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Appendix A

Special Quasi Random Structures (SQS)

The present work uses the ATAT software to generate the SQS of binary, ternary and quaternary systems. For binary, ternary, and quaternary systems, SQS of size 16 atoms, 120 atoms, and 160 atoms was used. Multiple instances were used to obtain the best SQS in each system.

Table A.1 Pair and multisite correlation function of SQS 16 atoms structure for mimicking random binary bcc alloys.

Clusters (Sites)	A=0.5, B=0.5	Random	A=0.25,B=0.75	Random
2	0	0	0.25	0.25
2	0	0	0.25	0.25
2	0	0	0.125	0.25
2	0	0	0.16667	0.25
2	0	0	0.22917	0.25
2	0	0	0.25	0.25
2	0	0	0.16667	0.25
2	0	0	0.33333	0.25
2	0	0	0.25	0.25
2	0	0	0.29167	0.25
2	0	0	0.375	0.25
2	0	0	0.25	0.25
3	0	0	0.125	0.125
3	0	0	0.125	0.125

3	0	0	0.0625	0.125
3	0	0	0.16667	0.125
3	0	0	0.125	0.125
3	0	0	-0.0833	0.125
3	0	0	0.125	0.125
3	0	0	0.0625	0.125
3	0	0	0.03125	0.125
3	0	0	0.10417	0.125
3	0	0	0.04167	0.125
3	0	0	0.08333	0.125
3	0	0	0.10417	0.125
3	0	0	0.0625	0.125
3	0	0	0.14583	0.125
3	0	0	0.0625	0.125
3	0	0	0.125	0.125
3	0	0	0.0625	0.125
3	0	0	0.0625	0.125
3	0	0	0.11458	0.125
3	0	0	0.1875	0.125
3	0	0	0.04167	0.125
3	0	0	0	0.125
3	0	0	0.09375	0.125
3	0	0	-0.0833	0.125
3	0	0	0	0.125

3	0	0	0.08333	0.125
3	0	0	0.125	0.125
3	0	0	0	0.125
3	0	0	0.08333	0.125
3	0	0	0.125	0.125
3	0	0	0.125	0.125
3	0	0	0.125	0.125
3	0	0	0.125	0.125
3	0	0	0.17708	0.125
3	0	0	0.11458	0.125
3	0	0	0.08333	0.125
3	0	0	0.08333	0.125
3	0	0	0.125	0.125
3	0	0	0.14583	0.125
3	0	0	0.0625	0.125
3	0	0	0.0625	0.125
3	0	0	0.08333	0.125
3	0	0	0.0625	0.125
3	0	0	0.10417	0.125
Objective_function= Perfect_match			Objective_function= -3.411417	

Table A.2 Pair and multisite correlation function of SQS of 120 atoms structure for mimicking random ternary bcc alloys.

A=0.2, B=0.4, C=0.2	A=0.25, B=0.125, C=0.625	A=0.3, B=0.2, C=0.5	A=0.333333, B=0.333333, C=0.333333
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Clusters (sites)	SQS	Random	SQS	Random	SQS	Random	SQS	Random
2	0.03906	0.04	0.015625	0.015625	0.001563	0.0025	-0.001563	0
2	0	0	0.056833	0.054127	0.013532	0.01299	-0.010825	0
2	-0.0047	0	0.1875	0.1875	0.067187	0.0675	-0.001563	0
2	0.0375	0.04	0.0125	0.015625	-0.00625	0.0025	0	0
2	0.00361	0	0.050518	0.054127	0.014434	0.01299	0	0
2	-0.0083	0	0.1875	0.1875	0.06875	0.0675	0	0
3	0.00703	0.008	0.001563	0.001953	0.00625	0.000125	-0.000781	0
3	-0.0036	0	0.006315	0.006766	-0.000902	0.00065	0.001353	0
3	0.00135	0	0.005413	0.006766	0	0.00065	-0.001353	0
3	-0.0016	0	0.025	0.023438	0.003125	0.003375	-0.002344	0
3	-0.0003	0	0.023438	0.023438	0.003125	0.003375	0.000781	0
3	-0.0023	0	0.08119	0.08119	0.014434	0.017537	-0.000451	0
4	0.00078	0.0016	0.002344	0.000244	0.004687	0.000006	0.000781	0
4	0.00023	0	0.001804	0.000846	-0.001128	0.000032	-0.004059	0
4	0.00078	0	0.003906	0.00293	-0.000781	0.000169	-0.000781	0
4	-0.0005	0	0.007031	0.00293	-0.002344	0.000169	0.005469	0
4	0.00293	0	0.013532	0.010149	-0.000226	0.000877	0.000451	0
4	-0.0008	0	0.033594	0.035156	0.00625	0.004556	0.000781	0
	Objective _function = -2.997993		Objective _function = -2.998540		Objective function= -3.461737		Objective _function = -2.998148	

