

Dielectric function calculations

11 dec

Used formulas

recap of last time

$$S_{tot}(E) = S_b(E)$$

$$S_b(E) = \frac{N_{ZLP}t}{\pi a_0 m_0 v^2} \text{Im} \left[\frac{-1}{\varepsilon(E)} \right] \ln \left[1 + \left(\frac{\beta}{\theta_E} \right)^2 \right]$$

$$\text{Re} \left[\frac{1}{\varepsilon(E)} \right] = \mathcal{C} \left\{ \text{sgn} \left[\mathcal{S}^{-1} \left\{ \text{Im} \left[\frac{-1}{\varepsilon(E)} \right] \right\} \right] \right\}$$

$$\theta_E = \frac{E}{\gamma m_0 v^2}$$

$$\frac{\int_0^\infty \frac{S(E)}{\ln \left[1 + \left(\frac{\beta}{\theta_E} \right)^2 \right]} \frac{dE}{E}}{\frac{\pi}{2} \left(1 - \operatorname{Re} \left[\frac{1}{\varepsilon(0)} \right] \right)} = \frac{N_{ZLPT}}{\pi a_0 m_0 v^2} \equiv K,$$

$$S_s(E) = \frac{2I_0 k_0^{-1} \left[\operatorname{Im} \left(\frac{-4}{1+\varepsilon} \right) - \operatorname{Im} \left(\frac{-1}{\varepsilon} \right) \right]}{\pi^2 a_0 m_0 v^2} \left[\frac{\tan^{-1}(\beta/\theta_E)}{\theta_E} - \frac{\beta}{\beta^2 + \theta_E^2} \right]$$

$$\hbar \mathbf{k}_0 = \gamma m_0 \mathbf{v}$$

$$\theta_E = \frac{E}{\gamma m_0 v^2}$$

Plan of attack

- Assume:

$$S_{tot}(E) = S_b'(E)$$

- Calculate ε' with KK-analysis

- Calculate

$$S_s'(E) = C_s(E) \left(\operatorname{Im} \left[\frac{-4}{1 + \varepsilon'(E)} \right] - \operatorname{Im} \left[\frac{-1}{\varepsilon'(E)} \right] \right)$$

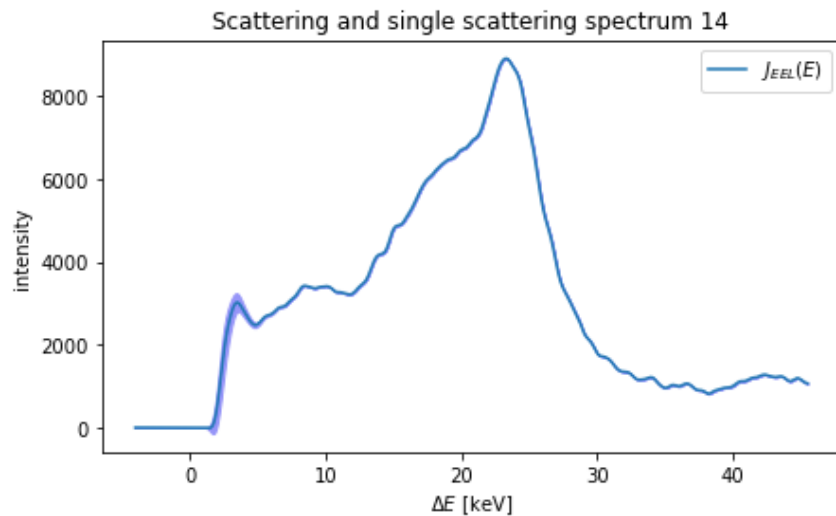
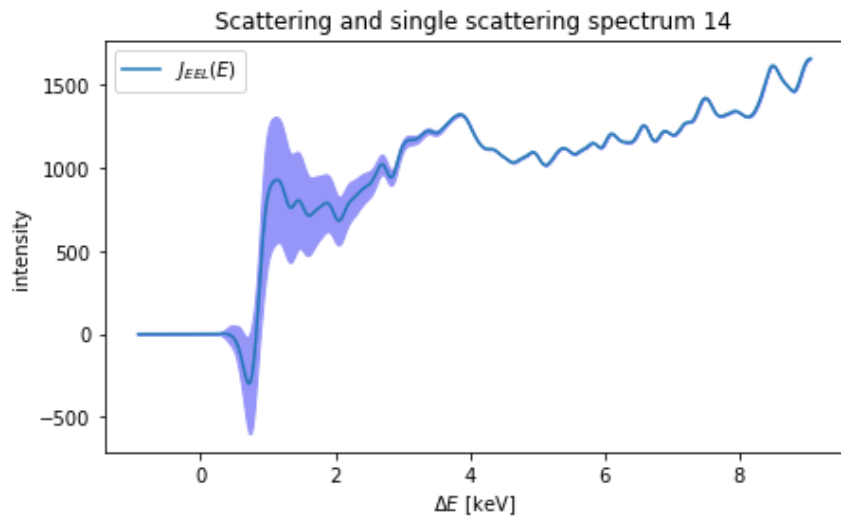
- Better approximation:

