

Supplementary Information for “first-principles prediction of high-entropy-alloy stability”

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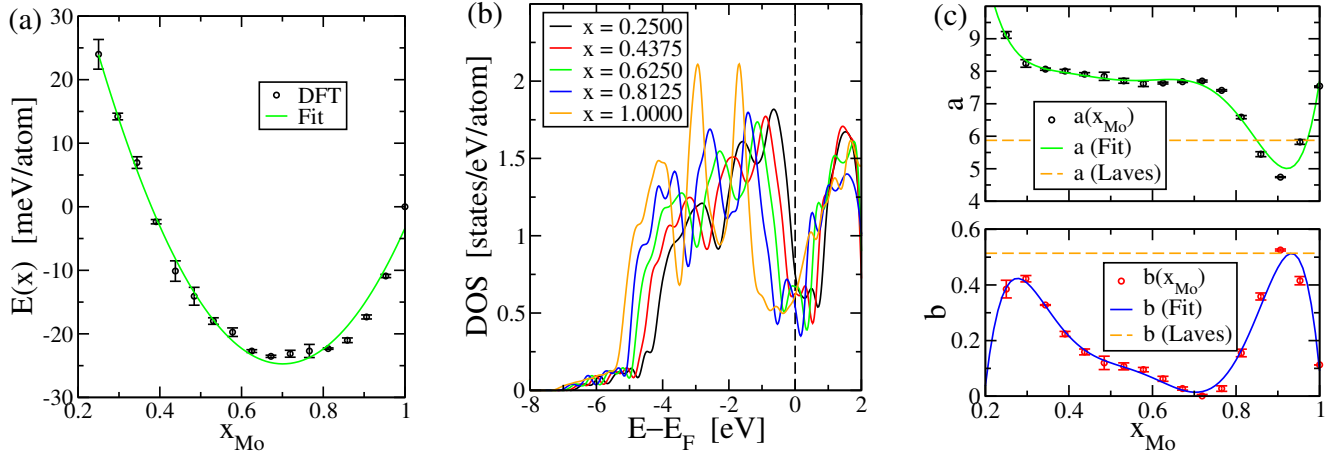


FIG. S1: (a) Formation enthalpies of BCC HEAs calculated from DFT at various compositions, x_{Mo} . (b) Electronic densities of states. (c) Coefficients of electronic free energy.

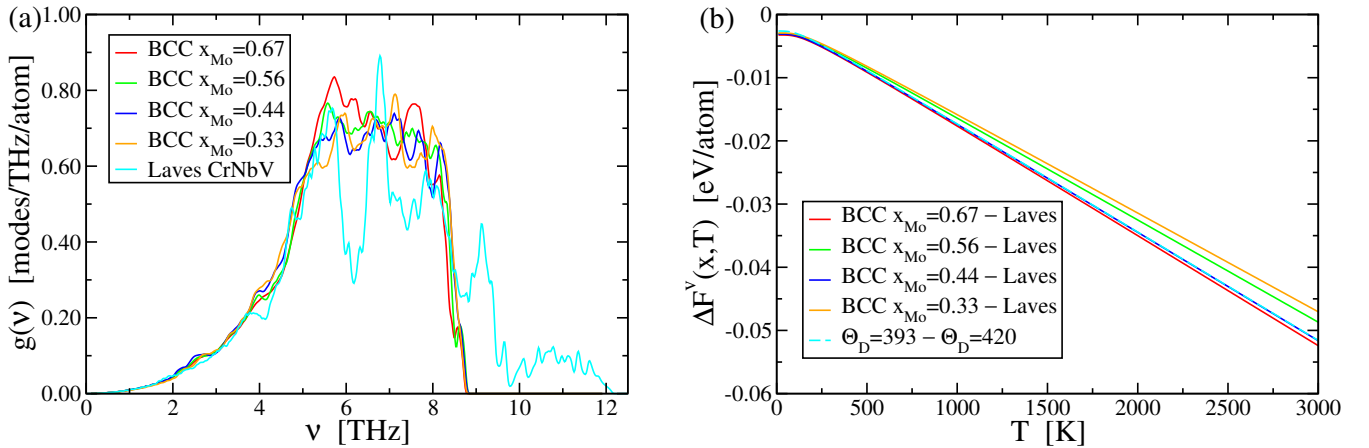


FIG. S2: (a) Vibrational densities of states for BCC cells of varying compositions, compared with the CrNbV Laves phase. (b) Vibrational free-energy differences between BCC and Laves phases.