Table A.3 Pair and multisite correlation function of SQS 160 atoms structure for mimicking random quaternary bcc alloys.

	A=0.125,B=0.125,C=0.3 75,D=0.375		A=0.125,B=0.25,C=0.25, D=0.375		A=0.2375,B=0.2375,C=0 .225,D=0.3		A=0.2625,B=0.2625,C=0 .275,D=0.2	
Clusters (sites)	SQS	Random	SQS	Random	SQS	Random	SQS	Random
2	0.0625	0.0625	0.01563	0.01563	0	0.00016	-0.0031	0.00016
2	0.0625	0.0625	0.01563	0.01563	0.00625	-0.0008	0.00156	-0.0008

2	0	0	0.03125	0.03125	0.01875	-0.0009	-0.0031	-0.0009
2	0.0625	0.0625	0.01563	0.01563	0	0.00391	0	0.00391
2	0	0	0.03125	0.03125	0	0.00469	0.01875	0.00469
2	0	0	0.0625	0.0625	0	0.00563	0	0.00563
2	0.05625	0.0625	0.00833	0.01563	-0.0063	0.00016	-0.0063	0.00016
2	0.04792	0.0625	0.01875	0.01563	0.01667	-0.0008	-0.0104	-0.0008
2	-0.0083	0	0.02917	0.03125	-0.0042	-0.0009	-0.0042	-0.0009
2	0.03958	0.0625	0.02083	0.01563	0.00625	0.00391	0.00208	0.00391
2	0.01667	0	0.025	0.03125	0.01667	0.00469	0.00417	0.00469
2	0.00833	0	0.05	0.0625	0.00833	0.00563	0.00833	0.00563
3	0.00781	0.01563	0.00417	0.00195	0.00417	-2E-06	-0.0167	2E-06
3	0.01667	0.01563	0.00885	0.00195	-0.001	0.00001	-0.0047	-1E-05
3	0.00313	0	0	0.00391	0.00938	1.2E-05	-0.0052	-1E-05
3	0.01094	0.01563	0.00208	0.00195	0.00104	0.00001	0.00104	-1E-05
3	0.01354	0.01563	-0.0078	0.00195	0	-5E-05	0.00313	4.9E-05
3	-0.0052	0	0.00208	0.00391	-0.0031	-6E-05	0.00781	5.9E-05
3	-0.001	0	0.00208	0.00391	-0.0042	1.2E-05	-0.0021	-1E-05
3	0.00625	0	-0.001	0.00391	-0.0104	-6E-05	0.01042	5.9E-05
3	0.00625	0	0.0125	0.00781	-0.0042	-7E-05	-0.0073	0.00007
3	-0.0057	0.01563	-0.0073	0.00195	-0.0021	-5E-05	-0.0104	4.9E-05
3	-0.0125	0	0.00104	0.00391	-0.001	-6E-05	0.00365	5.9E-05
3	0.01823	0.01563	-0.001	0.00195	0.00313	0.00024	0.00417	-0.0002
3	0.00833	0	0.00729	0.00391	0.00104	0.00029	0.00313	-0.0003
3	0.01771	0	-0.0042	0.00391	0.00417	0.00029	0.00417	-0.0003

