Supporting information

First-principles determination of the crystallography of the low-temperature phase for NbRu and TaRu shape memory alloys

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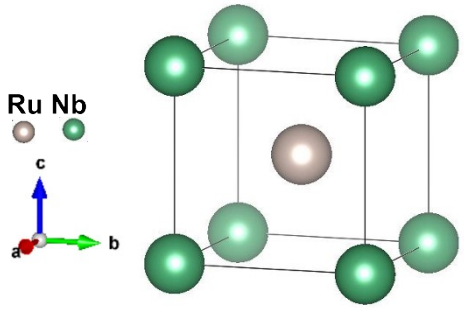

Figure S1. The crystallographic of the cubic phase (Pm-3m) for NbRu alloy. The structural parameters a = b = c = 3.180 Å, and α = β = γ = 90^0. Nb atom locate at Wyckoff position (1a): (0.0, 0.0, 0.0), whereas Ru atom locate at Wyckoff position (1b): (0.5, 0.5, 0.5).

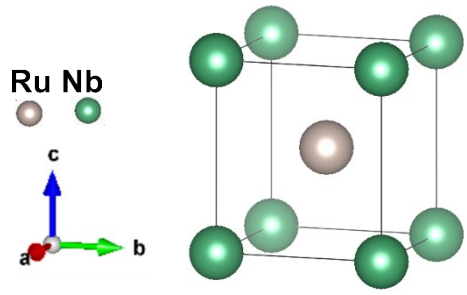

Figure S2. The crystallographic of the tetragonal phase (P4/mmm) for NbRu alloy. The structural parameters a = b = 3.062 Å, c = 3.431 Å, and α = β = γ = 90^0. Nb atom locate at Wyckoff position (1a): (0.0, 0.0, 0.0), whereas Ru atom locate at Wyckoff position (1d): (0.5, 0.5, 0.5).

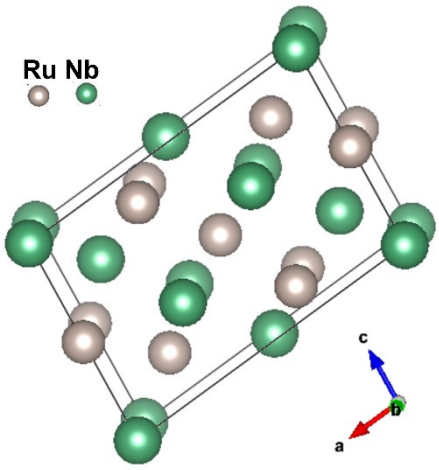

Figure S3. The crystallographic of the monoclinic phase (P2/m) for NbRu alloy. The structural parameters are listed in table S1.

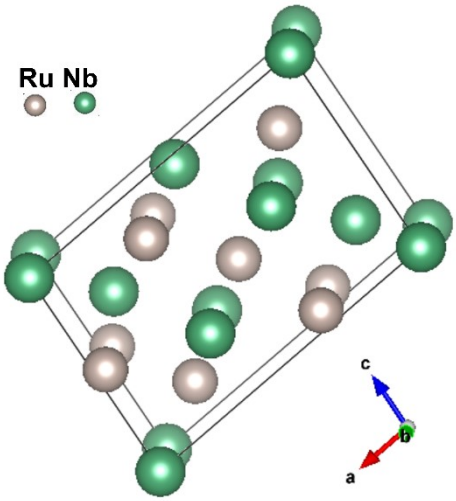

Figure S4. The crystallographic of the monoclinic phase ($P2_1/m$) for NbRu alloy. The structural parameters are listed in table S1.

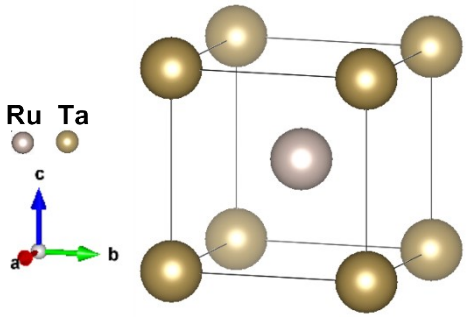

Figure S5. The crystallographic of the cubic phase (Pm-3m) for TaRu alloy. The structural parameters a = b = c = 3.164 Å, and $\alpha = \beta = \gamma = 90^0$. Ta atom locate at Wyckoff position (1a): (0.0, 0.0, 0.0), whereas Ru atom locate at Wyckoff position (1b): (0.5, 0.5, 0.5).

