

Supporting information

Table S1 comparison the reported method with TEMUC3 developed by X.Z. Li(Li, 2019). The real primitive cell of the Al_5Co_2 phase was reported to be $a=0.77$ nm, $b=1.08$ nm, $c=1.7$ nm, $\alpha=161.5^\circ$, $\beta=76.85^\circ$, and $\gamma=110.94^\circ$. This cell was converted to a reciprocal cell as the input cell of Niggli Reduction Tools ($a^*=1.5006$ nm⁻¹, $b^*=3.2834$ nm⁻¹, $c^*=2.0006$ nm⁻¹, $\alpha^*=17.57^\circ$, $\beta^*=67.92^\circ$, and $\gamma^*=62.71$). It indicates that the reported method is well consistent with TEMUC3.

	TEMUC3	The reported method
Input cell	0.76, 1.71, 1.08, 161.6, 69.33, 116.49	1.5006, 3.2834, 2.0006, 17.57, 67.92, 62.71
Reduced cell*		1.3197, 1.5002, 1.5006, 60.11, 89.96, 89.93
Reduced cell		7.5773, 7.6884, 7.6863, 119.89, 90.00, 90.06
Niggli matrix		57.42, 59.11, 59.08, -29.45, -0.00, -0.06 Criteria (B=C, -B/2, 0, 0)
Unit cell	7.6, 7.6, 7.6, 89.95, 89.98, 119.8	7.6884, 7.6863, 7.5773, 90.00, 90.06, 119.89

Table S2 The list of the symmetry constraint unit cell, the evaluated errors of the input cell, and the Bravais criteria of the example 2 for convenient to choosing the Bravais lattice in the box “Unit Cell List” of Niggli Reduction Tools.

	Sym. unit cell	Evaluated errors of the input cell	Bravais criteria
cF	5.4199, 5.4199, 5.4199 90.00, 90.00, 90.00	-0.0103, -0.0806, -0.0927 0.04, 0.94, 0.86	A=B=C, A/2, A/2, A/2
hR	3.9142, 3.9142, 9.2175 90.00, 90.00, 120.00	-0.0390, 0.0817, 0.0163 -0.14, 0.08, -0.19	A=B=C, D, D, D
	3.8762, 3.8762, 9.2707 90.00, 90.00, 120.00	0.0486, 0.0068, -0.0338 -0.07, 0.94, 0.85	A=B, A/2, A/2, A/2
oI	3.8466, 3.7715, 5.4866 90.00, 90.00, 90.00	0.0089, -0.0867, -0.0777 -0.04, 0.91, 0.77	B=C, D, A/2, A/2
mC	6.5935, 3.9058, 3.7298 90.00, 124.10, 90.00	-0.0149, 0.0656, 0.0053 -0.11, 0.29, 0.19	A=B, D, D, F
	6.5373, 3.7715, 3.8466 90.00, 123.05, 90.00	0.0020, -0.0015, 0.0116 -0.18, -0.87, -1.11	B=C, D, E, E
	6.6972, 3.8466, 3.7715 90.00, 125.00, 90.00	0.0089, -0.0413, -0.0543 -0.11, 1.06, 0.89	None, D, A/2, A/2
aP	3.8466, 3.8169, 3.7298 59.95, 62.34, 61.28	0.0000, 0.0000, 0.0000 -0.00, 0.00, 0.00	None

Li, X. Z. (2019). *Micron* **117**, 1-7.