Supplementary Information

Experimental and Theoretical Determination of the Grüneisen Parameter to Analyze the Density Effect on Anharmonicity and Thermal Conductivity in the NbCoSb System

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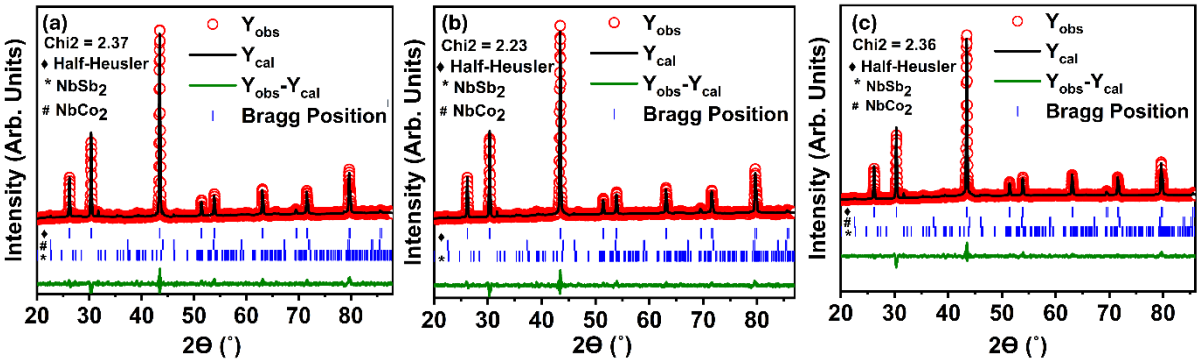

FIG. S1(a), (b), and (c) represent the Rietveld refinement data for the samples HP-65, HP-80, and HP-90, respectively.

Table S1 shows the chi2, lattice parameter, phase fraction, and crystallite size for the HP-65, HP-80, and HP-90 samples.

Sample	Chi2	Lattice Parameter (Å)	Fraction of phase			Crystallite size (nm)
			HH	$NbSb_2$	$NbCo_2$	
HP-65	2.37	5.891	97.18	1.85	0.97	59.8
HP-80	2.23	5.891	97.83	1.49	0.67	65.7
HP-90	2.36	5.891	97.73	1.60	0.67	65.1

Table S2 represents the Nominal and EPMA composition of the HP-65, HP-80, and HP-90 samples.

Nominal Composition	1st run	2nd run	3rd run	Average EPMA
$Nb_{0.83}CoSb$ (HP-65)	$Nb_{0.80}Co_{1.03}Sb_{1.00}$	$Nb_{0.79}Co_{1.03}Sb_{1.01}$	$Nb_{0.79}Co_{1.02}Sb_{1.01}$	$Nb_{0.79}Co_{1.03}Sb_{1.01}$
$Nb_{0.83}CoSb$ (HP-80)	$Nb_{0.80}Co_{1.02}Sb_{1.01}$	$Nb_{0.79}Co_{1.03}Sb_{1.00}$	$Nb_{0.79}Co_{1.03}Sb_{1.01}$	$Nb_{0.79}Co_{1.03}Sb_{1.01}$
$Nb_{0.83}CoSb$ (HP-90)	$Nb_{0.80}Co_{1.02}Sb_{1.01}$	$Nb_{0.79}Co_{1.02}Sb_{1.01}$	$Nb_{0.80}Co_{1.03}Sb_{1.00}$	$Nb_{0.80}Co_{1.02}Sb_{1.01}$

Table S3 represents the density values at room temperature and 1023 K for the HP-65, HP-80, and HP-90 samples.

Sample	Density (g/cm^3) at 300K	Density (g/cm^3) at 1023K
HP-65	7.85	7.70
HP-80	7.98	7.81
HP-90	8.07	7.89

Table S4. DFT computed atomic density and experimental mass density (gm/cm^3) of three vacancy configurations at 300 K.

System	Atomic density (Theory) gm/cm^3	Mass density (Experimental) gm/cm^3
Co vacancy	8.39	8.07 (HP-90)
Nb vacancy	8.11	7.98 (HP-80)
Nb-Co vacancy	7.64	7.85 (HP-65)

Table S5. Elastic constant (C_{3D}), deformation potential constant (E_1), m* (m_o), and DOS derivative (eV^{-1}) (conduction band) values computed at 300 K for Co, Nb, and Nb-Co vacancy systems.

System	C_{3D} (J/m^3) $\times 10^{11}$	E_1 (eV)	m* (m_o)	DOS derivative (eV^{-1}) (conduction band)
Co vacancy	30.18	1.20	1.8	3.05
Nb vacancy	0.10	0.36	0.46	146
Nb-Co vacancy	4.16	0.48	8.3	75.96

Table S6. Computed ICOHP values for atomic pairs near the vacancy position in Nb, Co, and Nb-Co vacancy structures.

System	Atomic pair	ICOHP
Co vacancy	Nb1 – Sb10	-1.83
	Nb1 – Sb11	-3.60
	Nb2 – Sb10	-3.74
	Nb2 – Sb11	-1.88
Nb vacancy	Co1 – Sb10	-1.70
	Nb1 – Sb11	-3.60
	Nb2 – Co1	-2.19
Nb-Co vacancy	Nb1 – Sb10	-1.73
	Nb1 – Sb11	-3.46
	Nb2 – Sb10	-3.32
	Nb2 – Sb11	-1.85

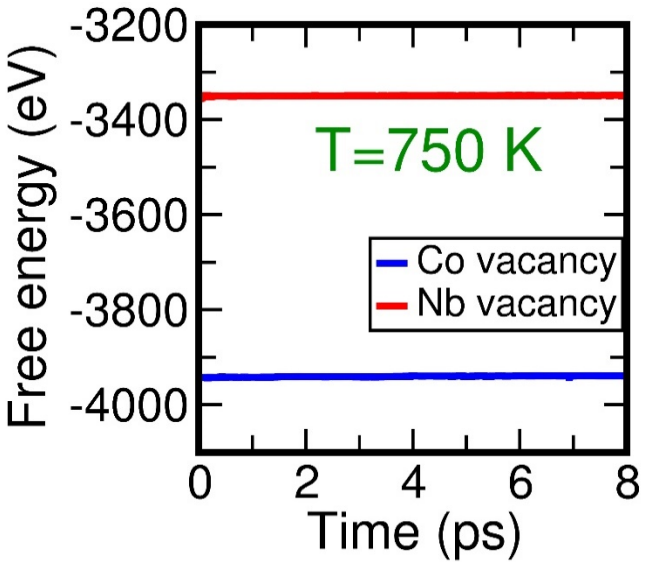

Figure S2. Time evolution of free energy up to 8 ps during AIMD simulations for both Nb and Co vacancy structures at 750 K.