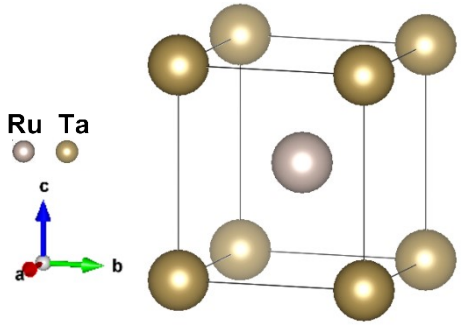

Figure S6. The crystallographic of the tetragonal phase (P4/mmm) for TaRu alloy. The structural parameters a = b = 3.049 Å, c = 3.407 Å, and $\alpha = \beta = \gamma = 90^0$. Ta atom locate at Wyckoff position (1a): (0.0, 0.0, 0.0), whereas Ru atom locate at Wyckoff position (1d): (0.5, 0.5, 0.5).

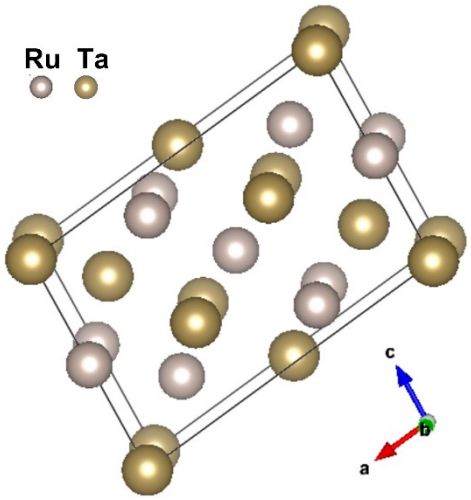

Figure S7. The crystallographic of the monoclinic phase (P2/m) for TaRu alloy. The structural parameters are listed in table S2.

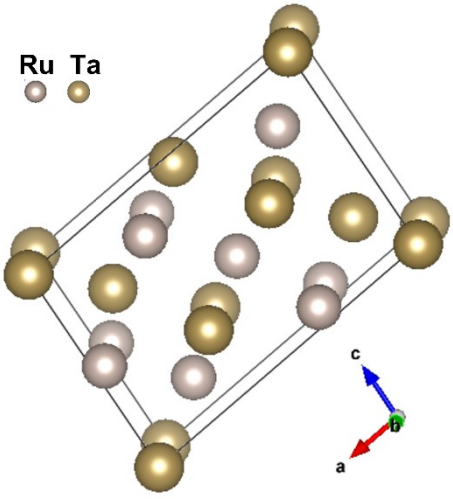

Figure S8. The crystallographic of the monoclinic phase ($P2_1/m$) for TaRu alloy. The structural parameters are listed in table S2.

Table S1 The convenient set of the atomic positions of the P2/m and the $P2_1/m$ monoclinic structures for NbRu. WP denotes the Wyckoff position. The lattice constants and angles for the P2/m monoclinic structure are a = 8.095 Å, b = 4.382 Å, c = 5.492 Å, $\alpha = 90^0$, $\beta = 97.6^0$ and $\gamma = 90^0$. On the other hand, the lattice constants and angles for the $P2_1/m$ monoclinic structure are a = 8.067 Å, b = 4.406 Å, c = 5.478 Å, $\alpha = 90^0$, $\beta = 97.1^0$ and $\gamma = 90^0$.

Atom	WP	P2/m			WP	$P2_1/m$		
		x	y	z		x	y	z
Nb-1	1a	0.0000	0.0000	0.0000	2e	0.0132	0.0000	0.0448
Nb-2	1e	0.5000	0.5000	0.0000	2e’	0.5013	0.5000	0.9786
Nb-3	2m	0.3233	0.0000	0.6212	2e’’	0.3089	0.0000	0.5997
Nb-4		0.6767	0.0000	0.3788	2e’	0.6654	0.0000	0.3547
Nb-5	2n	0.8541	0.5000	0.7287	2e’’	0.8578	0.5000	0.7336
Nb-6		0.1459	0.5000	0.2713	2e	0.1535	0.5000	0.2885
Ru-1	1c	0.0000	0.0000	0.5000	2e	0.9786	0.0000	0.5311
Ru-2	1h	0.5000	0.5000	0.5000	2e’	0.5015	0.5000	0.4899
Ru-3	2m	0.3503	0.0000	0.1390	2e’’	0.3589	0.0000	0.1197
Ru-4		0.6497	0.0000	0.8610	2e’	0.6652	0.0000	0.8434
Ru-5	2n	0.8083	0.5000	0.2086	2e’’	0.8077	0.5000	0.2136
Ru-6		0.1917	0.5000	0.7914	2e	0.1881	0.5000	0.8022

