Phase Separation and Superconductivity in $Fe_{1+x}Te_{0.5}Se_{0.5}$

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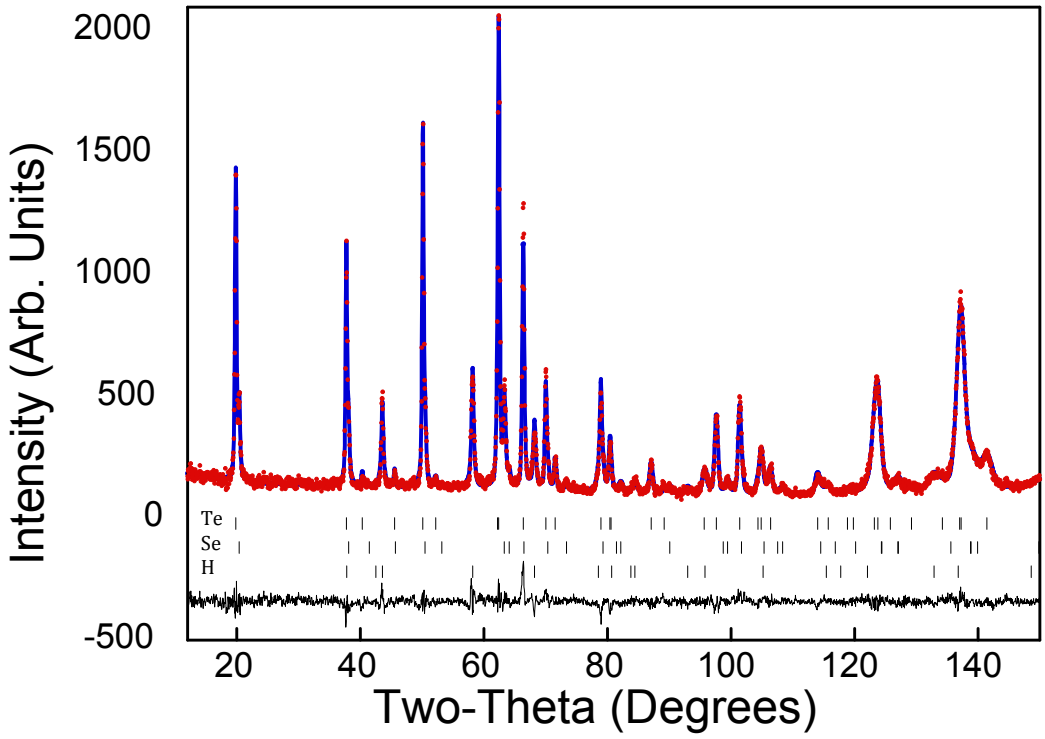
Supplementary Information

