Mechanical properties and behavior of the Ti-45Nb alloy subjected to extreme conditions

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Supplementary Information

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Supplementary Figures

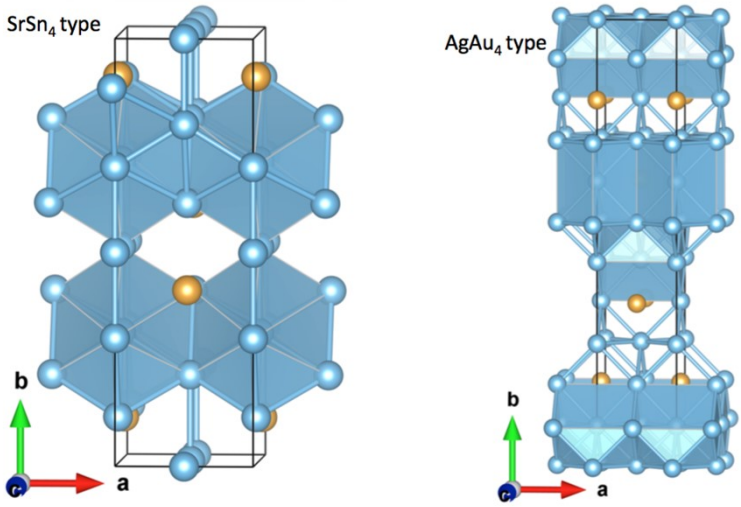

Figure S1. Different sublattice visualizations of both the $SrSn_4$ type and $AgAu_4$ Ti_4Nb structure modifications.

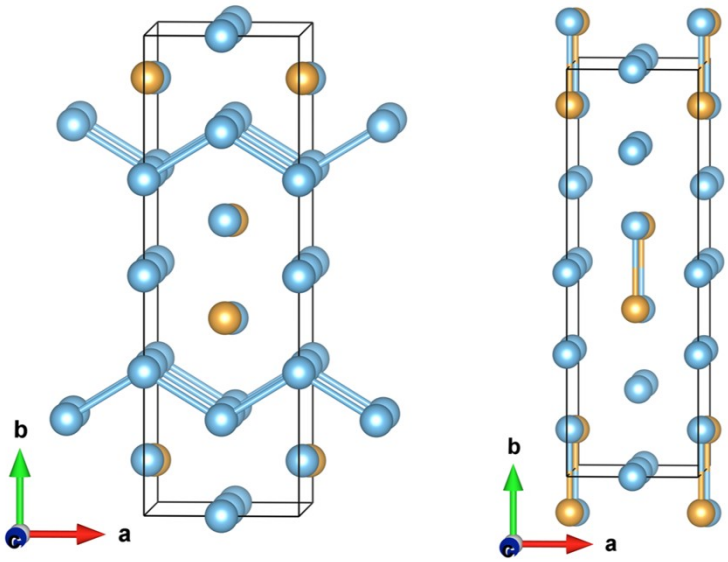

Figure S2. Shortest Ti-Ti and Nb-Ti inter-nuclear separations in $SrSn_4$ type Ti_4Nb structure modification.

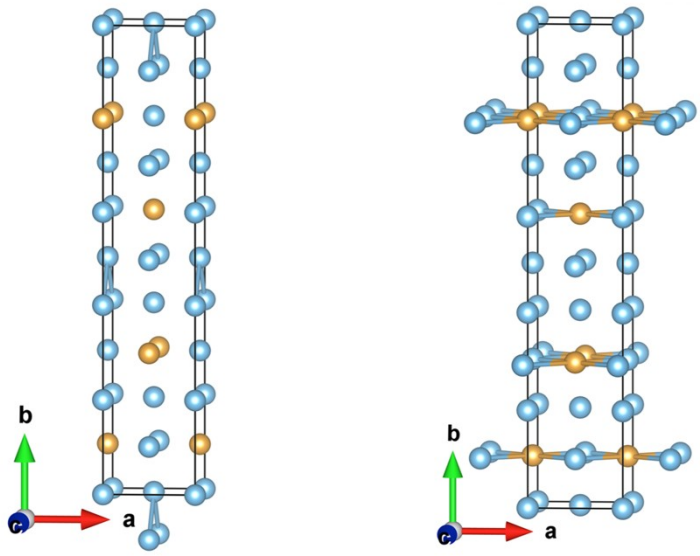

Figure S3. Shortest Ti-Ti and Nb-Ti inter-nuclear separations in $AgAu_4$ type of Ti_4Nb structure modification.