Table S2 The convenient set of the atomic positions of the P2/m and the $P2_1/m$ monoclinic structures for TaRu. WP denotes the Wyckoff position. The lattice constants and angles for the P2/m monoclinic structure are a = 8.048 Å, b = 4.369 Å, c = 5.452 Å, $\alpha = 90^0$, $\beta = 97.4^0$ and $\gamma = 90^0$. On the other hand, the lattice constants and angles for the $P2_1/m$ monoclinic structure are a = 8.029 Å, b = 4.391 Å, c = 5.436 Å, $\alpha = 90^0$, $\beta = 97.0^0$ and $\gamma = 90^0$.

Atom	WP	P2/m	WP	$P2_1/m$

		x	y	z		x	y	z
Ta-1	1a	0.0000	0.0000	0.0000	2e	0.0118	0.0000	0.0433
Ta-2	1e	0.5000	0.5000	0.0000	2e’	0.5012	0.5000	0.9806
Ta-3	2m	0.3242	0.0000	0.6255	2e’,	0.3108	0.0000	0.6035
Ta-4		0.6758	0.0000	0.3745	2e’	0.6655	0.0000	0.3527
Ta-5	2n	0.8519	0.5000	0.7250	2e’,	0.8559	0.5000	0.7298
Ta-6		0.1481	0.5000	0.2750	2e	0.1549	0.5000	0.2900
Ru-1	1c	0.0000	0.0000	0.5000	2e	0.9786	0.0000	0.5312
Ru-2	1h	0.5000	0.5000	0.5000	2e’	0.5017	0.5000	0.4908
Ru-3	2m	0.3489	0.0000	0.1408	2e’,	0.3578	0.0000	0.1222
Ru-4		0.6511	0.0000	0.8592	2e’	0.6650	0.0000	0.8425
Ru-5	2n	0.8088	0.5000	0.2069	2e’,	0.8089	0.5000	0.2111
Ru-6		0.1912	0.5000	0.7931	2e	0.1881	0.5000	0.8021

Table S3 The standard set of the atomic positions of the $P2_1/m$ monoclinic structure for NbRu. WP denotes the Wyckoff position. The corresponding structural parameters are a = 8.067 Å, b = 4.406 Å, c = 5.478 Å, $\alpha = 90^0$, $\beta = 97.1^0$ and $\gamma = 90^0$.

Atom	WP	$P2_1/m$		
		x	y	z
Nb-1 and Nb-6	2e	0.9299	0.7500	0.8782
Nb-2 and Nb-4	2e’	0.4180	0.2500	0.8120
Nb-3 and Nb-5	2e’’	0.2256	0.7500	0.4331
Ru-1 and Ru-6	2e	0.8953	0.7500	0.3645
Ru-2 and Ru-4	2e’	0.4182	0.2500	0.3233
Ru-3 and Ru-5	2e’’	0.2756	0.7500	0.9531

Table S4 The standard set of the atomic positions of the $P2_1/m$ monoclinic structure for TaRu. WP denotes the Wyckoff position. The corresponding structural parameters are a = 8.029 Å, b = 4.391 Å, c = 5.436 Å, $\alpha = 90^0$, $\beta = 97.0^0$ and $\gamma = 90^0$.

Atom	WP	$P2_1/m$		
		x	y	z
Ta-1 and Ta-6	2e	0.9285	0.7500	0.8767
Ta-2 and Ta-4	2e’	0.4179	0.2500	0.8140
Ta-3 and Ta-5	2e’’	0.2275	0.7500	0.4369
Ru-1 and Ru-6	2e	0.8953	0.7500	0.3646
Ru-2 and Ru-4	2e’	0.4184	0.2500	0.3242
Ru-3 and Ru-5	2e’’	0.2745	0.7500	0.9556