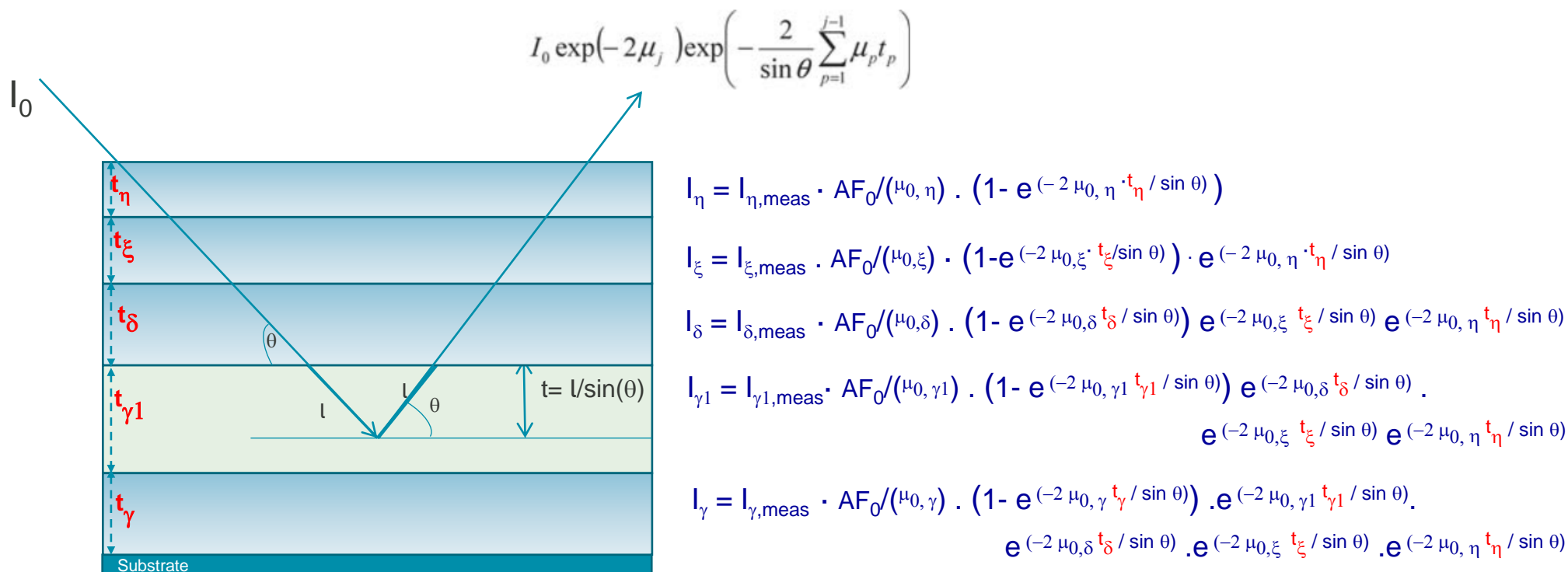


SIMPLE CALCULATION FOR LAYERS

Implemented explicit forms



Intensity corrections for the layered structure related scales and other correction factors



$$I_{\eta} = I_{\eta, \text{meas}} \cdot AF_0 / (\mu_{0, \eta}) \cdot (1 - e^{(-2 \mu_{0, \eta} \cdot t_{\eta} / \sin \theta)})$$

$$I_{\xi} = I_{\xi, \text{meas}} \cdot AF_0 / (\mu_{0, \xi}) \cdot (1 - e^{(-2 \mu_{0, \xi} \cdot t_{\xi} / \sin \theta)}) \cdot e^{(-2 \mu_{0, \eta} \cdot t_{\eta} / \sin \theta)}$$

$$I_{\delta} = I_{\delta, \text{meas}} \cdot AF_0 / (\mu_{0, \delta}) \cdot (1 - e^{(-2 \mu_{0, \delta} \cdot t_{\delta} / \sin \theta)}) \cdot e^{(-2 \mu_{0, \xi} \cdot t_{\xi} / \sin \theta)} \cdot e^{(-2 \mu_{0, \eta} \cdot t_{\eta} / \sin \theta)}$$

$$I_{\gamma 1} = I_{\gamma 1, \text{meas}} \cdot AF_0 / (\mu_{0, \gamma 1}) \cdot (1 - e^{(-2 \mu_{0, \gamma 1} \cdot t_{\gamma 1} / \sin \theta)}) \cdot e^{(-2 \mu_{0, \delta} \cdot t_{\delta} / \sin \theta)} \cdot e^{(-2 \mu_{0, \xi} \cdot t_{\xi} / \sin \theta)} \cdot e^{(-2 \mu_{0, \eta} \cdot t_{\eta} / \sin \theta)}$$

$$I_{\gamma} = I_{\gamma, \text{meas}} \cdot AF_0 / (\mu_{0, \gamma}) \cdot (1 - e^{(-2 \mu_{0, \gamma} \cdot t_{\gamma} / \sin \theta)}) \cdot e^{(-2 \mu_{0, \gamma 1} \cdot t_{\gamma 1} / \sin \theta)} \cdot e^{(-2 \mu_{0, \delta} \cdot t_{\delta} / \sin \theta)} \cdot e^{(-2 \mu_{0, \xi} \cdot t_{\xi} / \sin \theta)} \cdot e^{(-2 \mu_{0, \eta} \cdot t_{\eta} / \sin \theta)}$$

