

Supplementary Information.

Mechanistic view for defect engineered VFeSb half-Heusler alloys

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Table S1. Refined Lattice Parameters, Structural Parameters, and Reliability Factors (with all non-excluded points for pattern) by Rietveld Analysis of XRD Patterns of $V_{1+x}Fe_{1+y}Sb$ ($0 < x, y < 0.1$) half-Heusler at 300 K.

Chemical Composition		Structural	Reliability Factors (%)				Density ($g.cm^{-3}$)	
Nominal	Refined	a (Å)	R _p	R _{wp}	R _{exp}	χ^2	Calculated	Experimental
VFeSb	$V_{1.00(1)}^{4a}Fe_{0.95(1)}^{4b}Fe_{0.05(1)}^{4d}Sb_{1.00(2)}^{4c}$	a = 5.8259(1)	7.7	10.6	6.1	2.96	7.677	7.5
$V_{0.90}FeSb$	$V_{0.90(2)}^{4a}Fe_{0.97(2)}^{4b}Fe_{0.09(1)}^{4d}Sb_{0.99(1)}^{4c}$	a = 5.8254(1)	9.9	14.1	8.8	2.56	7.706	7.6
$V_{0.95}FeSb$	$V_{0.95(2)}^{4a}Fe_{0.96(1)}^{4b}Fe_{0.06(1)}^{4d}Sb_{0.99(1)}^{4c}$	a = 5.8258(1)	8.9	12.0	7.1	2.81	7.696	7.5
$V_{1.05}FeSb$	$V_{1.00(1)}^{4a}Fe_{0.94(1)}^{4b}Fe_{0.06(1)}^{4d}Sb_{0.99(1)}^{4c}$	a = 5.8260(1)	8.9	11.9	7.1	2.80	7.674	7.4
$V_{1.10}FeSb$	$V_{1.00(2)}^{4a}Fe_{0.93(1)}^{4b}Fe_{0.03(1)}^{4d}Sb_{0.97(2)}^{4c}$	a = 5.8262(1)	8.4	11.4	7.2	2.49	7.616	7.4
$VFe_{0.90}Sb$	$V_{1.00(2)}^{4a}Fe_{0.90(1)}^{4b}Fe_{0.02(1)}^{4d}Sb_{0.98(1)}^{4c}$	a = 5.8256(1)	11.2	16.4	8.4	3.84	7.581	7.4
$VFe_{0.95}Sb$	$V_{1.00(1)}^{4a}Fe_{0.90(1)}^{4b}Fe_{0.05(1)}^{4d}Sb_{1.00(1)}^{4c}$	a = 5.8258(1)	7.8	10.7	8.1	1.77	7.677	7.5
$VFe_{1.05}Sb$	$V_{1.00(1)}^{4a}Fe_{0.95(2)}^{4b}Fe_{0.08(2)}^{4d}Sb_{0.99(1)}^{4c}$	a = 5.8263(1)	8.2	11.3	6.2	3.32	7.715	7.6
$VFe_{1.10}Sb$	$V_{1.00(2)}^{4a}Fe_{0.99(1)}^{4b}Fe_{0.08(1)}^{4d}Sb_{0.99(2)}^{4c}$	a = 5.8265(1)	7.7	10.6	6.0	3.10	7.778	7.7

