HyperSpy-quantification

December 19, 2022

1 Quantification in HyperSpy

[1]:
```
import hyperspy.api as hs
```

1.1 Quantification with linear background removal

[2]:
```
path="data/2022-09-06_EDS-SEM-APREO/"
file = "GaAs_30kV.emsa"
s = hs.load(path+file, signal_type='EDS_TEM')
s.add_elements(['As', 'Ga'])
# s.plot(xray_lines=True)
```

[3]:
```
bw = s.estimate_background_windows(windows_width=2)
iw =  s.estimate_integration_windows(windows_width=2)
# s.plot(xray_lines=True, background_windows=bw, integration_windows=iw)
```

[4]:
```
s_intensities = s.get_lines_intensity(background_windows=bw,␣
 ↪integration_windows=iw)
k_factors = [4.191, 3.268] # As, Ga
quant = s.quantification(s_intensities, 'CL', factors=k_factors)
print(f'{file} quantification\nAs: {quant[0].data[0]:.2f} %, Ga: {quant[1].
 ↪data[0]:.2f} %')
```

```
[########################################] | 100% Completed | 118.19 ms
GaAs_30kV.emsa quantification
As: 56.95 %, Ga: 43.05 %
```

1.2 Quantification with intensity from model fit

[5]:
```
# model fit
m = s.create_model(auto_background=False)
m.add_polynomial_background(order=6)
m.add_family_lines(['As_Ka', 'Ga_Ka'])

m.fit()
'm'
# m.plot(True)
```

[5]: 'm'

[6]:
```
m_intensities = m.get_lines_intensity()
for bs in m_intensities:
    print(bs.metadata.Sample.xray_lines)
k_factors = [4.191, 3.268] # As, Ga
m_intensities[0::2] # selects As Ka and Ga Ka
quant = s.quantification(m_intensities[0::2], 'CL', factors=k_factors)
print(f'{file} quantification with model fit')
print(f'As: {quant[0].data[0]:.2f} %, Ga: {quant[1].data[0]:.2f} %')
```

```
['As_Ka']
['As_La']
['Ga_Ka']
['Ga_La']
[########################################] | 100% Completed | 109.13 ms
GaAs_30kV.emsa quantification with model fit
As: 41.31 %, Ga: 58.69 %
```

1.3 Quantification with intensity from model fit, after calibration

[7]:
```
# quanitfication after calibration in HyperSpy

m.calibrate_energy_axis(calibrate='scale')
m.calibrate_energy_axis(calibrate='offset')

m_intensities = m.get_lines_intensity()
for bs in m_intensities:
    print(bs.metadata.Sample.xray_lines)

k_factors = [4.191, 3.268] # As, Ga
m_intensities[0::2] # selects As Ka and Ga Ka
quant = s.quantification(m_intensities[0::2], 'CL', factors=k_factors)
print(f'{file} quantification with model fit')
print(f'As: {quant[0].data[0]:.2f} %, Ga: {quant[1].data[0]:.2f} %')

# m.plot(True)
```

```
['As_Ka']
['As_La']
['Ga_Ka']
['Ga_La']
[########################################] | 100% Completed | 106.70 ms
GaAs_30kV.emsa quantification with model fit
As: 41.34 %, Ga: 58.66 %
```