3	0.00417	0	-0.0104	0.00781	0.01042	0.00035	0.00833	-0.0004
3	-0.0188	0	0.00833	0.00781	-0.0208	-7E-05	-0.0021	0.00007
3	0.00208	0	0.00833	0.00781	0.00417	0.00035	0.0125	-0.0004
3	-0.0042	0	-0.0083	0.01563	0	0.00042	-0.0167	-0.0004
4	-0.0083	0.00391	0.00729	0.00024	0.00104	0	-0.001	0
4	0.00417	0.00391	0.00625	0.00024	-0.0021	0	-0.0031	0
4	0.00677	0	-0.0021	0.00049	0.00313	0	0	0
4	0.00833	0.00391	-0.0031	0.00024	-0.001	1E-06	0.00208	1E-06
4	-0.001	0	-0.0016	0.00049	0.00417	1E-06	-0.0016	1E-06
4	-0.0021	0	0.00104	0.00098	0.00625	1E-06	0.00104	1E-06
4	-0.0021	0.00391	-0.0052	0.00024	0.00104	1E-06	-0.001	1E-06
4	0.00208	0.00391	-0.0021	0.00024	-0.0021	-3E-06	0.00208	-3E-06
4	-0.0026	0	0.00729	0.00049	0.00521	-4E-06	-0.0042	-4E-06
4	-0.0068	0	0	0.00049	0.00417	1E-06	-0.0052	1E-06
4	0	0	-0.0057	0.00049	-0.001	-4E-06	-0.0052	-4E-06
4	0.00313	0	0	0.00098	-0.0021	-4E-06	0.00365	-4E-06
4	-0.0292	0	-0.0083	0.00098	-0.0021	1E-06	-0.0021	1E-06
4	0.00208	0	-0.0042	0.00098	0	-4E-06	-0.0021	-4E-06
4	0.00625	0	0.00833	0.00195	-0.0042	-5E-06	-0.0104	-5E-06
4	0.00417	0.00391	-0.001	0.00024	0.00104	1.5E-05	-0.001	1.5E-05
4	0.00469	0	0.00104	0.00049	0.00625	1.8E-05	0	1.8E-05
4	0	0	0.02396	0.00098	-0.0021	2.2E-05	0.00208	2.2E-05
4	0	0	0	0.00098	0.00208	2.2E-05	-0.0063	2.2E-05
4	-0.0021	0	0	0.00195	0.00833	2.6E-05	0.00833	2.6E-05

4	0	0	-0.0667	0.00391	0	3.2E-05	0	3.2E-05
Objective_ function= - 3.457481			Objective_ function= - 3.457324		Objective_ function= - 2.995539		Objective_ function= - 2.995240	

Details of correlation functions for quaternary bcc structure in the CV basis using tetrahedron approximation

Jindal and Lele (Jindal and Lele 2023) have developed a basis (CV basis) by carefully selecting the required number of cluster variables (CVs) as CECs. The advantage of this basis is that CECs of the lower order system remain invariant in this basis and can be straightforwardly extended to multicomponent systems. This basis is used in this work for the determination of CECs of the multicomponent Nb-Ti-V-Zr system using CECs of the subsystems. Using tetrahedron approximation of CVM, we will briefly give details of CFs used in CV basis for a disordered quaternary bcc structure. A total of 55 CFs (including 4-point CFs) are used in this description. The irregular tetrahedron cluster in the bcc structure is shown in Figure 1-2. Clusters and sub-clusters used in tetrahedron approximation for bcc structure: point (1), I-n pair (12), II-n pair (13), triangle (123), and tetrahedron (1234). Table B.1 gives the list of clusters and corresponding CFs and CECs.