$$S_b''(E) = S_{tot}(E) - S_s'(E)$$

- Calculate ε'' with KK-analysis
- Calculate S_s''
- Approximate S_b'''
 - Calculate ε''' with KK-analysis
 - Calculate S_s'''
 - Approximate S_b''''

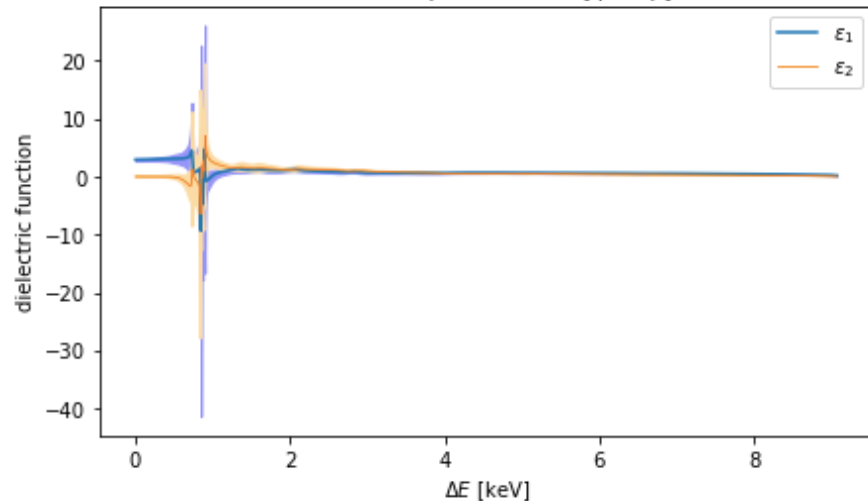
Repeat until convergence

EELS