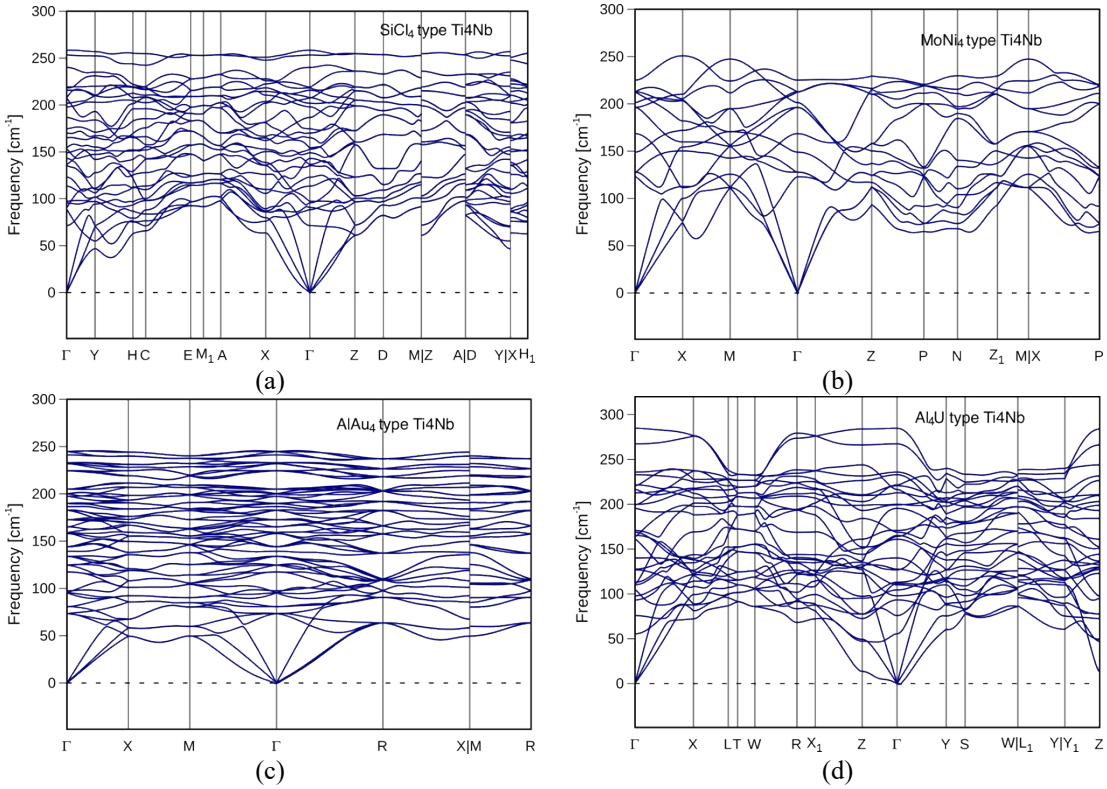

Figure S4. The calculated phonon dispersion spectra of (a) $SiCl_4$ type monoclinic $P2_1/m$ (no. 11), (b) $MoNi_4$ type tetragonal $I4/m$ (no. 87), (c) $AlAu_4$ type cubic $P2_13$ (no. 198), and (d) Al_4U type orthorhombic $Imma$ (no. 74) Ti_4Nb modifications.