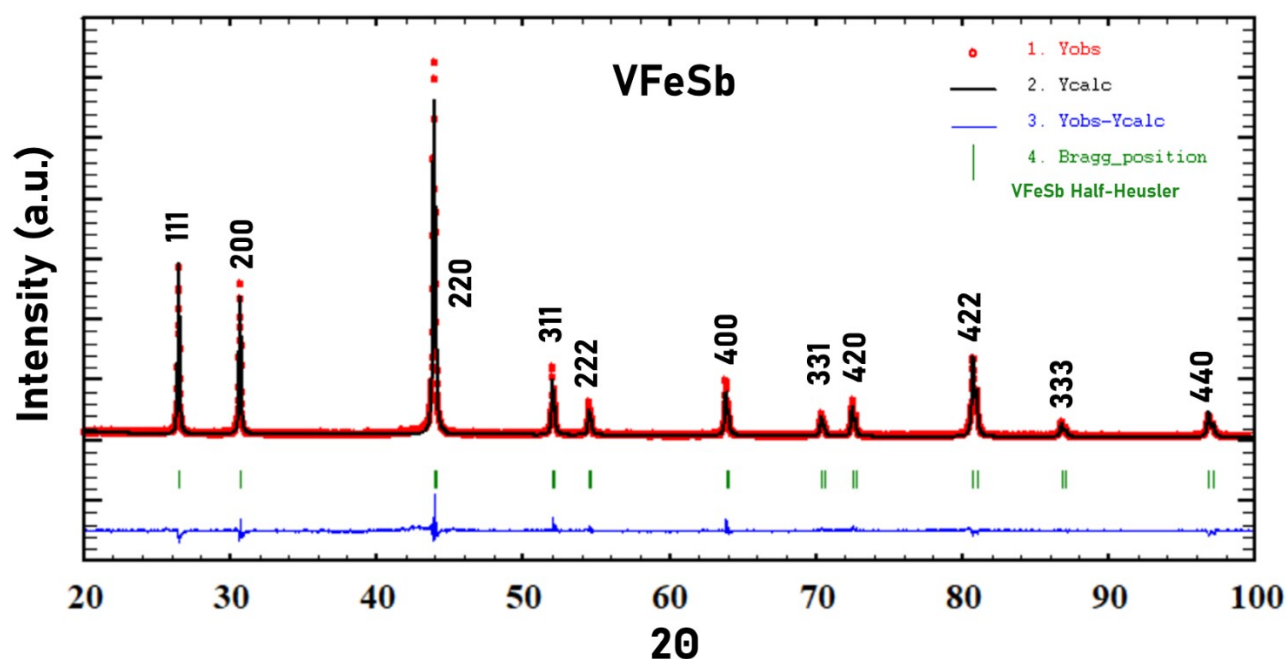


Figure S1. Rietveld refined XRD pattern of VFeSb half-Heusler.

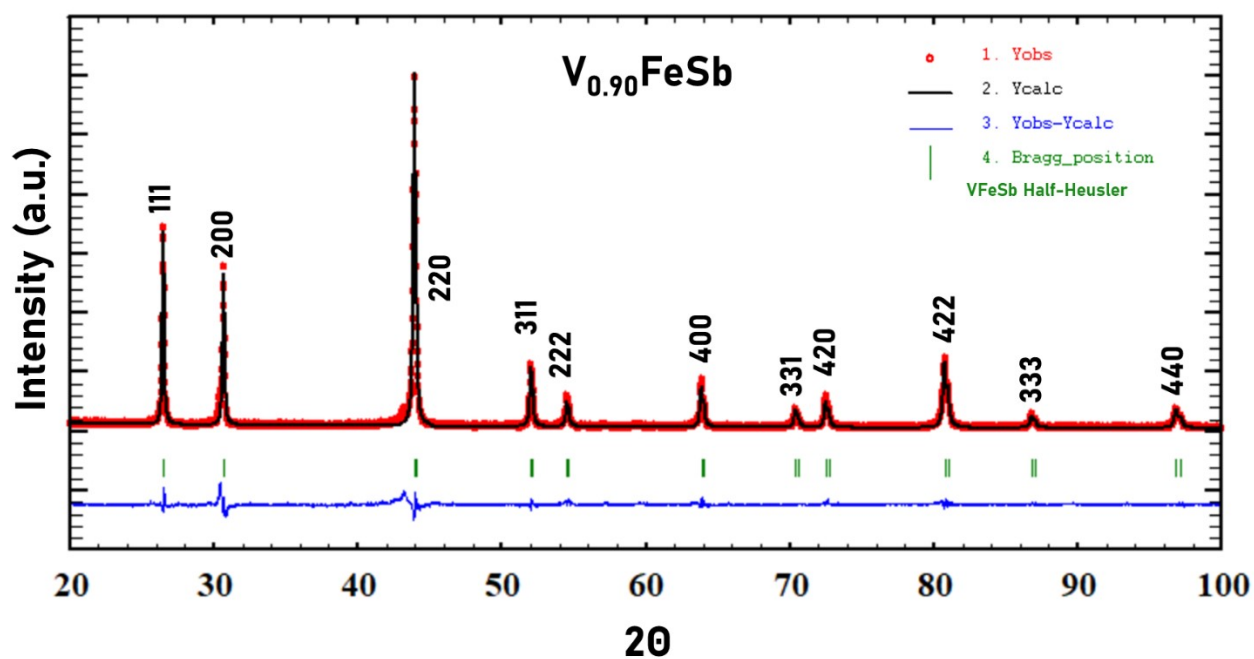


Figure S2. Rietveld refined XRD pattern of V_{0.90}FeSb half-Heusler.