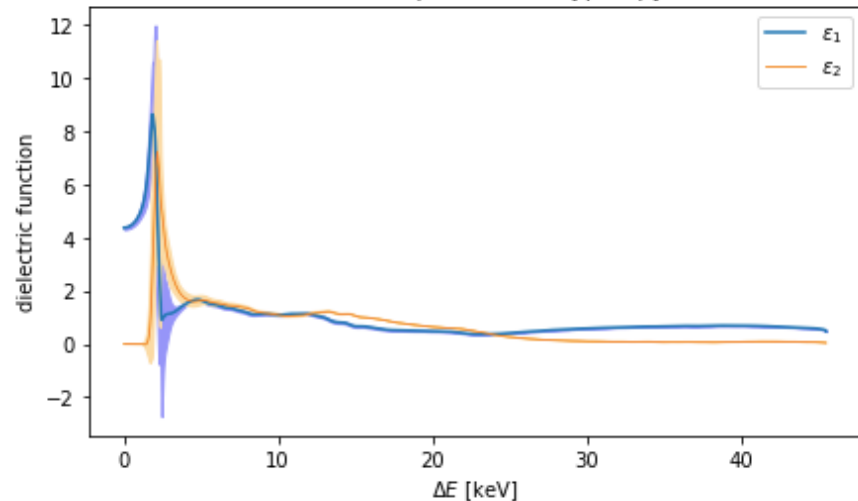


First iteration

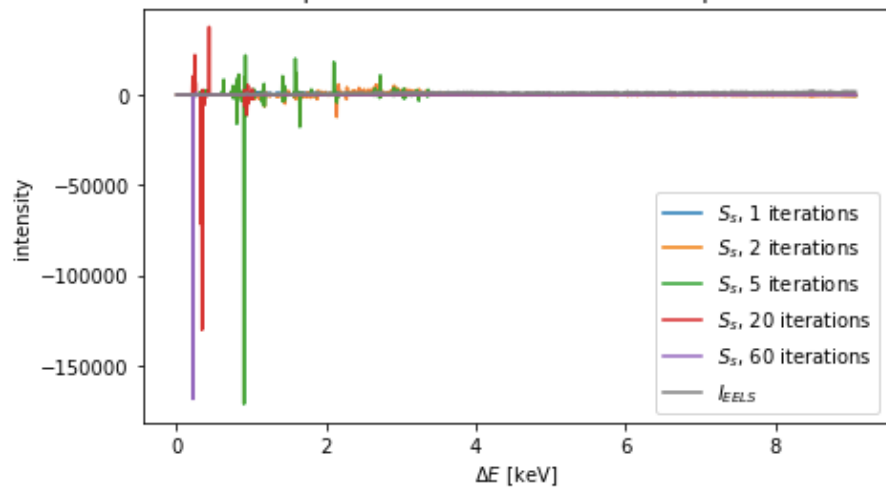
error in dielectric function specimen 3, hyperspy, no iterations: 1



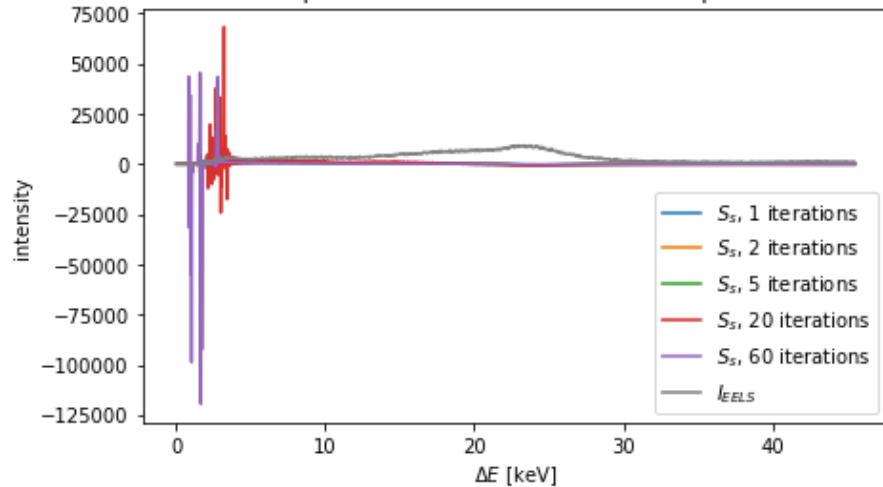
error in dielectric function specimen 4, hyperspy, no iterations: 1



