

SUPPORTING INFORMATION

Modulating Hardness in $\text{Sc}_2(\text{Ru}_{5-x}\text{TM}_x)\text{B}_4$ through Empirical Considerations and Computational Analysis

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Table S1. Selected Crystallographic Data for Sc₂Ru₅B₄ and Sc₂(Ru_{4.2}Re_{0.8})B₄

Formula	Sc ₂ Ru ₅ B ₄	Sc ₂ (Ru _{4.2} Re _{0.8})B ₄
Mass (g mol ⁻¹)	1277.02	1412.48
Space group; <i>Z</i>	<i>Pbam</i> (55); 2	<i>Pbam</i> (55); 2
<i>a</i> (Å)	8.4743(2)	8.486(1)
<i>b</i> (Å)	9.9738(2)	9.984(1)
<i>c</i> (Å)	2.9985(1)	3.0197(4)
<i>V</i> (Å ³)	253.44(1)	255.86(6)
crystal color, shape	gray, plate	gray, plate
data collection temp. (K)	296	296
radiation source, λ (Å)	Mo K, 0.71073	Mo K, 0.71073
ρ _{calc} (g cm ⁻³)	8.367	9.167
μ (mm ⁻¹)	16.85	33.14
absorption correction	multi-scan	analytical
θ _{min} , θ _{max}	6.31, 56.63	6.31, 58.10
refinement method	<i>F</i> ²	<i>F</i> ²
<i>hkl</i> ranges	-11 ≤ <i>h</i> ≤ 11 -13 ≤ <i>k</i> ≤ 13 -4 ≤ <i>l</i> ≤ 4	0 ≤ <i>h</i> ≤ 11 0 ≤ <i>k</i> ≤ 13 0 ≤ <i>l</i> ≤ 4
no. of reflections; <i>R</i> _{int}	3974; 0.0292	442; 0
no. of unique reflections	369	395
no. of parameters	37	31
<i>R</i> (<i>F</i>) for <i>F</i> _o ² > 4σ (<i>F</i> _o ²)	0.0182	0.0161
<i>R</i> _w (<i>F</i> _o ²)	0.05	0.0371
Goodness of fit	1.028	1.151
Δρ _{max} , Δρ _{min} (e ⁻ /Å ³)	0.75, -1.00	1.34, -1.01

Table S2. Equivalent isotropic displacement parameters for Sc₂Ru₅B₄ and Sc₂(Ru₄Re)B₄

Compound	Atom	Wyckoff	<i>x</i>	<i>y</i>	<i>z</i>	<i>U</i> _{equiv.}	Occ.
(a) Sc ₂ Ru ₅ B ₄	Sc	4h	0.8424(1)	0.3187(1)	0.5	0.0161(3)	1
	Ru	4g	0.59569(4)	0.26207(4)	1	0.0144(2)	1
	Ru	2c	1	0.5	0	0.0141(2)	0.998(3)
	Ru	4g	0.33922(4)	0.45209(4)	1	0.0147(2)	1

	B	4h	0.1488(6)	0.3973(6)	0.5	0.015(1)	1
	B	4h	0.5347(8)	0.4104(7)	0.5	0.022(1)	1
(b) Sc ₂ (Ru _{4.2} Re _{0.8})B ₄	Sc	4h	0.8424(1)	0.6814(1)	0.5	0.0050(2)	1
	Ru	4g	0.34037(3)	0.54696(3)	1	0.0033(1)	0.601(3)
	Ru	2c	1	0.5	0	0.0028(2)	1
	Ru	4g	0.59602(5)	0.73909(4)	1	0.0031(2)	1
	Re	4g	0.34037(3)	0.54696(3)	1	0.0033(1)	0.399(3)
	B	4h	0.5352(7)	0.5898(6)	0.5	0.005(1) ^a	1
	B	4h	0.149(6)	0.6009(6)	0.5	0.006(1) ^a	1