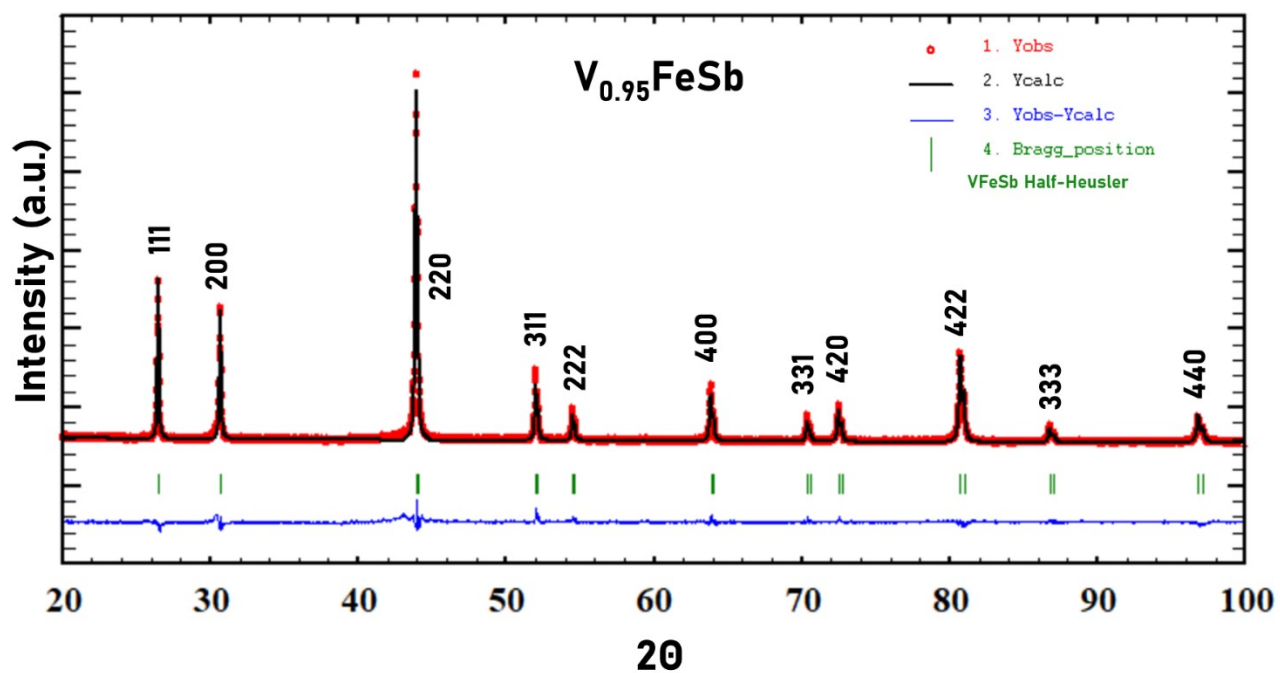


Figure S3. Rietveld refined XRD pattern of V_{0.95}FeSb half-Heusler.