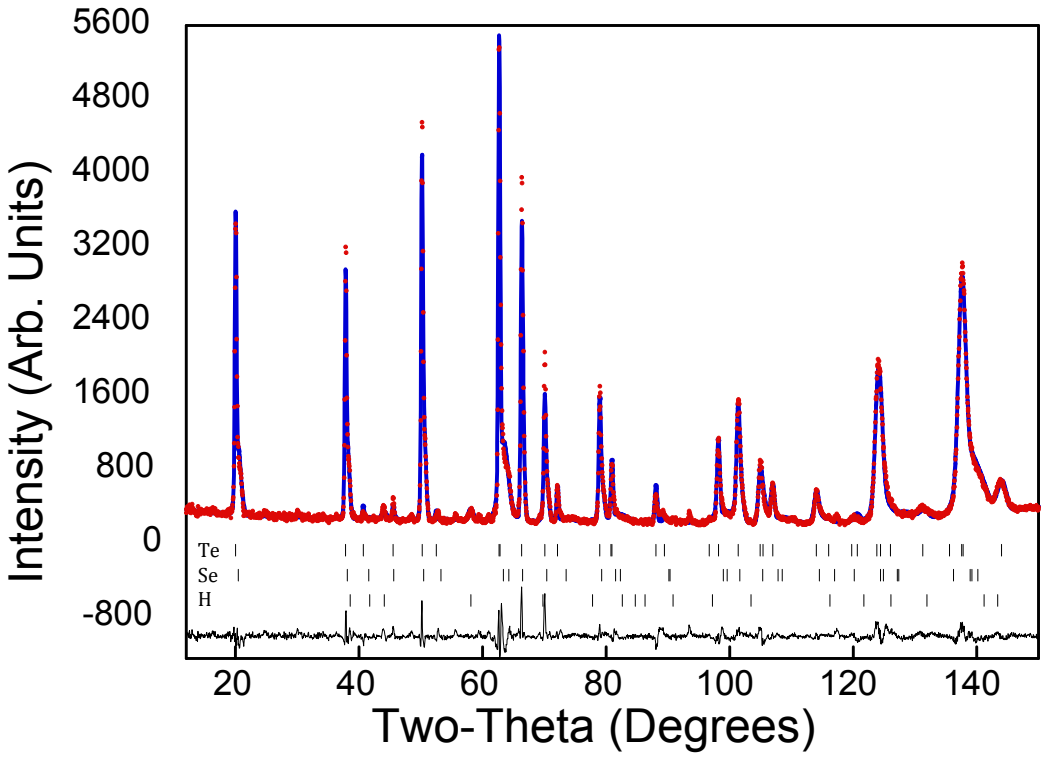
Quenched from 800 °C



Phase	Label	*a* (Å)	*b* (Å)	Formula	Phase Fraction
Te-rich	Te	3.79793(6)	6.0343(2)	$FeTe_{0.67(3)}Se_{0.33(3)}$	48(1) %
Se-rich	Se	3.7907(2)	5.8748(5)	$FeTe_{0.4(1)}Se_{0.6(1)}$	29(2) %
Hexagonal	H	3.7081(2)	5.832(4)	FeSe	23(1)

R-factor = 5.98%, χ^2 = 1.18%

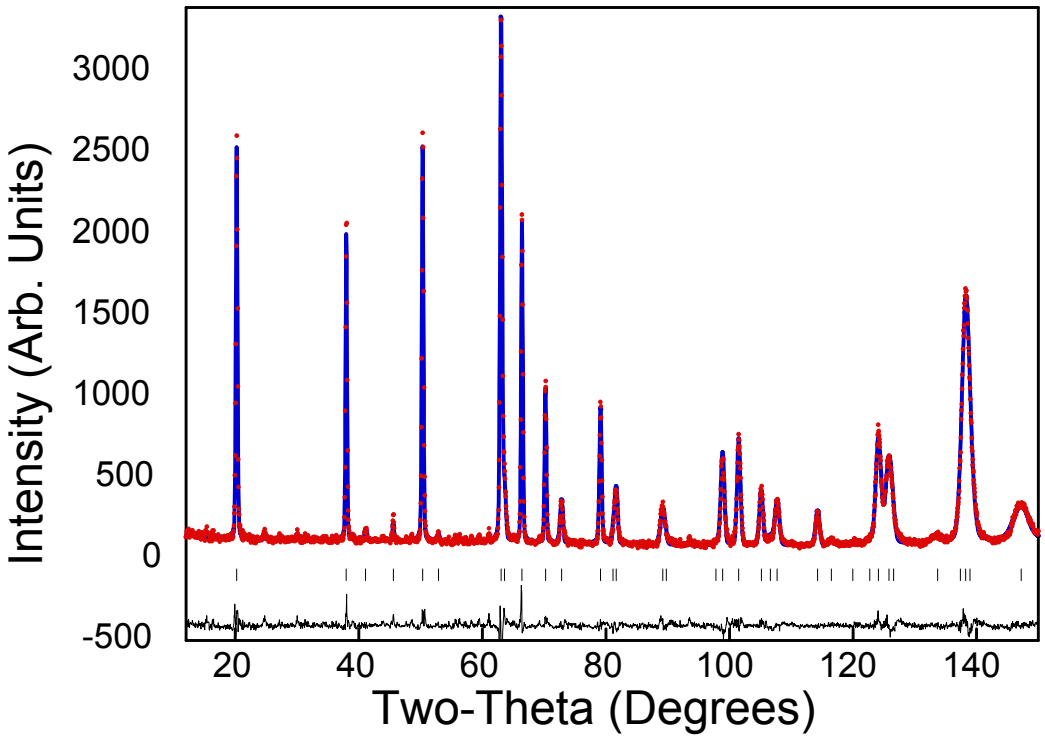
Quenched from 440 °C



Phase	Label	*a* (Å)	*b* (Å)	Formula	Phase Fraction
Te-rich	Te	3.79859(5)	5.9792(1)	$FeTe_{0.52(3)}Se_{0.48(3)}$	51(2) %
Se-rich	Se	3.7910(1)	5.861(1)	$FeTe_{0.41(5)}Se_{0.59(5)}$	44(2) %
Hexagonal	H	3.6347(9)	5.836(2)	FeSe	5(1)