For point CFs, the entire set of point cluster variables is used in the description. The I-neighbour (v_{2PR1}) and II-neighbour (v_{2PR2}) pair CFs are defined as follows,

$$v_{2PR1} = \rho_{12}^{PR} = \rho_{12}^{RP}, \quad P < R \quad \text{B.1}$$

$$v_{2PR2} = \rho_{13}^{PR} = \rho_{13}^{RP}, \quad P < R \quad \text{B.2}$$

Where ρ_{12}^{RP} is CV corresponds to the probability of finding elements R and P on the 12-type pair cluster. Similarly, Triangle CFs are defined as follows,

$$v_{3PR} = \rho_{123}^{RPR} - \rho_{123}^{PRP} \quad \text{B.3}$$

and

$$v_{3PRT1} = \rho_{123}^{RPT}, \quad v_{3PRT2} = \rho_{123}^{PRT}, \quad v_{3PRT3} = \rho_{123}^{PTR} \quad \text{B.4}$$

ρ_{123}^{RPR} denotes the CV corresponding to finding elements $R, P,$ and R on sites 1, 2, and 3, respectively.

Tetrahedron CFs are chosen as follows,

$$v4PR = \rho_{1234}^{PRPR} \quad \text{B.5}$$

$$v4PRT1 = \rho_{1234}^{PRPT} ; v4PRT2 = \rho_{1234}^{PRTR} ; v4PRT3 = \rho_{1234}^{PTRT} \quad \text{B.6}$$

$$v4MPRT1 = \rho_{1234}^{MRPT} ; v4MPRT2 = \rho_{1234}^{MPRT} ; v4MPRT3 = \rho_{1234}^{MPTR} \quad \text{B.6}$$

Table B.1 CFs for CE using tetrahedron approximation for bcc structure.

Cluster Type	CFs	CECs
Point	xP, \dots	..
I-n Pair	$v2NbTi1$	$e2NbTi1$
	$v2NbV1$	$e2NbV1$
	$v2NbZr1$	$e2NbZr1$
	$v2TiV1$	$e2TiV1$
	$v2TiZr1$	$e2TiZr1$
	$v2VZr1$	$e2VZr1$
	II-n Pair	$v2NbTi2$
$v2NbV2$		$e2NbV2$
$v2NbZr2$		$e2NbZr2$
$v2TiV2$		$e2TiV2$
$v2TiZr2$		$e2TiZr2$
$v2VZr2$		$e2VZr2$
Triangle	$v3NbTiV1$	$e3NbTiV1$
	$v3NbTiV2$	$e3NbTiV2$
	$v3NbTiV3$	$e3NbTiV3$
	$v3NbTiZr1$	$e3NbTiZr1$
	$v3NbTiZr2$	$e3NbTiZr2$
	$v3NbTiZr3$	$e3NbTiZr3$
	$v3NbVZr1$	$e3NbVZr1$
	$v3NbVZr2$	$e3NbVZr2$
	$v3NbVZr3$	$e3NbVZr3$
	$v3TiVZr1$	$e3TiVZr1$
	$v3TiVZr2$	$e3TiVZr2$
	$v3TiVZr3$	$e3TiVZr3$
	$v3NbTi$	$e3NbTi$
	$v3NbV$	$e3NbV$
	$v3NbZr$	$e3NbZr$

	<i>v3TiV</i>	<i>e3TiV</i>
	<i>v3TiZr</i>	<i>e3TiZr</i>
	<i>v3VZr</i>	<i>e3VZr</i>
Tetrahedron	<i>v4NbTiVZr1</i>	<i>e4NbTiVZr1</i>
	<i>v4NbTiVZr2</i>	<i>e4NbTiVZr2</i>
	<i>v4NbTiVZr3</i>	<i>e4NbTiVZr3</i>
	<i>v4NbTiV1</i>	<i>e4NbTiV1</i>
	<i>v4NbTiV2</i>	<i>e4NbTiV2</i>
	<i>v4NbTiV3</i>	<i>e4NbTiV3</i>
	<i>v4NbTiZr1</i>	<i>e4NbTiZr1</i>
	<i>v4NbTiZr2</i>	<i>e4NbTiZr2</i>
	<i>v4NbTiZr3</i>	<i>e4NbTiZr3</i>
	<i>v4NbVZr1</i>	<i>e4NbVZr1</i>
	<i>v4NbVZr2</i>	<i>e4NbVZr2</i>
	<i>v4NbVZr3</i>	<i>e4NbVZr3</i>
	<i>v4TiVZr1</i>	<i>e4TiVZr1</i>
	<i>v4TiVZr2</i>	<i>e4TiVZr2</i>
	<i>v4TiVZr3</i>	<i>e4TiVZr3</i>
	<i>v4NbTi2</i>	<i>e4NbTi2</i>
	<i>v4NbV2</i>	<i>e4NbV2</i>
	<i>v4NbZr2</i>	<i>e4NbZr2</i>
	<i>v4TiV2</i>	<i>e4TiV2</i>
	<i>v4TiZr2</i>	<i>e4TiZr2</i>
	<i>v4VZr2</i>	<i>e4VZr2</i>