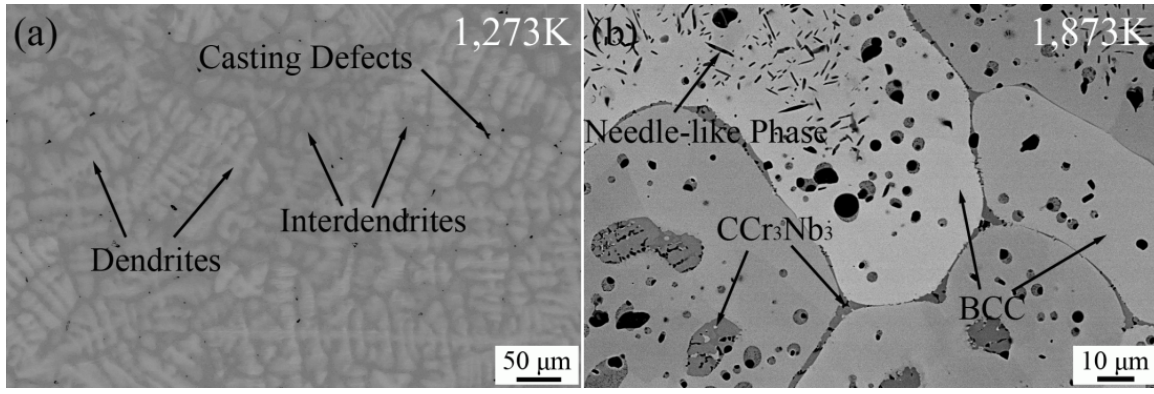


FIG. S3: Electron micrographs of the (a) Cr-Mo-Nb-V sample following $T = 1,273\text{K}$ anneal, and (b) following $T = 1,873\text{K}$.