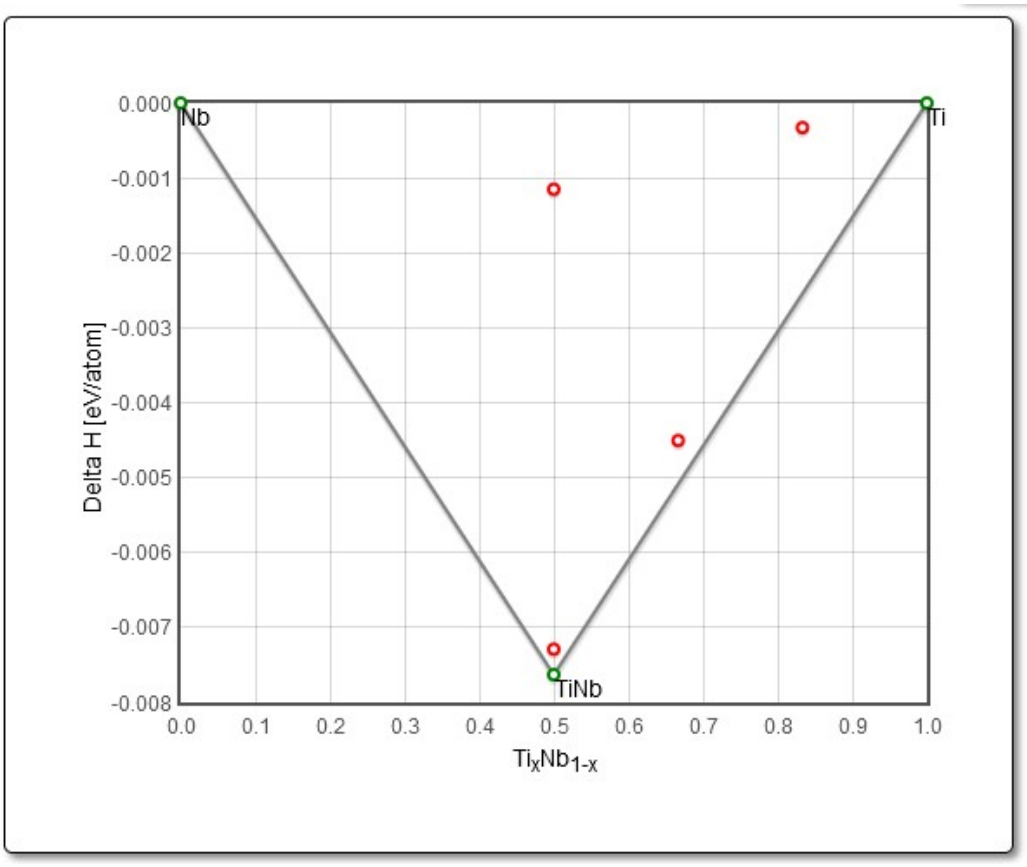

Figure S5. The phase diagram of Ti-Nb was explored using the Open Quantum Materials Database (OQMD) [S1,S2].

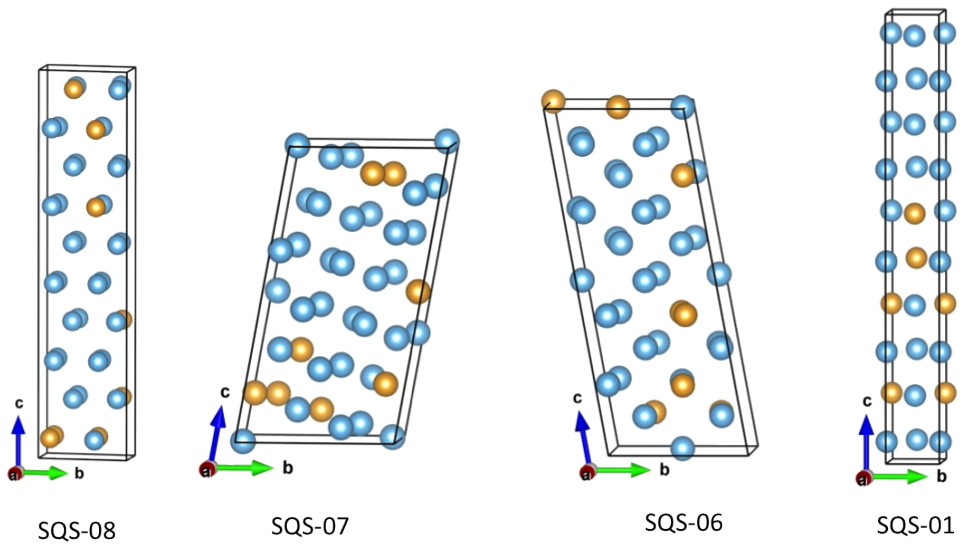

Figure S6. The energetically most favorable random structures from DFT computed disordered intermetallic phases using the Special Quasi-random Structures (SQS), and pseudo-random distributions in supercells in Ti_4Nb chemical system.

Supplementary Tables

Table S1. Calculated elements of elastic stiffness constants (C_{ij}) of $SiCl_4$ type of Ti_4Nb structure modification.