R-factor = 5.75%, χ^2 = 2.79%

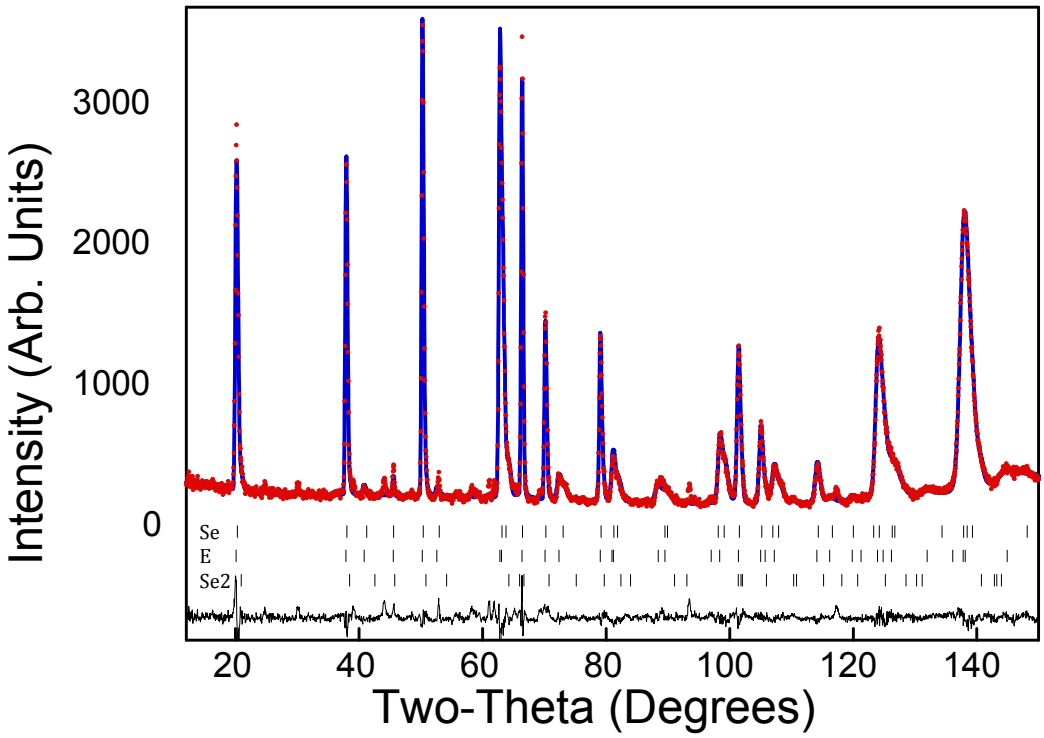
Cooled over 12 hours



Phase	*a* (Å)	*b* (Å)	Formula	Phase Fraction
Single Phase	3.79510(3)	5.9294(1)	$FeTe_{0.57(2)}Se_{0.43(2)}$	100 %