^amodeled with isotropic atomic displacement parameters

Table S3. Refined harmonic displacement parameters for Sc₂Ru₅B₄ and Sc₂(Ru₄Re)B₄

Compound	Site	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
(a) Sc ₂ Ru ₅ B ₄	Sc1	0.0150(5)	0.0182(5)	0.0152(5)	0	0	-0.0013(3)
	Ru1	0.0141(3)	0.0142(3)	0.0149(3)	0	0	-0.0002(1)
	Ru2	0.0135(3)	0.0143(4)	0.0145(3)	0	0	0.0005(2)
	Ru3	0.0144(3)	0.0148(3)	0.0150(3)	0	0	0.0002(1)
	B1	0.013(2)	0.017(3)	0.013(3)	0	0	-0.001(2)
	B2	0.025(3)	0.021(3)	0.022(3)	0	0	0.003(2)
(b) Sc ₂ (Ru _{4.2} Re _{0.8})B ₄	Sc1	0.0032(5)	0.0081(5)	0.0036(5)	0	0	0.0006(4)
	Ru1	0.0026(2)	0.0047(2)	0.0028(2)	0	0	-0.0001(1)
	Ru2	0.0015(3)	0.0041(3)	0.0027(3)	0	0	-0.0002(2)
	Ru3	0.0024(2)	0.0040(2)	0.0030(2)	0	0	0.0001(2)

Re1 0.0026(2) 0.0047(2) 0.0028(2) 0 0 -0.0001(1)

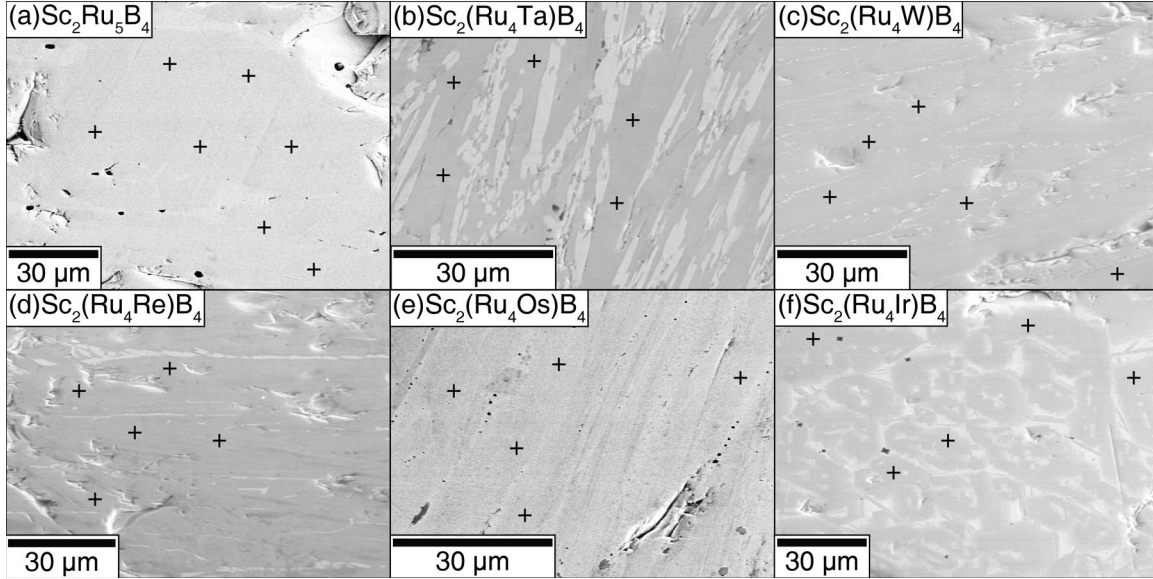


Figure S1: Backscattered electron micrographs of (a) $\text{Sc}_2\text{Ru}_5\text{B}_4$, (b) $\text{Sc}_2(\text{Ru}_4\text{Ta})\text{B}_4$, (c) $\text{Sc}_2(\text{Ru}_4\text{W})\text{B}_4$, (d) $\text{Sc}_2(\text{Ru}_4\text{Re})\text{B}_4$, (e) $\text{Sc}_2(\text{Ru}_4\text{Os})\text{B}_4$, and (f) $\text{Sc}_2(\text{Ru}_4\text{Ir})\text{B}_4$. Plus signs indicate the spots selected for EDS analysis.