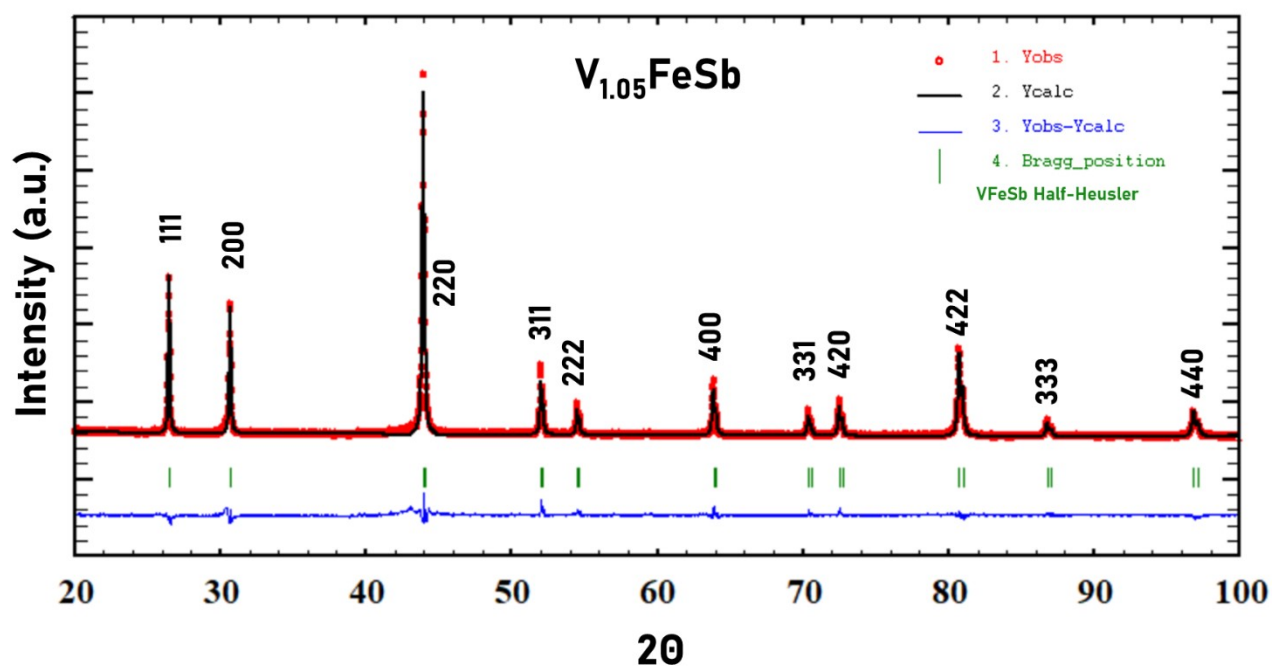


Figure S4. Rietveld refined XRD pattern of V_{1.05}FeSb half-Heusler.