R-factor = 6.24%, χ^2 = 1.37%

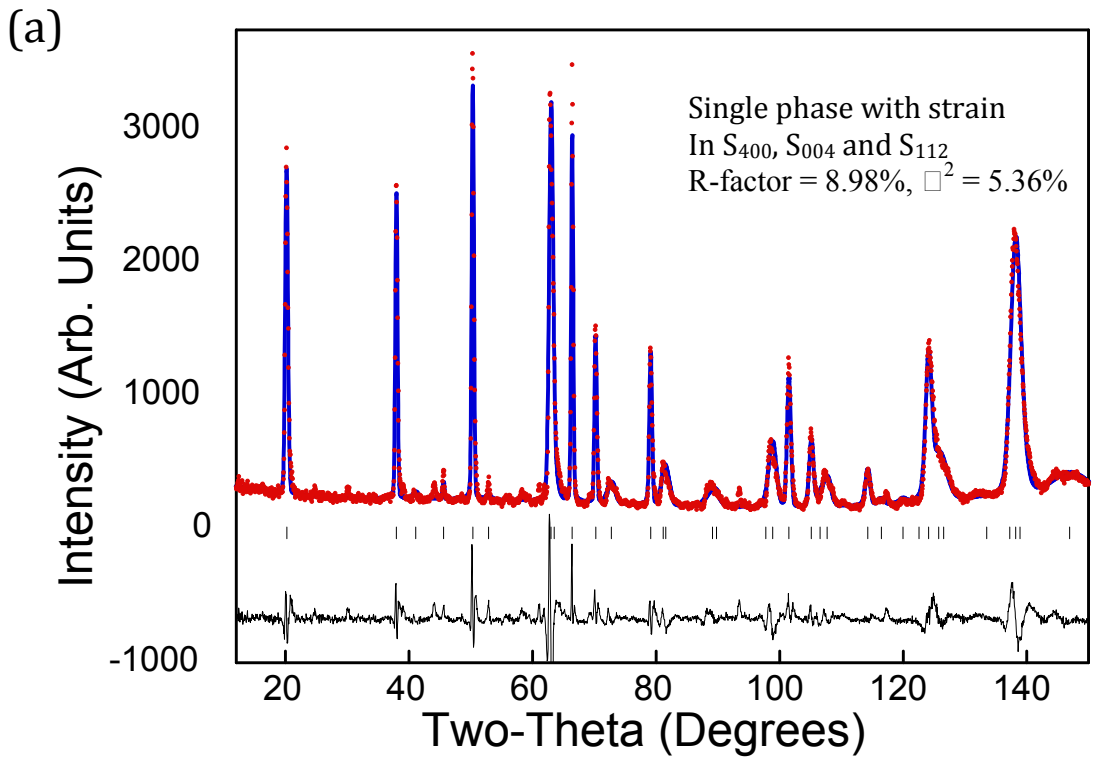
Slow cooled over 2 weeks

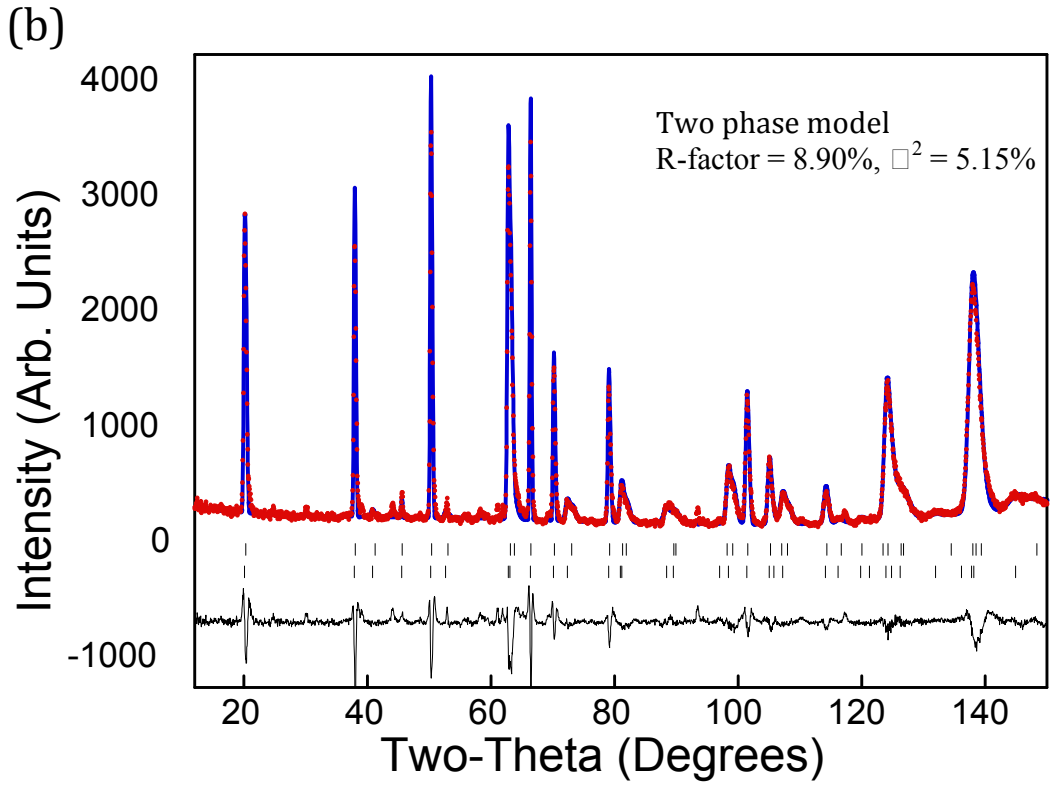


Phase	Label	*a* (Å)	*b* (Å)	Formula	Phase Fraction
Se-rich	Se	3.79391(9)	5.9025(8)	$FeTe_{0.26(2)}Se_{0.74(2)}$	53(2) %
Equal	E	3.7974(1)	5.9616(3)	$FeTe_{0.47(2)}Se_{0.53(2)}$	38(2) %
Se-rich 2	Se2	3.7805(5)	5.727(2)	$FeTe_{0.30(7)}Se_{0.70(7)}$	9(1) %

R-factor = 5.44%, χ^2 = 2.21%

Rietveld refinement fits obtained for the sample slow cooled over two weeks with (a) single phase model with strain and (b) a two pha e model both of *P4/nmm* symmetry.





Comparison of selected reflections between 2 and 3 phase model for sample cooled for 2 weeks, showing that although the third phase of P4/nmm symmetry is a minor phase it has a very significant impact on the fit