surface plasmons for different iterations, specimen 3

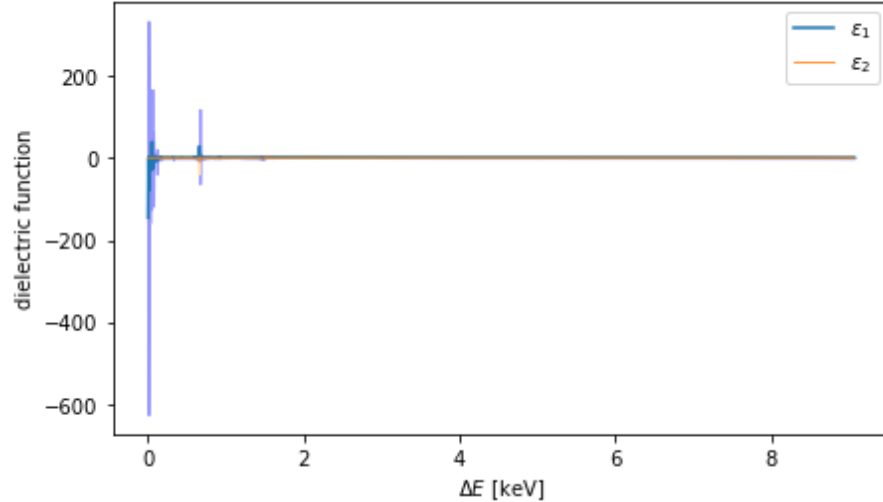


surface plasmons for different iterations, specimen 4

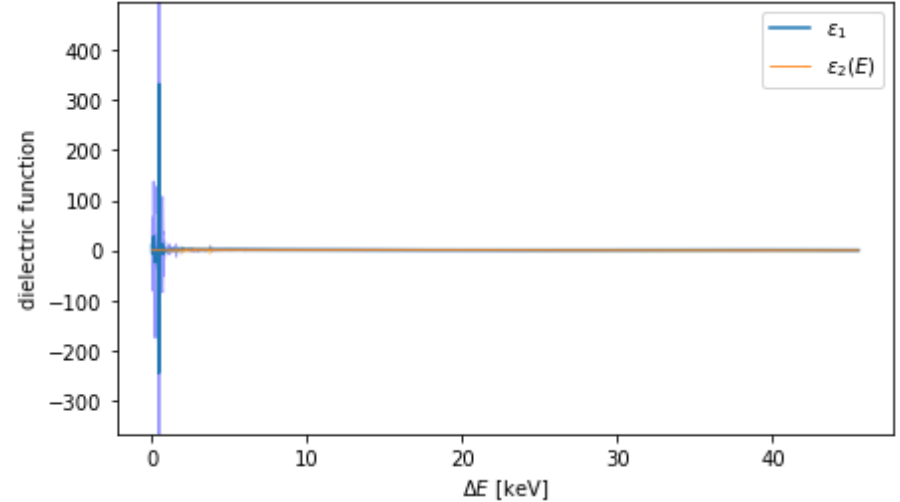


Next iterations

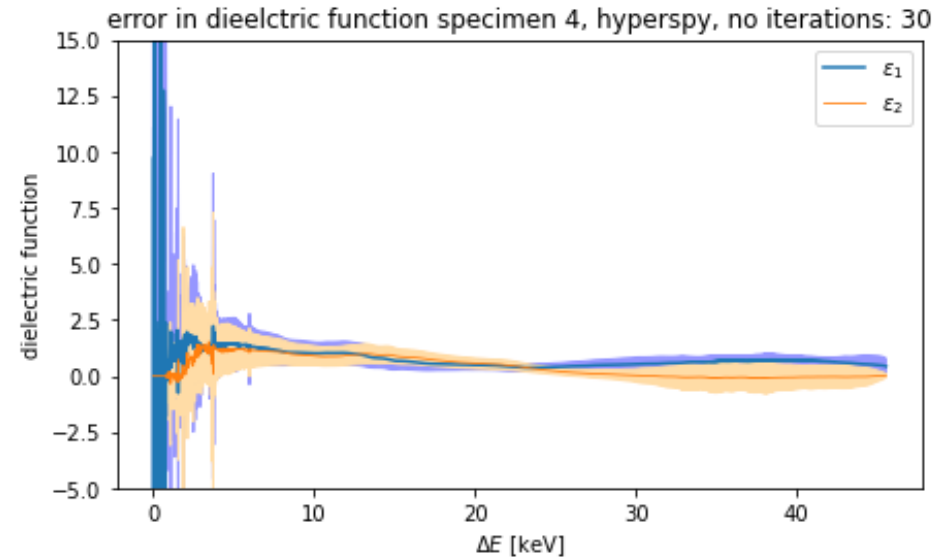