C_{ij}	1	2	3	4	5	6
1	171.31132	77.89224	100.64795	0	0	-18.52067
2	77.89224	193.51518	93.84969	0	0	13.1342
3	100.64795	93.84969	168.21474	0	0	14.22477
4	0	0	0	30.46738	-2.79035	0
5	0	0	0	-2.79035	27.4789	0
6	-18.52067	13.1342	14.22477	0	0	52.20065

Table S2. Calculated elements of elastic stiffness constants (C_{ij}) of Al_4U type of Ti_4Nb structure modification.

C_{ij}	1	2	3	4	5	6
1	166.86316	90.28352	115.15573	0	0	0
2	90.28352	210.70015	65.34569	0	0	0
3	115.15573	65.34569	176.91473	0	0	0
4	0	0	0	51.71654	0	0
5	0	0	0	0	1.40389	0
6	0	0	0	0	0	40.31661

Table S3. Calculated elements of elastic stiffness constants (C_{ij}) of $SrSn_4$ type of Ti_4Nb structure modification.

C_{ij}	1	2	3	4	5	6
1	165.90573	122.4832	86.20536	0	0	0
2	122.4832	171.03558	61.48785	0	0	0
3	86.20536	61.48785	219.61556	0	0	0
4	0	0	0	42.00439	0	0
5	0	0	0	0	9.24459	0
6	0	0	0	0	0	55.83283

Table S4. Calculated elements of elastic stiffness constants (C_{ij}) of $AgAu_4$ type of Ti_4Nb structure modification.

C_{ij}	1	2	3	4	5	6
1	132.65354	115.49458	108.99595	0	0	0
2	115.49458	130.08758	114.5786	0	0	0
3	108.99595	114.5786	132.5739	0	0	0
4	0	0	0	57.257	0	0
5	0	0	0	0	56.66673	0
6	0	0	0	0	0	66.01973

Table S5. Calculated elements of elastic stiffness constants (C_{ij}) of $MoNi_4$ type of Ti_4Nb structure modification.

C_{ij}	1	2	3	4	5	6
1	146.22201	98.04278	113.12769	24.40402	0	0
2	98.04278	146.22201	113.12769	-24.40402	0	0
3	113.12769	113.12769	133.79409	0	0	0
4	24.40402	-24.40402	0	39.98464	0	0
5	0	0	0	0	57.15968	0
6	0	0	0	0	0	57.15968

Table S6. Calculated elements of elastic stiffness constants (C_{ij}) of $AlAu_4$ type of Ti_4Nb structure modification.

C_{ij}	1	2	3	4	5	6
1	115.9925	110.023	110.023	0	0	0
2	110.023	115.9925	110.023	0	0	0
3	110.023	110.023	115.9925	0	0	0
4	0	0	0	38.2506	0	0
5	0	0	0	0	38.2506	0
6	0	0	0	0	0	38.2506

Table S7. Calculated phase diagram of Ti-Nb with three stable phases (Ti, Nb, and TiNb) investigated using the Open Quantum Materials Database (OQMD) [S1,S2].

Stable phases

ID	Spacegroup	Formation Energy [eV/atom]	Stability [eV/atom]	Prototype	# of atoms	Project	Finish Time	Reference
Nb	Im-3m	0	0	A2_W	1	None		
Ti	P6/mmm	0	0	BiIn2	3	None		Chebotareva, E.s., Nuzhdina, S.g.(1973). Observation of omega-titanium in a composite hard facing alloy based on fine-grain diamonds. Fizika Metallov i Metallovedenie, 36.
TiNb	P21/m	-0.008	0		12	None		

Table S8. Calculated phase diagram of Ti-Nb with all possible phases of pure Ti with computed negative (or slightly positive) formation energies (E_f) explored using the Open Quantum Materials Database (OQMD). [S1,S2]