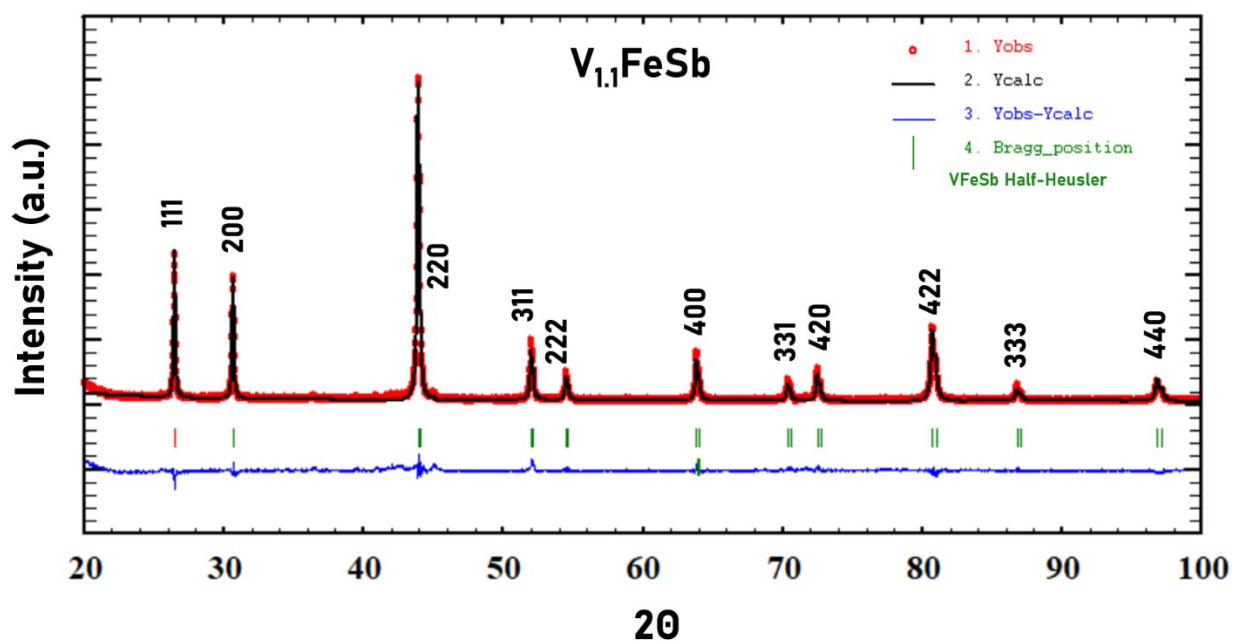


Figure S5. Rietveld refined XRD pattern of V_{1.1}FeSb half-Heusler.

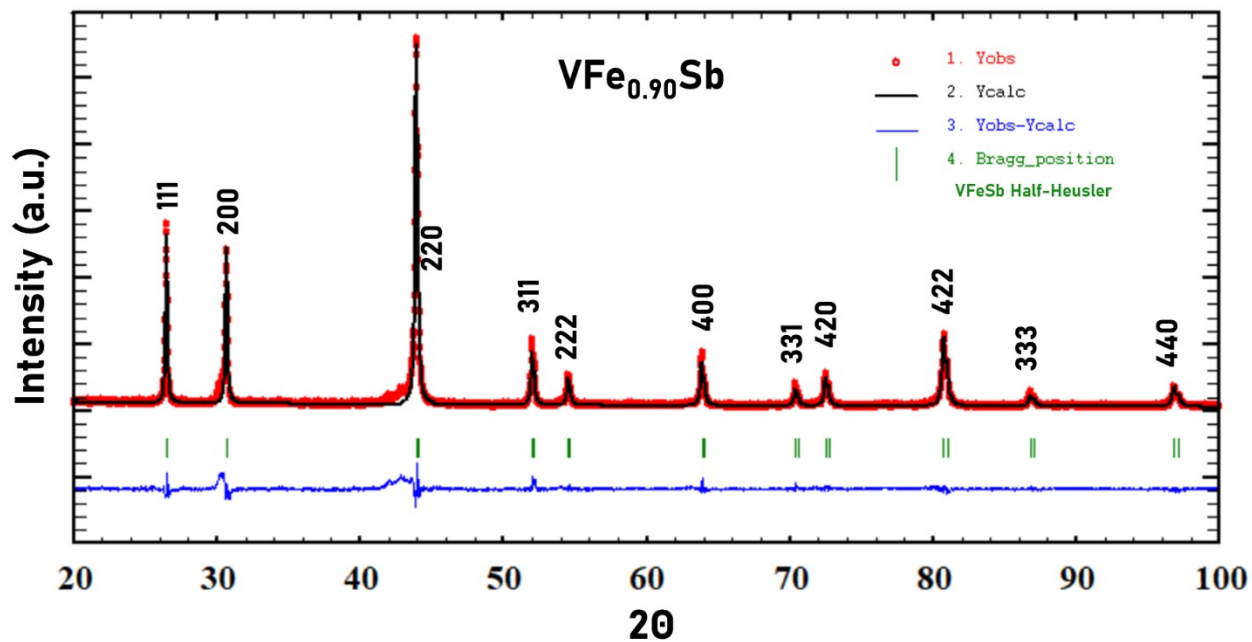


Figure S6. Rietveld refined XRD pattern of VFe_{0.90}Sb half-Heusler.

