Phase separation in fluorite-related $U_{1-y}Ce_yO_{2-x}$: a re-examination by x-ray and neutron diffraction.

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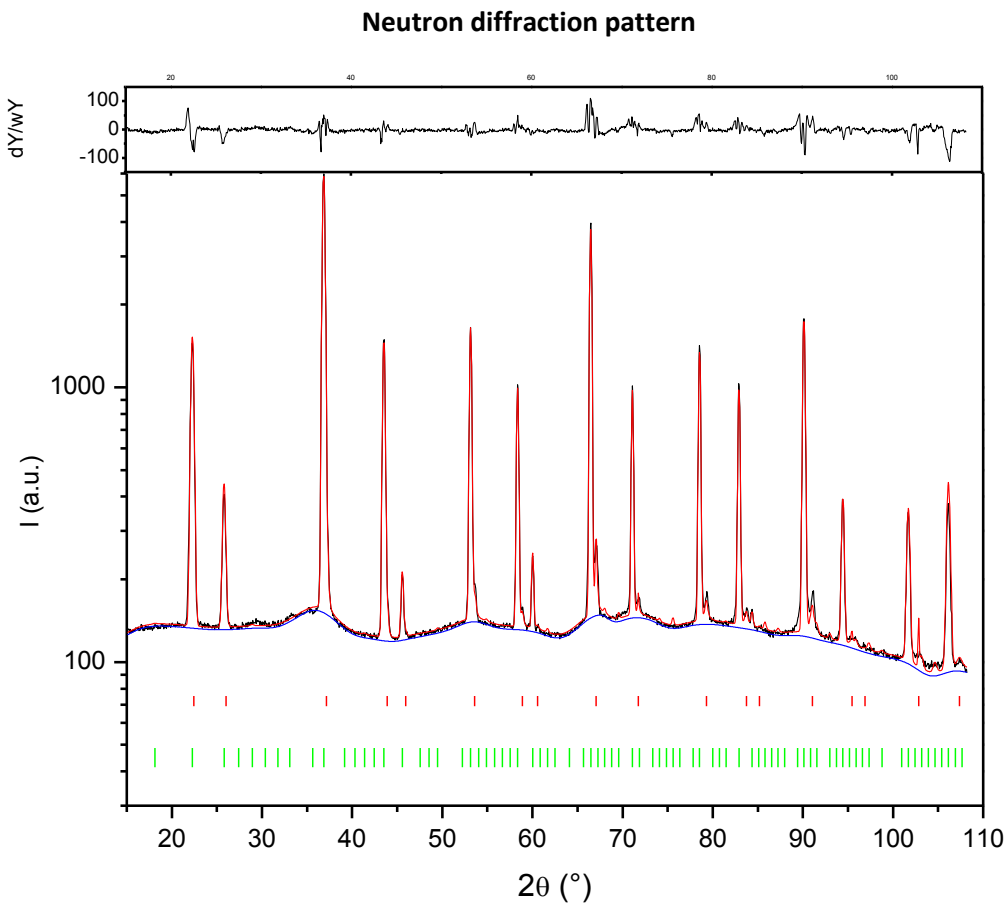

Fig-1a: Rietveld refinement (red line) of neutron diffraction pattern (black line). The background is pollted in blue and the the normalized difference between the refined and experimental intensities is plotted in the insert. Red sticks and green sticks display the positions of different Bragg peaks associated with the fluorite stoichiometric phase $(U0_{.56}Ce_{0.44})O_2$ and the sub stoichiomertric C-type bixbyite structure $(U0_{.56}Ce_{0.44})O_{1.935}$ (results of refinements are summarized in table 2).

Crystallographic Data (powder)

Chemical formula: $(U0_{.56}Ce_{0.44})O_{1.935}$

Formula weight: 225.09 g/mol

Temperature: 300K

Wavelength: 0.12299 nm

Crystal system : Ia-3

Space group: 206

a=10.9838(4) A

b=10.9838(4) A

c=10.9838(4) A

α=90°

β=90°

γ=90°

V=1325.12 A^3

Z=32

d=0.7601 A -4.7113 A

χ^2=2.15

R_p=0.0296

R_{wp}=0.0444