Ti

9315	Ti	P6/mmm	0	0	BiIn2	3	None	Chebotareva, E.s., Nuzhdina, S.g.(1973). Observation of omega-titanium in a composite hard facing alloy based on fine-grain diamonds. Fizika Metallov i Metallovedenie, 36.
2031311	Ti	Ibam	0.003	0.003		6	None	Zarkevich, N.a., Johnson, D.d.(2016). Titanium alpha-omega phase transformation pathway and a predicted metastable structure. Physical Review, Serie 3. B - Condensed Matter (18,1978-), 93.
755845	Ti	P63/mmc	0.014	0.014		24	None	
8079	Ti	P63/mmc	0.014	0.014	Mg	2	None	Wood, R.m.(1962). The lattice constants of high purity alpha titanium. Review of Scientific Instruments, 33.
2016208	Ti	P63/mmc	0.014	0.014	hcp#Mg	2	None	Bulanova, M., Fartushna, I., Meleshevich, K., Samelyuk, A. (2014). Isothermal section at 850?C of the Ti - Dy - Al system in the Ti - Ti Al - Dy Al2 - Dy region. Journal of Alloys Compd., 598.
52003	Ti	P63/mmc	0.014	0.014	Mg	2	None	Hull, A.w.(2002). Crystal structure of Ti and Zr. Golden Book of Phase Transitions, Wroclaw, 1.
755836	Ti	P63/mmc	0.014	0.014		6	None	
755844	Ti	P63/mmc	0.014	0.014		6	None	
755851	Ti	P63/mmc	0.014	0.014		2	None	
755831	Ti	P63/mmc	0.014	0.014		4	None	
755833	Ti	P63/mmc	0.014	0.014		2	None	
755850	Ti	P63/mmc	0.014	0.014		2	None	
755840	Ti	P63/mmc	0.014	0.014		2	None	
1215380	Ti	P63/mmc	0.014	0.014	A3_Mg	2	None	
755821	Ti	P63/mmc	0.014	0.014		4	None	
755848	Ti	Pmm2	0.014	0.014		12	None	
117514	Ti	P63/mmc	0.014	0.014	Mg	2	None	Singh, R.k., Srivastava, A., Chauhan, M.(2011). Pressure induced phase transitions in transition metal nitrides: ab initio study. Physica Status Solidi, Sectio B: Basic Research, 248.
755847	Ti	P63/mmc	0.014	0.014		2	None	
755838	Ti	P63/mmc	0.014	0.014		2	None	
755837	Ti	Pmmn	0.014	0.014		12	None	
755826	Ti	Cmcm	0.014	0.014		4	None	
755846	Ti	Cmcm	0.014	0.014		4	None	
755824	Ti	Cmcm	0.014	0.014		4	None	
755841	Ti	Cmcm	0.014	0.014		4	None	
755832	Ti	P63/mmc	0.014	0.014		2	None	
755829	Ti	P63/mmc	0.014	0.014		2	None	
117243	Ti	P63/mmc	0.014	0.014	Mg	2	None	Chattaraj, D., Parida, S.c., Majumder, C.(2011). Structural and electronic properties of U2 Ti: a first principles study. Physica B: Condensed Matter (Amsterdam, 152, 1988-), 406.

