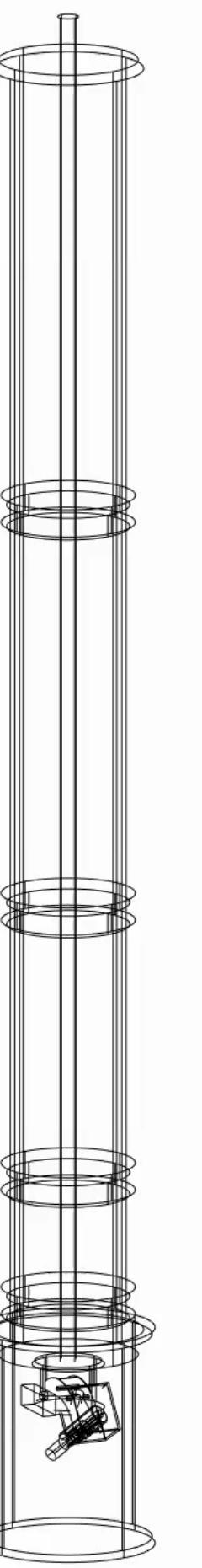
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Building a sample



Image from NIST webpage

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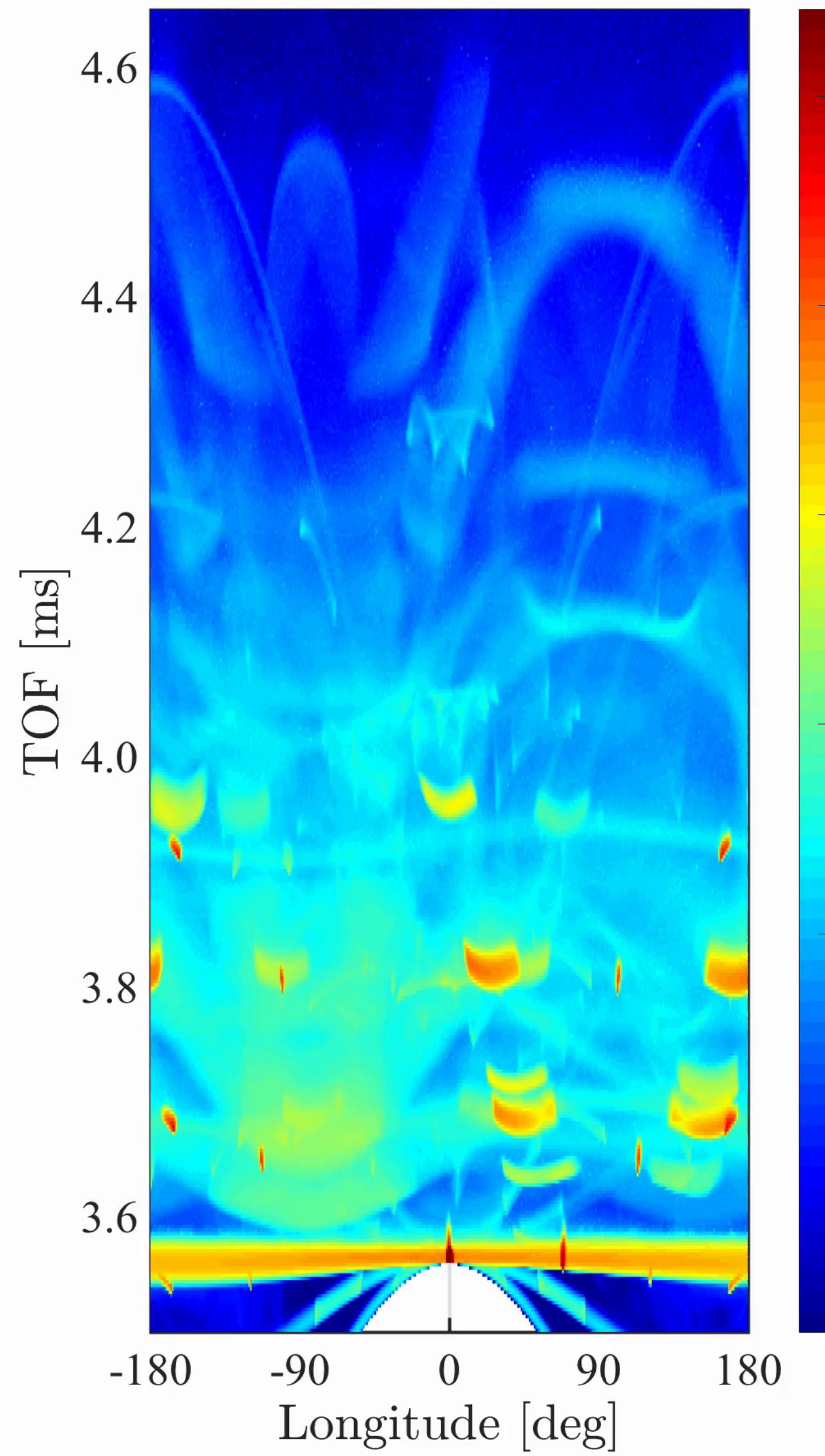
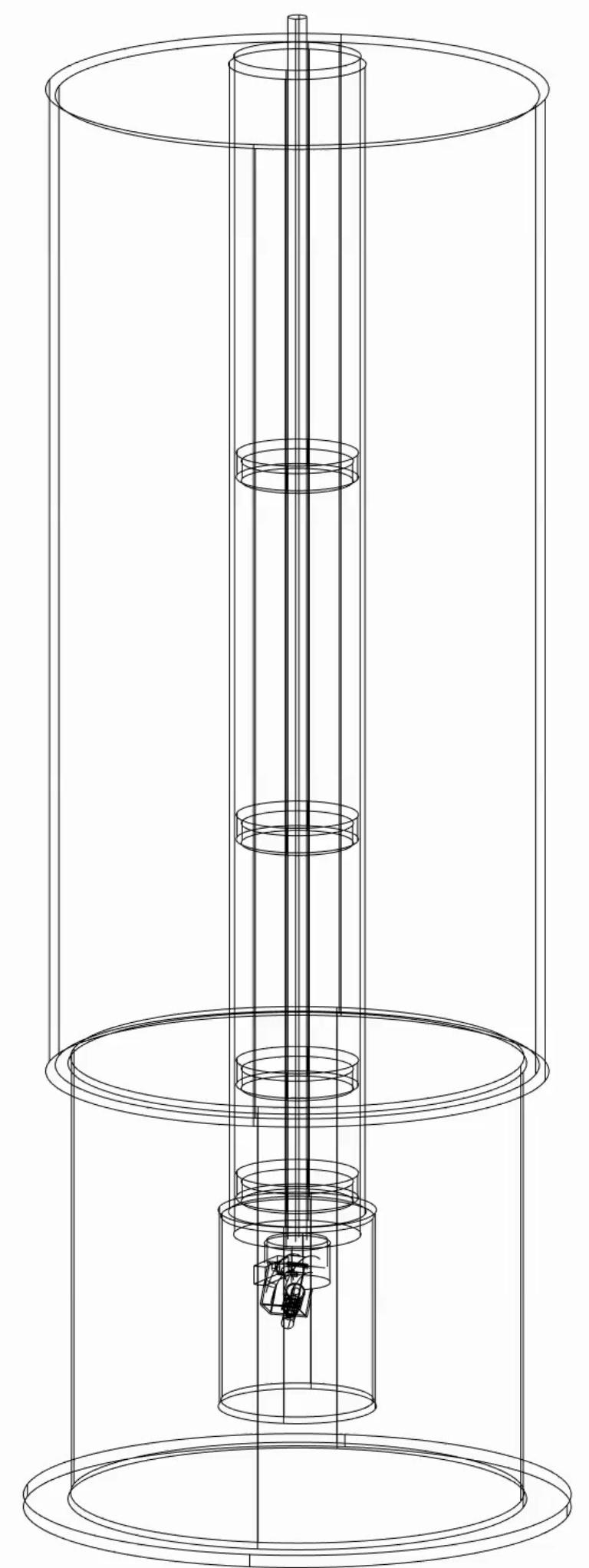


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