**Transformation of CECs in the orthogonal basis for the disordered bcc (A2)
structure to CECs in the CV basis**

For a binary system P-Q, enthalpy of mixing H_{mc} in the orthogonal basis can be written as

$$H_{mc} = 4C_2^{PQ}(u_2^{PQ} - 1) + 3C_3^{PQ}(u_3^{PQ} - 1) + 12C_4^{PQ}(u_4^{PQ} + x_P - x_Q) + 6C_5^{PQ}(u_5^{PQ} - 1) \quad C.1$$

The above expression may be compared with a similar expression on the CV basis.

$$H_{mc} = e_{21PQ} \cdot v_{21PQ} + e_{22PQ} \cdot v_{22PQ} + e_{3PQ} \cdot v_{3PQ} + e_{4PQ} \cdot v_{4PQ} \quad C.2$$

The CVCFs can be expressed in terms of orthogonal basis CFs as follows.

$$v_{21PQ} = \rho_{12}^{PR} = \frac{1}{4}\langle(1 - \sigma_1)(1 + \sigma_2)\rangle = \frac{1}{4}(1 - u_2^{PQ})$$

$$v_{22PQ} = \rho_{13}^{PR} = \frac{1}{4}\langle(1 - \sigma_1)(1 + \sigma_3)\rangle = \frac{1}{4}(1 - u_3^{PQ})$$

+ similar relations for triangle and tetrahedron CFs

Substituting these in Eqn. (124), we have

$$H_{mc} = \frac{1}{4}e_{21PQ} \cdot (1 - u_2^{PQ}) + \frac{1}{4}e_{22PQ} \cdot (1 - u_3^{PQ}) + \dots \quad C.3$$

A comparison of Eqns. (C.1) and (C.3) leads to the following equivalence between the CECs on the orthogonal basis and the CECs on the CV basis:

$$e_{21PQ} = -16 \cdot C_2^{PQ} \quad C.4$$

$$e_{22PQ} = -12 \cdot C_3^{PQ}$$

$$e_{3PQ} = -48 \cdot C_4^{PQ}$$

$$e_{4PQ} = 96 \cdot C_5^{PQ}$$

Similar relations hold for binary subsystems of higher-order systems.

Determination of equiatomic composition in quaternary system.

A 3-D tetrahedron contour can be drawn using commercially available Origin software or any freely available software to represent the quaternary composition. However, it is challenging to visualize changes in the tetrahedron contour space.

To overcome this issue, a 2-D heat map is more useful. The four vertices of the square represent the four pure elements. The edges of the square will represent the binary compositions. The central point of the square will represent the equiatomic composition.

The following figure will represent it.