755823	Ti	P63/mmc	0.014	0.014		14	None	
755839	Ti	P63/mmc	0.014	0.014		2	None	
755842	Ti	P63/mmc	0.014	0.014		2	None	
755834	Ti	Cmcm	0.014	0.014		8	None	
755835	Ti	P63/mmc	0.014	0.014		14	None	
755825	Ti	P63/mmc	0.014	0.014		2	None	
110171	Ti	P63/mmc	0.014	0.014	Mg	2	None	De wijs, G.a., Van setten, M.j., Er, S., Brocks, G.(2010). First-principles modelling of magnesium titanium hydrides. Journal of Physics: Condensed Matter, 22.
87084	Ti	P63/mmc	0.014	0.014	Mg	2	None	Novoselova, T., Malinov, S., Sha, W., Zhecheva, A.(2004). High-temperature synchrotron X-ray diffraction study of phases in a gamma Ti Al alloy. Materials Science and Engineering, 371.
755830	Ti	P63/mmc	0.014	0.014		10	None	
755827	Ti	P63/mmc	0.014	0.014		10	None	
755828	Ti	Cmcm	0.014	0.014		12	None	
755822	Ti	Pm	0.014	0.014		12	None	
755849	Ti	Pm	0.014	0.014		12	None	
2030140	Ti	P63/mmc	0.014	0.014	hcp#Mg	2	None	Richter, Manuel, Schoenecker, Stephan, Li, Xiaoqing, Koepernik, Klaus, Johansson, Boerje, Vitos, Levente(2015). Metastable cubic and tetragonal phases of transition metals predicted by density-functional theory. RSC Advances, 5.
1215291	Ti	Cmcm	0.016	0.016	A20_alpha_U	2	None	
1216096	Ti	R-3m	0.039	0.039	C19_alpha_Sm	3	None	
1214579	Ti	Fm-3m	0.070	0.070	A1_Cu	1	None	
676147	Ti	Fm-3m	0.070	0.070		1	None	Haglund, J., Fernandez guillermet, F., Grimvall, G., Korling, M. (1993). Theory of bonding in transition-metal carbides and nitrides. Physical Review, Serie 3. B - Condensed Matter (18,1978-), 48.
1484872	Ti	I4/mmm	0.070	0.070		1	None	
1215737	Ti	I4/mmm	0.070	0.070	A6_In	1	None	
1215915	Ti	P3121	0.073	0.073	A8_Se	3	None	
1214668	Ti	R-3m	0.074	0.074	A10_Hg	1	None	
8390	Ti	Im-3m	0.114	0.114	W	1	None	Spreadborough, J., Christian, J.w.(1959). The measurement of the lattice dimensions and Debye temperatures of titanium and silver by X-ray methods. Proceedings of the Physical Society, London, 74.
1215202	Ti	Im-3m	0.114	0.114	A2_W	1	None	
1214935	Ti	P4132	0.124	0.124	A13_beta_Mn	20	None	
1215113	Ti	Cmca	0.157	0.157	A17_Black_P	4	None	
1215024	Ti	Pm-3n	0.193	0.193	A15_beta_W	8	None	
1280389	Ti	Pm-3n	0.193	0.193		8	None	
1577532	Ti	I-43m	0.197	0.197		29	None	
1214846	Ti	I-43m	0.198	0.198	A12_alpha_Mn	29	None	
1214757	Ti	Cmca	0.242	0.242	A11_Ga	4	None	
1484703	Ti	R-3m	0.253	0.253		13	None	
1485151	Ti	Fd-3m	0.269	0.269		6	None	
1485752	Ti	P63/mmc	0.283	0.283		12	None	
1215648	Ti	I41/amd	0.405	0.405	A5_Sn	2	None	
1216004	Ti	P63/mmc	0.896	0.896	A9_Graphite_C	4	None	
1215559	Ti	Fd-3m	2.116	2.116	A4_Diamond_C	2	None	
1215826	Ti	R-3m	3.159	3.159	A7_As	2	None	

Table S9. Calculated phase diagram of Ti-Nb with all possible phases of pure Nb with computed negative (or slightly positive) formation energies (E_f) explored using the Open Quantum Materials Database (OQMD) [S1,S2].

Nb

1215170	Nb	Im-3m	0	0	A2_W	1	None	
1521870	Nb	Im-3m	0	0		1	None	
1521875	Nb	Im-3m	0	0		1	None	
685533	Nb	Im-3m	0.000	0.000		1	None	Neuburger, M.c.(1936). Praezisionsmessung der Gitterkonstante von sehr reinem Niob. Zeitschrift fuer Kristallographie, Kristallgeometrie, Kristallphysik, Kristallchemie (-144,1977), 93.
1215883	Nb	P3121	0.076	0.076	A8_Se	3	None	
1214992	Nb	Pm-3n	0.105	0.105	A15_beta_W	8	None	
1280310	Nb	Pm-3n	0.105	0.105		8	None	
2030157	Nb	I4/mmm	0.145	0.145	In	1	None	Richter, Manuel, Schoenecker, Stephan, Li, Xiaoqing, Koepernik, Klaus, Johansson, Boerje, Vitos, Levente(2015). Metastable cubic and tetragonal phases of transition metals predicted by density-functional theory. RSC Advances, 5.
1215705	Nb	I4/mmm	0.147	0.147	A6_In	1	None	
1214814	Nb	I-43m	0.167	0.167	A12_alpha_Mn	29	None	
2030113	Nb	R-3m	0.174	0.174	W6Fe7	13	None	Santos, V. O. D., Petrilli, H. M., Schoen, C. G., Eleno, L. T.(2015 Thermodynamic modelling of the Nb-Ni-Si phase diagram based on the 1073 K isothermal section using ab initio calculations. Comouter coupling of phase diagrams and thermochemistry, 51.
1215259	Nb	Cmcm	0.198	0.198	A20_alpha_U	2	None	
1801139	Nb	P6/mmm	0.202	0.202		3	None	
2031499	Nb	P6/mmm	0.202	0.202		3	None	Tanaka, Isao, Ikeda, Yuji(2016). Stability of the omega structur of transition elements. Physical Review, Serie 3. B - Condensed Matter (18,1978-), 93.
1214903	Nb	P4132	0.213	0.213	A13_beta_Mn	20	None	
1214636	Nb	R-3m	0.268	0.268	A10_Hg	1	None	
1215438	Nb	P63/mmc	0.291	0.291	A3p_La	4	None	
1216064	Nb	R-3m	0.293	0.293	C19_alpha_Sm	3	None	
2029911	Nb	P63/mmc	0.296	0.296	hcp#Mg	2	None	Zhang, X., Arroyave, R., Junkaew, A., Ham, B.(2015). Investigation of interfaces in Mg/Nb multilayer thin films. Computational Materials Science, Elsevier, 108.
1215348	Nb	P63/mmc	0.297	0.297	A3_Mg	2	None	
1214547	Nb	Fm-3m	0.322	0.322	A1_Cu	1	None	
676151	Nb	Fm-3m	0.322	0.322		1	None	Haglund, J., Fernandez guillermet, F., Grimvall, G., Korling, M. (1993). Theory of bonding in transition-metal carbides and nitrides. Physical Review, Serie 3. B - Condensed Matter (18,1978-), 48.
1215794	Nb	R-3m	0.324	0.324	A7_As	2	None	
1215081	Nb	Cmca	0.344	0.344	A17_Black_P	4	None	
1214725	Nb	Cmca	0.442	0.442	A11_Ga	4	None	
1215616	Nb	I41/amd	0.601	0.601	A5_Sn	2	None	