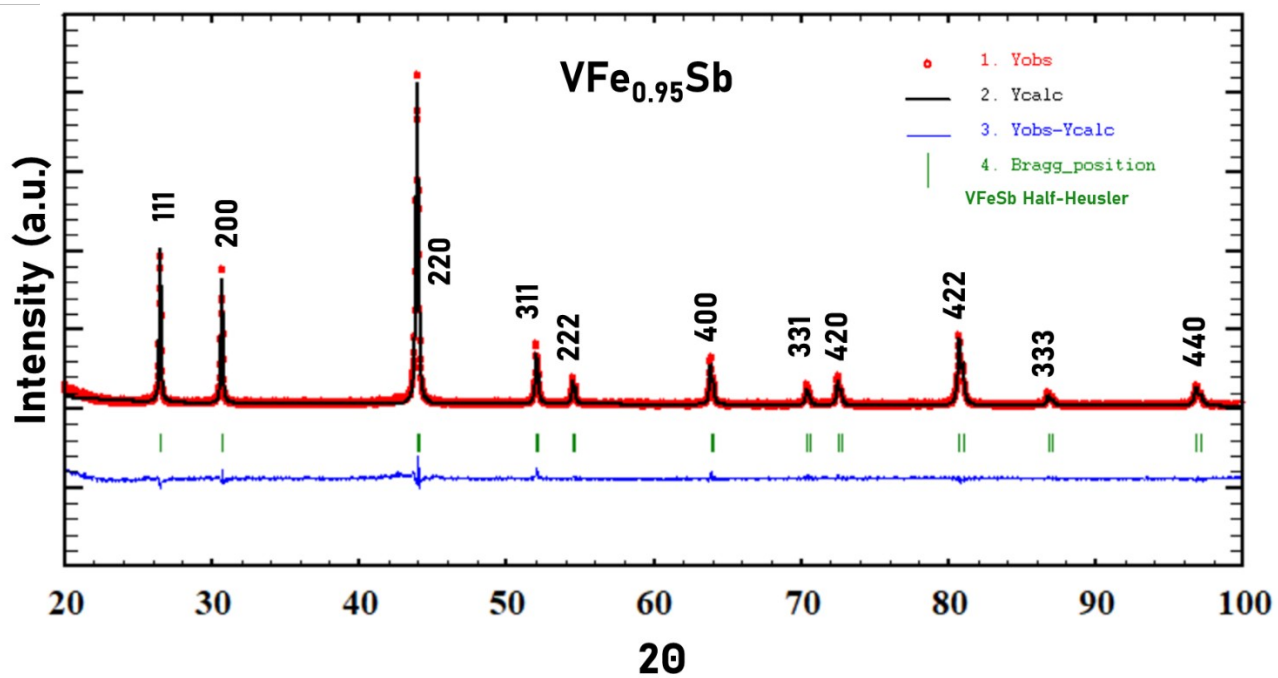


Figure S7. Rietveld refined XRD pattern of VFe_{0.95}Sb half-Heusler.