Table S4. Unit Cell Parameters for $\text{Sc}_2(\text{Ru}_4\text{TM})\text{B}_4$ ($\text{TM} = \text{Ru}, \text{Ta}, \text{W}, \text{Mo}, \text{Re}, \text{Os}, \text{and Ir}$)

sample	a, Å	b, Å	c, Å	volume, Å ³	α	β	γ
$\text{Sc}_2\text{Ru}_5\text{B}_4$	8.4865(2)	2.9930(8)	9.9714(2)	253.277(8)	90.000	90.000	90.000
$\text{Sc}_2\text{Ru}_4\text{TaB}_4$	8.5049(9)	3.0162(2)	9.9588(8)	255.47(2)	90.000	90.000	90.000
$\text{Sc}_2\text{Ru}_4\text{WB}_4$	8.5319(2)	3.02155(7)	9.9617(2)	256.813(8)	90.000	90.000	90.000
$\text{Sc}_2\text{Ru}_4\text{ReB}_4$	8.4667(2)	3.00785(9)	9.964(3)	253.76(1)	90.000	90.000	90.000
$\text{Sc}_2\text{Ru}_4\text{OsB}_4$	8.4950(4)	2.9979(1)	9.986(4)	254.33(1)	90.000	90.000	90.000
$\text{Sc}_2\text{Ru}_4\text{IrB}_4$	8.5937(2)	2.98087(8)	9.9286(6)	254.34(1)	90.000	90.000	90.000

Table S5. Ideal stress and strain values of $\text{Sc}_2\text{Ru}_5\text{B}_4$ for various tensile systems derived from stress-strain curves

applied tensile	ideal stress (Gpa)	strain
[100]	32.7	0.27
[010]	46.5	0.32
[001]	34.2	0.24
[101]	28.4	0.17
[110]	27.4	0.17

[111]	23.4	0.17
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Table S6. Ideal stress and strain values of Sc₂Ru₅B₄ for various shear systems derived from stress-strain curves

applied tensile	ideal stress (Gpa)	strain
(100)[001]	21.1	0.30
(100)[010]	18.3	0.21
(100)[011]	17.2	0.23
(100)[0-11]	17.2	0.23
(001)[100]	21.1	0.30
(001)[110]	18.6	0.23
(001)[010]	20.0	0.21
(001)[-100]	21.1	0.30
(001)[-110]	18.6	0.23
(011)[01-1]	24.2	0.30
(011)[100]	17.2	0.23
(011)[1-11]	22.5	0.25
(011)[11-1]	20.6	0.30
(110)[-110]	24.5	0.49
(110)[001]	18.6	0.23
(110)[1-11]	21.8	0.32
(110)[1-10]	26.2	0.35
(010)[001]	20.0	0.21
(010)[-100]	18.3	0.21
(010)[101]	18.6	0.17
(111)[-110]	21.8	0.32
(111)[-101]	20.2	0.21
(111)[01-1]	20.6	0.30
(111)[0-11]	22.5	0.25
(111)[11-2]	14.7	0.14
(111)[-1-12]	22.0	0.23

Table S7. Ideal stress and strain values of Sc₂(Ru₄Ta)B₄ for various shear systems derived from stress-strain curves

applied tensile	ideal stress (Gpa)	strain
(100)[001]	21.4	0.25
(100)[010]	17.7	0.14
(100)[011]	19.3	0.21
(100)[0-11]	19.3	0.21

(001)[100]	21.4	0.25
(001)[110]	16.2	0.14
(001)[010]	19.4	0.17
(001)[-100]	21.4	0.25
(001)[-110]	16.2	0.14
(011)[01-1]	20.8	0.32
(011)[100]	19.3	0.21
(011)[1-11]	22.4	0.23
(011)[11-1]	19.7	0.39
(110)[-110]	24.4	0.42
(110)[001]	16.2	0.14
(110)[1-11]	20.1	0.32
(110)[1-10]	22.0	0.39
(010)[001]	19.7	0.17
(010)[-100]	17.7	0.14
(010)[101]	20.0	0.17
(111)[-110]	20.1	0.32
(111)[-101]	19.7	0.17
(111)[01-1]	19.7	0.39
(111)[0-11]	22.4	0.23
(111)[11-2]	21.2	0.23
(111)[-1-12]	20.7	0.21

Table S8. Ideal stress and strain values of $\text{Sc}_2(\text{Ru}_4\text{W})\text{B}_4$ for various shear systems derived from stress-strain curves

applied tensile	ideal stress (Gpa)	strain
(100)[001]	20.4	0.23
(100)[010]	19.3	0.14
(100)[011]	20.8	0.19
(100)[0-11]	20.8	0.19
(001)[100]	20.4	0.23
(001)[110]	19.7	0.17
(001)[010]	21.6	0.19
(001)[-100]	20.4	0.23
(001)[-110]	19.6	0.17
(011)[01-1]	23.5	0.32
(011)[100]	20.8	0.19
(011)[1-11]	23.5	0.21
(011)[11-1]	20.6	0.35
(110)[-110]	24.6	0.42