Table S10. Calculated phase diagram of Ti-Nb with all possible phases of mixed Ti-Nb compounds with computed negative (or slightly positive) formation energies (E_f) explored using the Open Quantum Materials Database (OQMD) [S1,S2].

Compounds contained in this region of phase space

ID	Composition	Spacegroup	Formation Energy [eV/atom]	Stability [eV/atom]	Prototype	# of atoms	Projects	Finish Time	Reference
			Nb-Ti						
754964	TiNb	P21/m	-0.008	0		12	None		
754958	TiNb	P21/m	-0.007	0.000		12	None		
754981	Ti_2Nb	Pm	-0.005	0.001		24	None		
1339573	$TiNb_{15}$	Pm-3m	0.001	0.002		16	None		
754972	Ti_5Nb	P-62m	-0.000	0.002		6	None		
754985	TiNb	Pm	-0.001	0.006		12	None		
754987	Ti_3Nb	Pmmn	0.003	0.007		8	None		
754976	TiNb	Pbcm	0.002	0.010		8	None		
754962	TiNb	Pmmn	0.003	0.011		16	None		
754959	Ti_4Nb_3	P21/m	0.005	0.011		14	None		
754960	TiNb	Pm	0.004	0.012		12	None		
754967	Ti_2Nb	Pmmn	0.007	0.012		12	None		
754956	TiNb	Pm	0.007	0.015		24	None		
312000	Ti_3Nb	Fm-3m	0.013	0.017	D0_3_BiF3	4	None		
754966	TiNb	Pm	0.010	0.017		10	None		
313047	$TiNb_3$	Fm-3m	0.014	0.018	D0_3_BiF3	4	None		
754978	Ti_3Nb	P21/m	0.017	0.020		8	None		
754963	TiNb	Pm	0.014	0.022		10	None		
323589	Ti_3Nb	P63/mmc	0.024	0.028	D0_19_Ni3Sn	8	None		
754975	Ti_3Nb	Cmcm	0.024	0.028		8	None		
754957	Ti_2Nb	Pmmn	0.023	0.028		12	None		
301458	Ti_3Nb	I4/mmm	0.027	0.031	D0_22_Al3Ti	4	None		
348075	Ti_3Nb	Pm-3m	0.031	0.035	L1_2_Cu3Au	4	None		
2030449	Ti_3Nb	Pm-3m	0.031	0.035	Auricupride#AuCu3	4	None		Li, Yang, Li, Jiahao, Liu, Baixin(2015). The atomistic mechanism of hcp-to-bcc martensitic transformation in the Ti-Nb system revealed by molecular dynamics simulations. Physical Chemistry Chemical Physics, 17.
1221332	TiNb	Pmma	0.031	0.038	B19_AuCd	4	None		
2030450	TiNb	Pm-3m	0.032	0.040	CsCl	2	None		Li, Yang, Li, Jiahao, Liu, Baixin(2015). The atomistic mechanism of hcp-to-bcc martensitic transformation in the Ti-Nb system revealed by molecular dynamics simulations. Physical Chemistry Chemical Physics, 17.