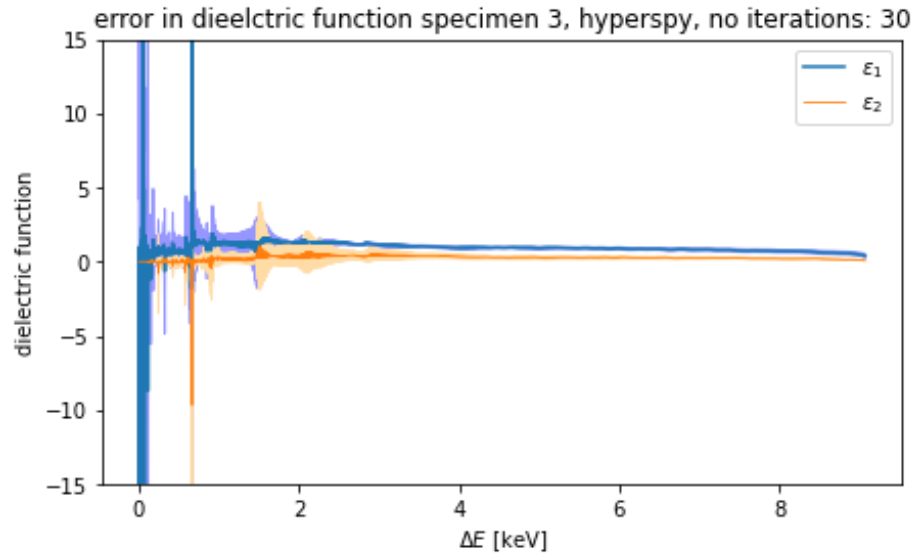
error in dielectric function specimen 3, hyperspy, no iterations: 30



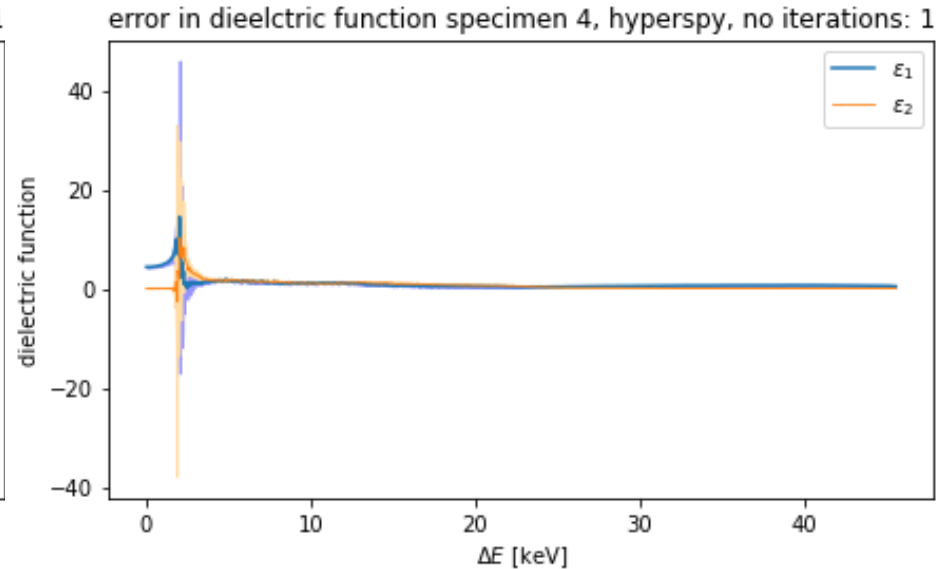
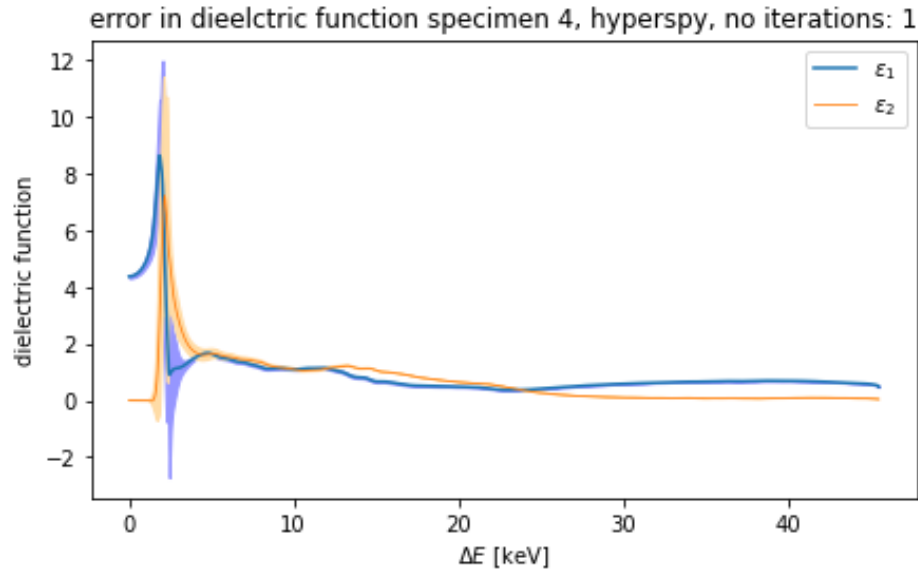
error in dielectric function specimen 4, hyperspy, no iterations: 30