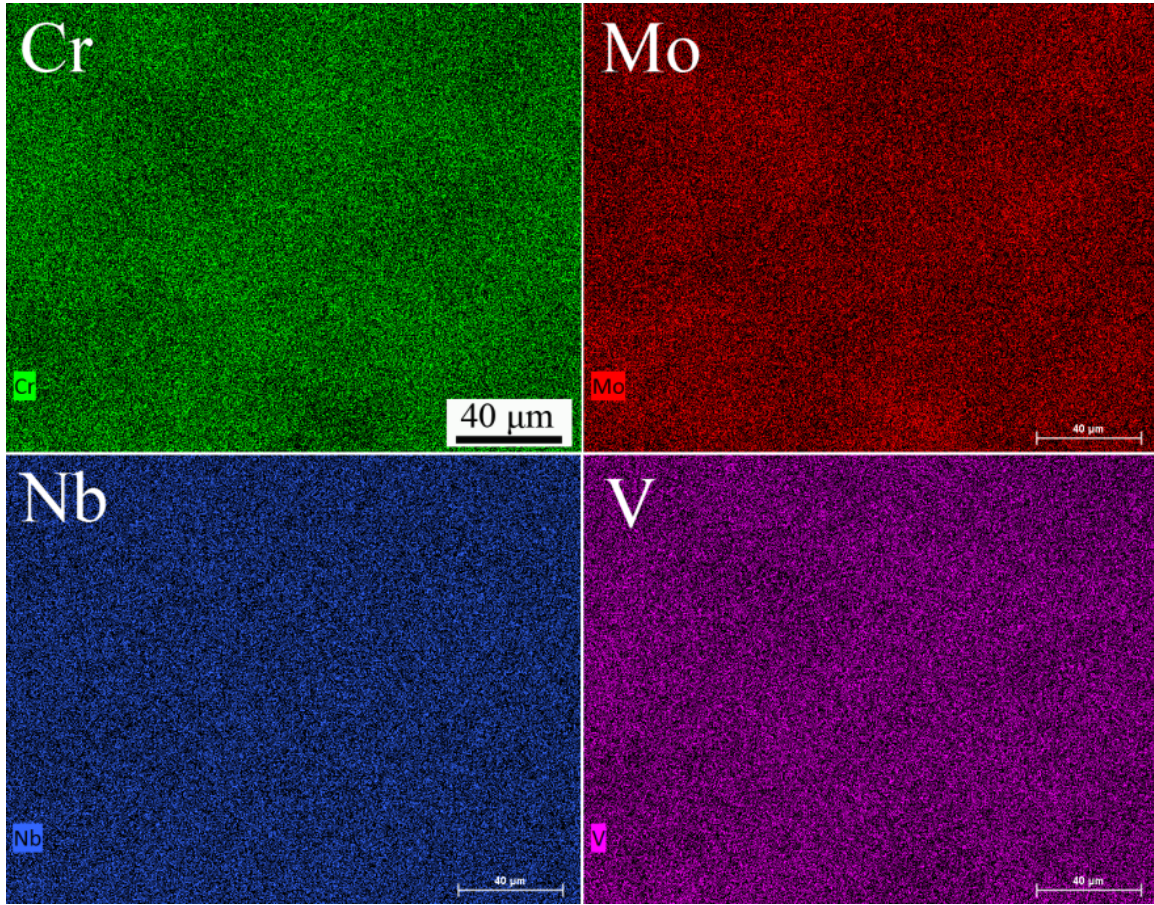


FIG. S4: The chemical distribution of constitutive elements after annealing the $T = 1,473\text{K}$ annealed sample at $T = 1,673\text{K}$ for 12 hours.

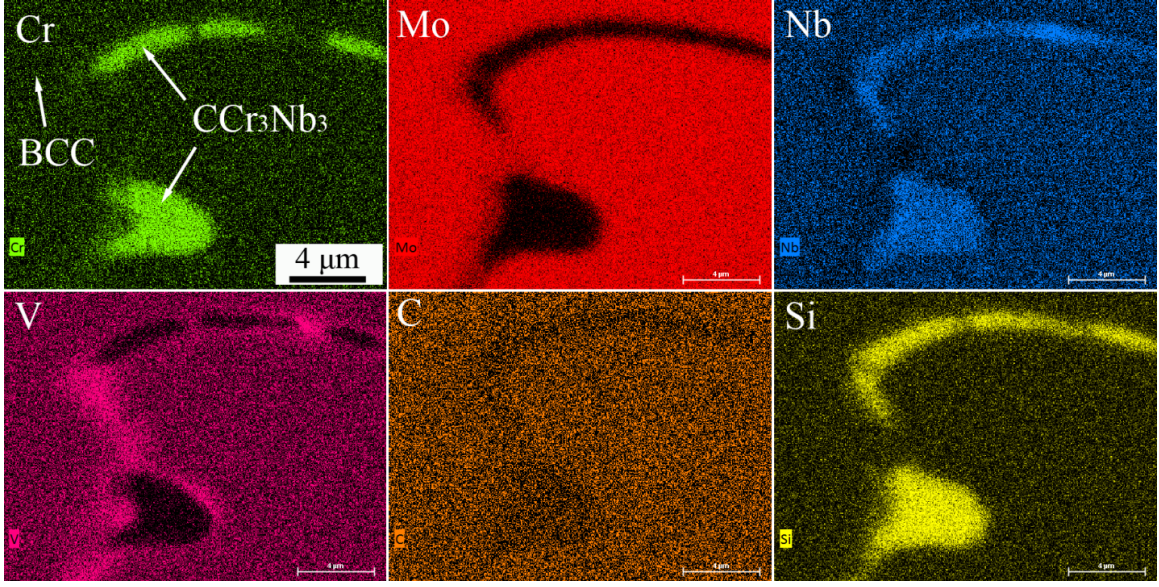


FIG. S5: The chemical distribution of the BCC and CCr_3Nb_3 phases in the $T = 1,873\text{K}$ -annealed state.