(110)[001]	19.7	0.17
(110)[1-11]	22.2	0.32
(110)[1-10]	25.2	0.37
(010)[001]	21.6	0.19
(010)[-100]	19.3	0.14
(010)[101]	21.6	0.19
(111)[-110]	22.2	0.32
(111)[-101]	24.5	0.23
(111)[01-1]	20.6	0.35
(111)[0-11]	23.5	0.21
(111)[11-2]	22.4	0.21
(111)[-1-12]	24.0	0.23

Table S9. Ideal stress and strain values of $\text{Sc}_2(\text{Ru}_4\text{Re})\text{B}_4$ for various shear systems derived from stress-strain curves

applied tensile	ideal stress (Gpa)	strain
(100)[001]	21.6	0.25
(100)[010]	20.9	0.19
(100)[011]	19.4	0.17
(100)[0-11]	19.4	0.17
(001)[100]	21.6	0.25
(001)[110]	21.0	0.19
(001)[010]	20.9	0.19
(001)[-100]	21.6	0.25
(001)[-110]	21.0	0.19
(011)[01-1]	24.0	0.32
(011)[100]	19.4	0.17
(011)[1-11]	23.2	0.21
(011)[11-1]	20.9	0.28
(110)[-110]	23.5	0.42
(110)[001]	21.0	0.19
(110)[1-11]	22.6	0.32
(110)[1-10]	27.5	0.37
(010)[001]	20.9	0.19
(010)[-100]	20.9	0.19
(010)[101]	21.8	0.19
(111)[-110]	22.6	0.32
(111)[-101]	23.3	0.21
(111)[01-1]	20.9	0.28
(111)[0-11]	23.2	0.21

(111)[11-2]	24.4	0.21
(111)[-1-12]	24.1	0.23

Table S10. Ideal stress and strain values of $\text{Sc}_2(\text{Ru}_4\text{Os})\text{B}_4$ for various shear systems derived from stress-strain curves

applied tensile	ideal stress (Gpa)	strain
(100)[001]	19.4	0.23
(100)[010]	19.5	0.21
(100)[011]	16.2	0.14
(100)[0-11]	16.3	0.14
(001)[100]	19.4	0.23
(001)[110]	18.8	0.23
(001)[010]	20.3	0.21
(001)[-100]	19.4	0.23
(001)[-110]	18.8	0.23
(011)[01-1]	23.3	0.30
(011)[100]	16.3	0.14
(011)[1-11]	21.5	0.21
(011)[11-1]	20.5	0.28
(110)[-110]	23.1	0.42
(110)[001]	18.8	0.23
(110)[1-11]	21.6	0.32
(110)[1-10]	26.8	0.35
(010)[001]	20.3	0.21
(010)[-100]	19.5	0.21
(010)[101]	19.5	0.19
(111)[-110]	21.6	0.32
(111)[-101]	19.9	0.19
(111)[01-1]	20.5	0.28
(111)[0-11]	21.5	0.21
(111)[11-2]	14.3	0.14
(111)[-1-12]	21.6	0.23

Table S11. Ideal stress and strain values of $\text{Sc}_2(\text{Ru}_4\text{Ir})\text{B}_4$ for various shear systems derived from stress-strain curves

applied tensile	ideal stress (Gpa)	strain
(100)[001]	21.5	0.35
(100)[010]	9.7	0.12
(100)[011]	16.6	0.21

(100)[0-11]	16.6	0.21
(001)[100]	21.5	0.35
(001)[110]	18.8	0.25
(001)[010]	12.7	0.14
(001)[-100]	21.1	0.35
(001)[-110]	18.8	0.25
(011)[01-1]	26.7	0.30
(011)[100]	16.6	0.21
(011)[1-11]	20.5	0.28
(011)[11-1]	21.4	0.32
(110)[-110]	26.8	0.51
(110)[001]	18.4	0.23
(110)[1-11]	21.6	0.30
(110)[1-10]	27.5	0.35
(010)[001]	12.7	0.14
(010)[-100]	9.8	0.12
(010)[101]	8.9	0.10
(111)[-110]	21.6	0.30
(111)[-101]	19.4	0.17
(111)[01-1]	21.4	0.32
(111)[0-11]	20.5	0.28
(111)[11-2]	10.0	0.12
(111)[-1-12]	19.5	0.25