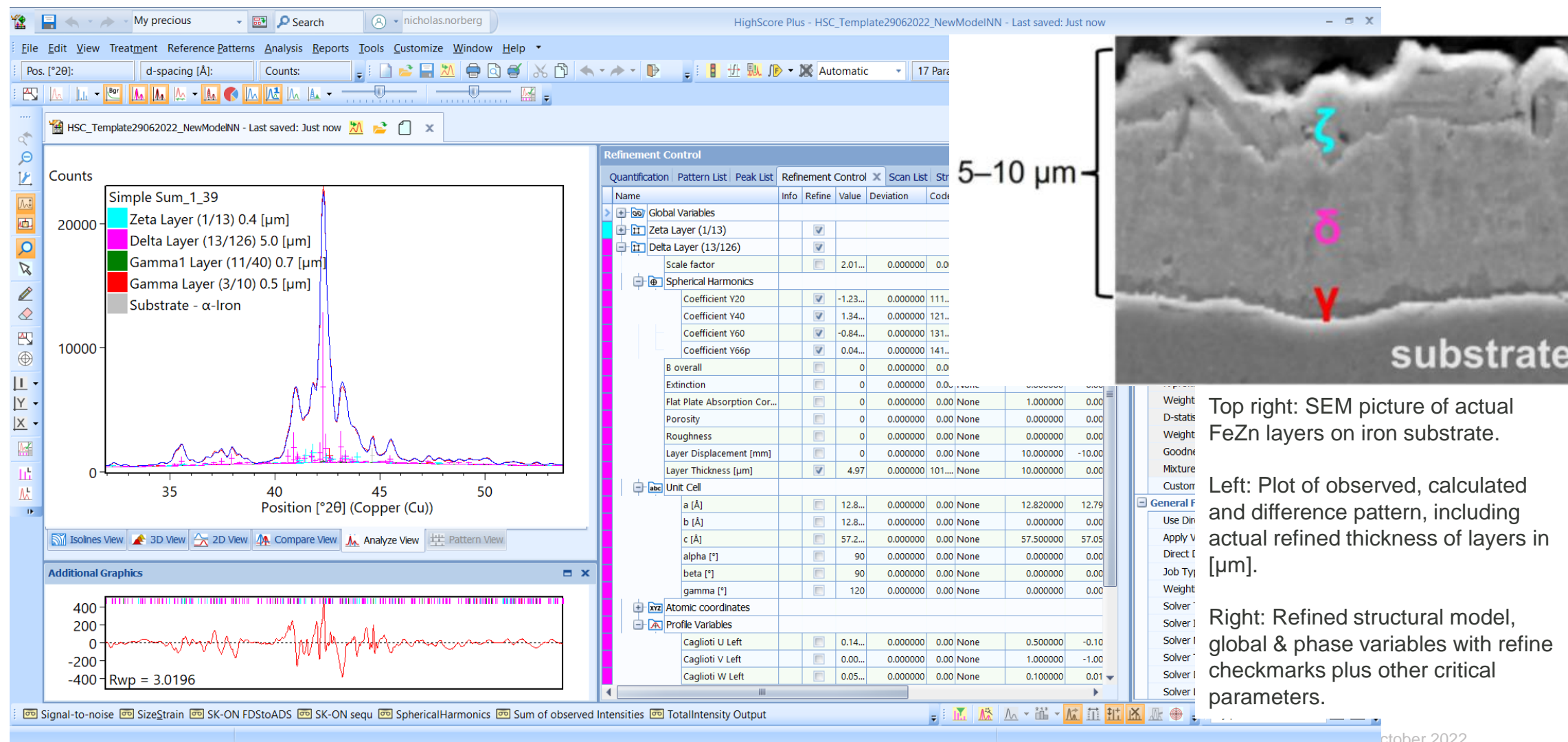
where, t_k : refinable parameters

$\mu_{0, \dots}$: Linear absorption coefficient [cm^{-1}]

and AF_0 : a supplied constant (depending on the instrument)

IMPLEMENTATION IN HIGHSCORE V5.2

Determination of layer thickness & many other parameters from XRD data



Top right: SEM picture of actual FeZn layers on iron substrate.

Left: Plot of observed, calculated and difference pattern, including actual refined thickness of layers in [μm].

Right: Refined structural model, global & phase variables with refine checkmarks plus other critical parameters.