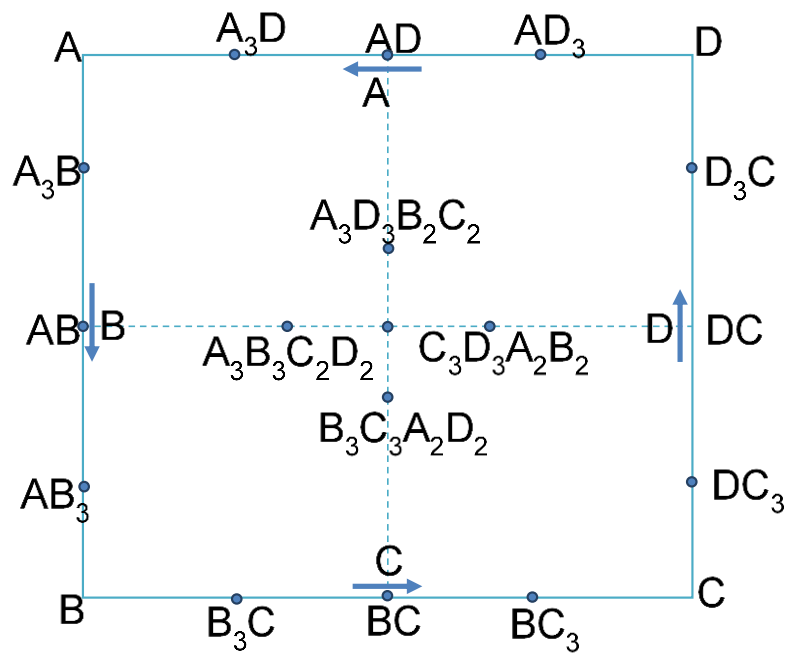


Figure: Representing the quaternary composition map with the $(AD)_m(BC)_n$.

The composition is chosen as $(AD)_m(BC)_n$. The ratio between A/D and B/C must be the same while selecting the composition. The details are given in the (Yang and Zhong 2021).

Calculated and CE fitted ground state energy

Nb-Ti	concentration	energy	fitted_energy
	0	0	-0.001549
	0.333333	-0.028465	-0.028386
	0.666667	-0.056876	-0.050412
	0.777778	-0.060645	-0.055265
	0.833333	-0.049933	-0.042833
	0.9	-0.031004	-0.027493
	1	0	0.000515

Nb-V	concentration	energy	fitted_energy
	0	0	-0.001246
	1	0	0.000633

Nb-Zr	concentration	energy	fitted_energy
	0	0	0.000468
	0.666667	-0.015888	-0.015548
	1	0	0.000435

Ti-V	concentration	energy	fitted_energy
	0	0	-0.002209
	0.125	-0.023339	-0.015959
	0.285714	-0.037251	-0.033615
	1	0	0.000059

Ti-Zr	concentration	energy	fitted_energy
	0	0	-0.008302
	0.333333	-0.075272	-0.076416
	0.5	-0.063176	-0.061435
	0.666667	-0.044498	-0.045632
	1	0	-0.001551

V-Zr	concentration	energy	fitted_energy
	0	0	0.063611
	1	0	0.032231

List of Research Papers

1. Kumar, Shanker, and Vikas Jindal. "Modeling Short-Range Ordering in Binary BCC Ti-X (X= Nb, V, Zr) Alloys using CE-CVM." *Journal of Phase Equilibria and Diffusion* 43, no. 4 (2022): 511-526.
2. Kumar, Shanker, and Vikas Jindal. "Thermodynamic Re-assessment of the Nb-Zr System Using the CE-CVM Model for Solid Solution Phases." *Journal of Phase Equilibria and Diffusion* 43, no. 3 (2022): 277-286.
3. Kumar, Shanker, and Vikas Jindal. "First-principles calculations and thermodynamic assessment of the Nb-V system using CE-CVM." *Calphad* 78 (2022): 102439.
4. Kumar, Shanker, Abhishek Kumar Thakur, Vikas Jindal, and Krishna Muralidharan. "A Neural Network Driven Approach for Characterizing the Interplay Between Short Range Ordering and Enthalpy of Mixing of Binary Subsystems in the NbTiVZr High Entropy Alloy." *Journal of Phase Equilibria and Diffusion* 44, no. 3 (2023): 520-538.
5. Kumar, Shanker, Albert Linda, Yagnesh Shadangi, and Vikas Jindal. "Influence of micro-segregation on the microstructure, and microhardness of MoNbTaxTi (1-x) W refractory high entropy alloys: Experimental and DFT approach." *Intermetallics* 164 (2024): 108080.