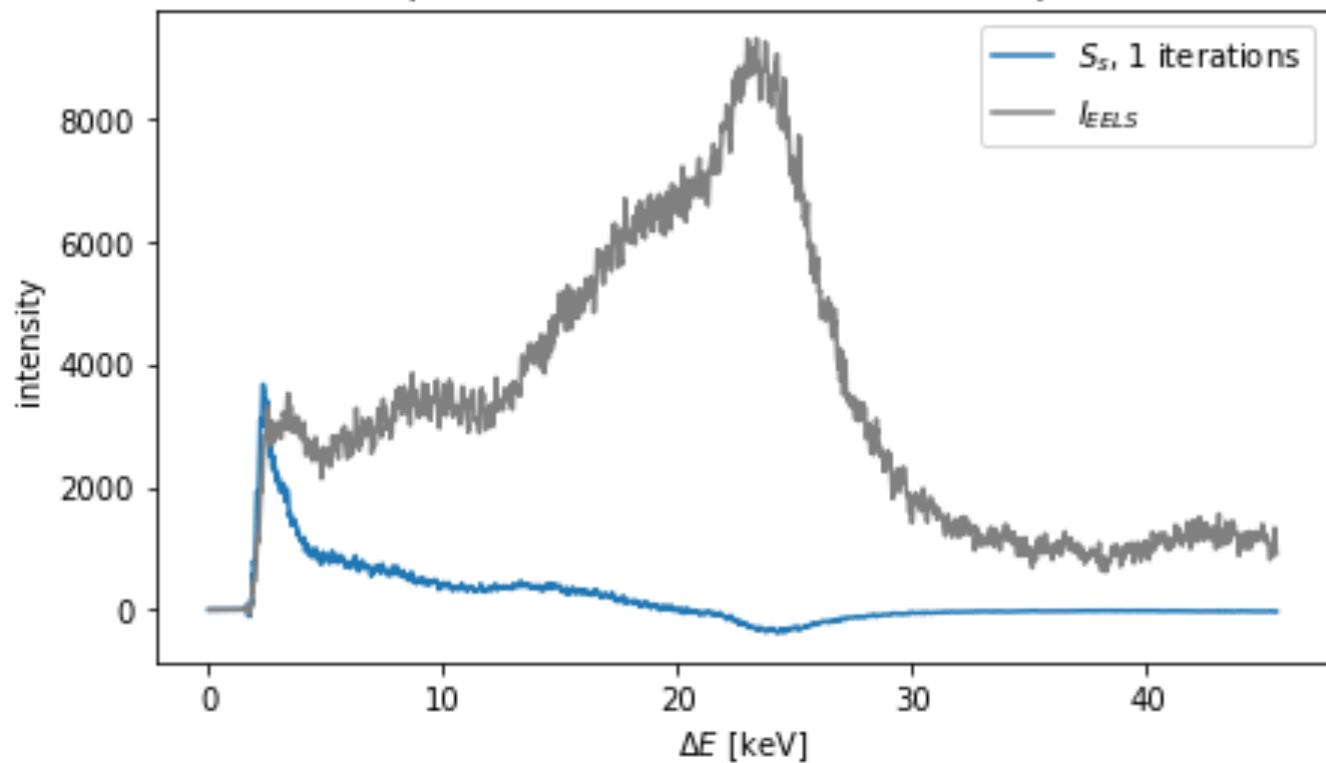
Equal axis over iterations



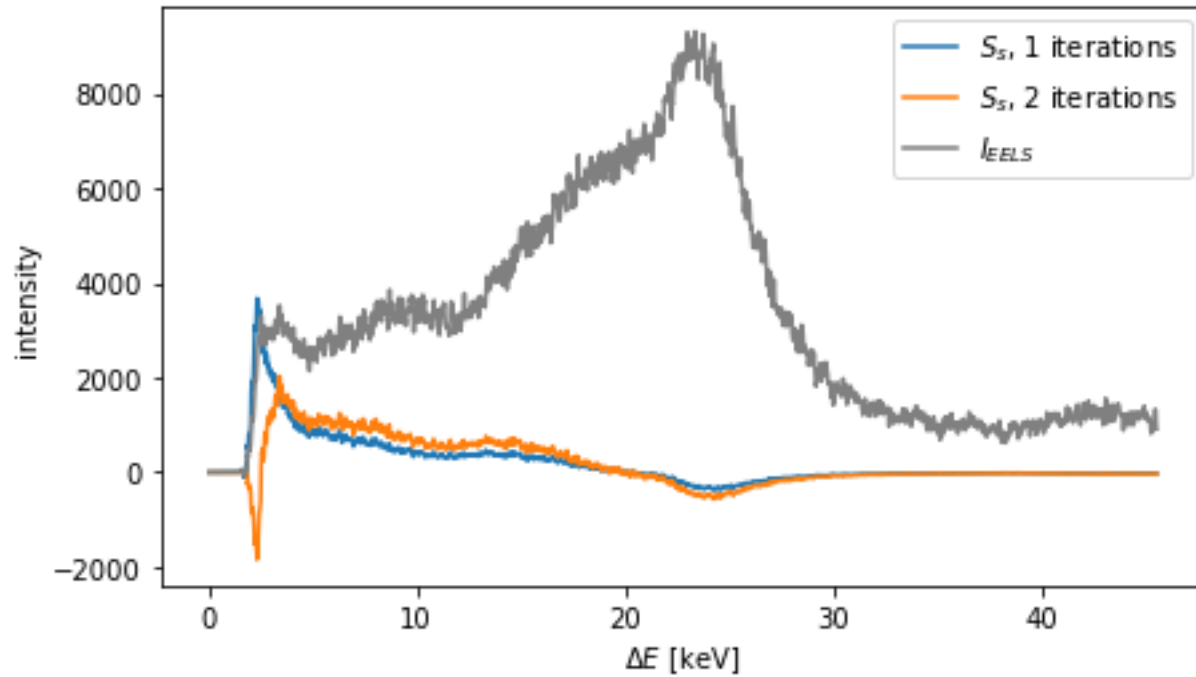
No smoothing

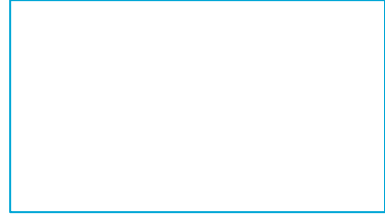


surface plasmons for different iterations, specimen 4



surface plasmons for different iterations, specimen 4





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