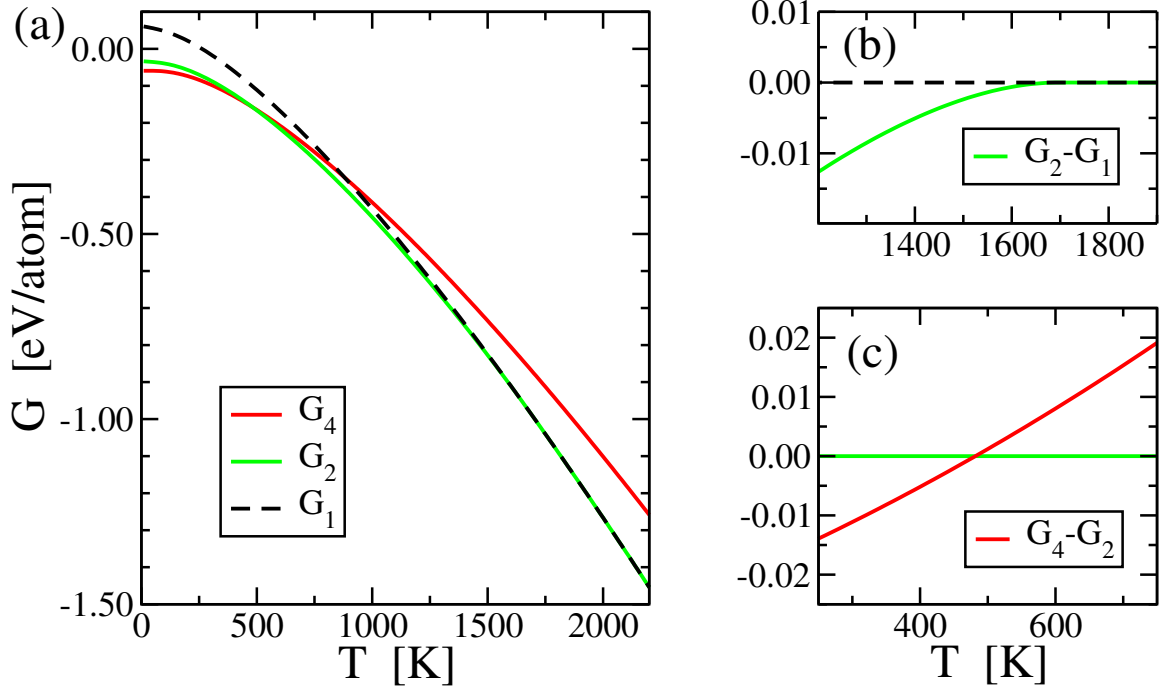


FIG. S6: Free energies for: (a) G_1 , a single-phase BCC high-entropy alloy; G_2 a two-phase mixture of the BCC medium entropy alloy with the coexisting Laves phase; G_4 a four-phase mixture of the Laves phase with chemically-ordered BCC-based structures. (b,c) Enlargements.

TABLE S1: Structures of competing phases. Lattice constants are given in Angstroms, and Wyckoff positions are in direct coordinates.

Compound	Cr ₂ V				
Pearson symbol	tI6				
Lattice constants	a = 2.87957, c = 8.68376				
Space group	I4/mmm #139				
Wyckoff	Cr	4e	0	0	0.17040
Wyckoff	V	2b	0	0	1/2
Compound	MoNb				
Pearson symbol	oC12				
Lattice constants	a = 13.80741, b = 3.23206, c = 4.55501				
Space group	Cmmm #65				
Wyckoff	Mo1	4h	0.17056	0	1/2
Wyckoff	Mo2	2a	0	0	0
Wyckoff	Nb1	2c	1/2	0	1/2
Wyckoff	Nb2	4g	0.66319	0	0
Compound	Mo ₄ V ₃				
Pearson symbol	hR7				
Lattice constants	a = 4.34264, c = 18.84620				
Space group	R3m:H #160				
Wyckoff	Mo1	3a	0	0	0.00020
Wyckoff	Mo2	3a	0	0	0.85778
Wyckoff	Mo3	3a	0	0	0.57079
Wyckoff	Mo4	3a	0	0	0.42837
Wyckoff	V1	3a	0	0	0.28729
Wyckoff	V2	3a	0	0	0.14128
Wyckoff	V3	3a	0	0	0.71429
Compound	CrNbV (disordered)				
Pearson symbol	cF24				
Lattice constants	a = 7.039				
Space group	Fd-3m #227				
Wyckoff	Nb	8a	0	0	0
Wyckoff	(Cr,V)	16d	5/8	5/8	5/8
Compound	CrNbV ordered				
Pearson symbol	oI12				
Lattice constants	a = 4.94026, b = 5.04117, c = 7.02909				
Space group	Imma #74				
Wyckoff	Nb	4e	1/2	1/2	0.12378
Wyckoff	Cr	4a	0	0	0
Wyckoff	V	4d	1/4	1/2	3/4

TABLE S2: Predicted structure of the carbide-impurity phase. Lattice constant is given in Angstroms, and Wyckoff positions are in direct coordinates.

Compound	CCr ₃ Nb ₃				
Pearson symbol	cF112				
Lattice constants	a = 11.55				
Space group	<i>Fd</i> $\bar{3}m$ #227				
Wyckoff	C	16d	1/4	1/2	1/4
Wyckoff	Cr1	16c	1/4	0	1/4
Wyckoff	Cr2	32e	0.453	0.797	0.453
Wyckoff	Nb	48f	0.625	0.432	0.625