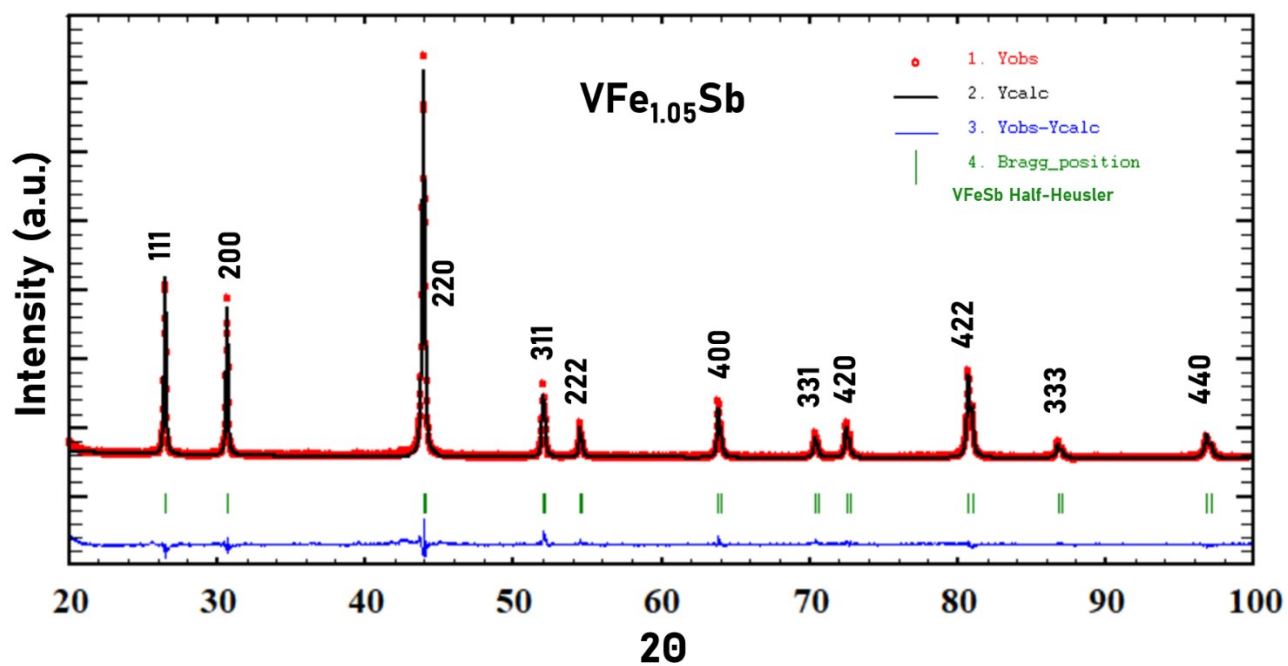


Figure S8. Rietveld refined XRD pattern of VFe_{1.05}Sb half-Heusler.

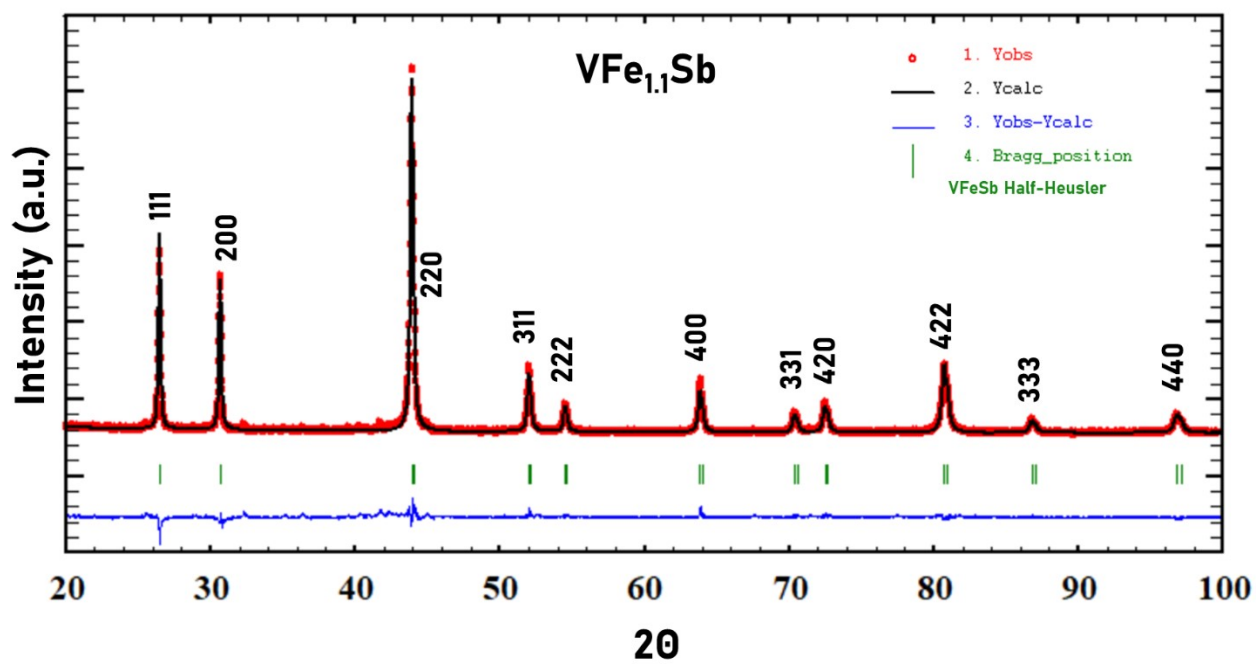


Figure S9. Rietveld refined XRD pattern of VFe_{1.1}Sb half-Heusler.

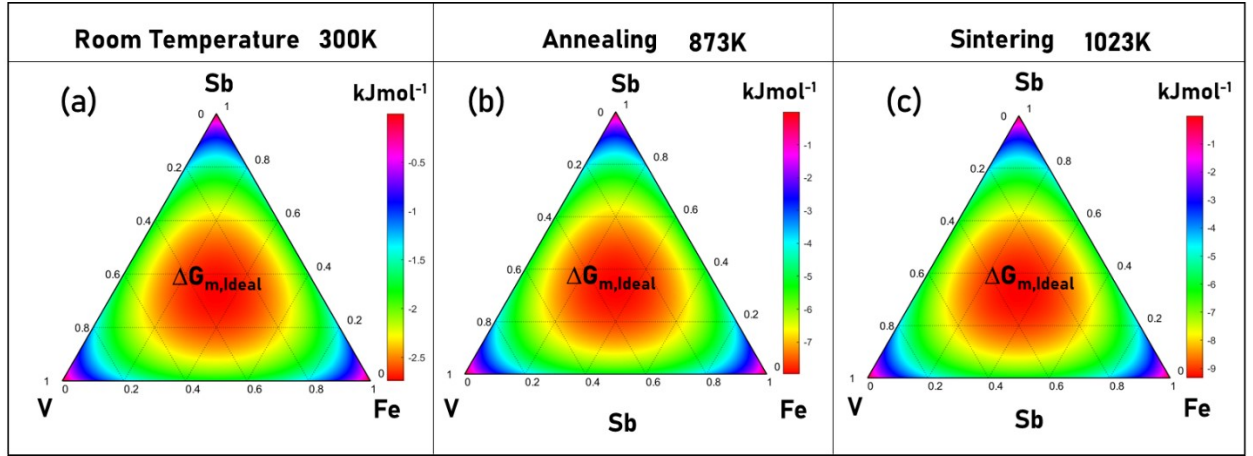


Figure S10. Ideal Gibbs free energy as a function of the V-Fe-Sb composition for (a) room temperature (300 K), (b) annealing temperature (873 K), and (c) maximum sintering (1023 K) temperature in VFeSb alloys.

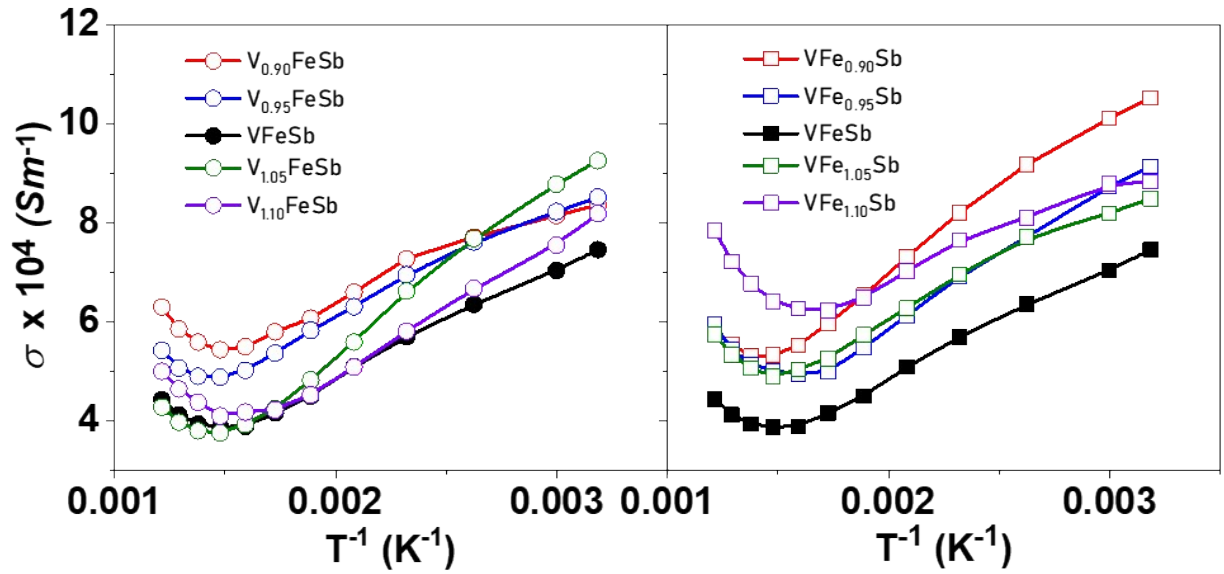


Figure S11. Temperature inverse dependence of electrical conductivity.