306941	TiNb	Pm-3m	0.032	0.040	B2_CsCl	2	None
1522342	TiNb	Pm-3m	0.032	0.040		2	None
754973	Ti_2Nb	Pmmn	0.037	0.043		12	None
754983	TiNb	Pmma	0.038	0.045		4	None
754969	TiNb	Pnma	0.051	0.059		8	None
754980	Ti_2Nb	Amm2	0.062	0.067		6	None
754965	TiNb	Pmmn	0.060	0.068		4	None
754984	Ti_2Nb	Cmcm	0.063	0.069		12	None
754961	TiNb	Pmmn	0.066	0.074		16	None
754977	TiNb	Pmmn	0.070	0.077		16	None
754986	TiNb	Pmm2	0.078	0.086		8	None
754970	TiNb	Pmm2	0.081	0.089		8	None
754971	Ti_4Nb_3	Pm	0.094	0.101		14	None
302505	$TiNb_3$	I4/mmm	0.104	0.108	D0_22_Al3Ti	4	None
1609956	Ti_2Nb	P63/mmc	0.111	0.116	C14_MgZn2	12	None
1235901	TiNb	P-6m2	0.114	0.122		2	None
1230497	TiNb	P-6m2	0.115	0.122	B_h_WC	2	None
754968	TiNb	Amm2	0.129	0.137		8	None
328025	TiNb	R-3m	0.133	0.141	L1_1_CuPt	2	None
1590660	Ti_2Nb	Fd-3m	0.144	0.149	C15_MgCu2	6	None
338483	TiNb	P4/mmm	0.178	0.185	L1_0_CuAu	2	None
347028	$TiNb_3$	Pm-3m	0.204	0.207	L1_2_Cu3Au	4	None
2030451	$TiNb_3$	Pm-3m	0.204	0.207	Auricupride#AuCu3	4	None
322542	$TiNb_3$	P63/mmc	0.206	0.210	D0_19_Ni3Sn	8	None
1609973	$TiNb_2$	P63/mmc	0.209	0.214	C14_MgZn2	12	None
1610063	$TiNb_2$	P63/mmc	0.221	0.226	C36_MgNi2	24	None
1520656	$TiNb_2$	Pnma	0.228	0.233		12	None
1591997	$TiNb_2$	Fd-3m	0.230	0.236	C15_MgCu2	6	None
428061	Ti_3Nb_2	R-3c	0.339	0.345	D5_1_Corundum_Al2O3	10	None
1106126	TiNb	Fm-3m	0.795	0.803	B1_NaCl	2	None
1233983	$TiNb_2$	P42/mnm	1.076	1.081	C4_Rutile_TiO2	6	None
1227011	TiNb	P63mc	1.516	1.524	B4_Zincblende_ZnS	4	None
1223526	TiNb	F-43m	2.388	2.395	B3_Sphalerite_ZnS	2	None
1239221	Ti_2Nb	Fd-3m	2.618	2.623	C9_SiO2	6	None
1239222	$TiNb_2$	Fd-3m	3.436	3.441	C9_SiO2	6	None

Li, Yang, Li, Jiahao, Liu, Baixin(2015). The atomistic mechanism of hcp-to-bcc martensitic transformation in the Ti-Nb system revealed by molecular dynamics simulations. Physical Chemistry Chemical Physics, 17.

Table S11. Calculated formation energies of various Ti_4Nb structure types computed using GGA-PBE functional. SQS-O1 corresponds to $Ti_{16}Nb_4$, SQS-02 to SQS-05 correspond to $Ti_{26}Nb_6$, SQS-06 to SQS-08 correspond $Ti_{32}Nb_8$, and SQS09 corresponds to $Ti_{64}Nb_{16}$. ΔE^1 is with reference to ground state Ti (hcp) and Nb (bcc). ΔE^2 is with reference to ground Ti state (bcc that is β-Ti) and Nb (bcc).

Structure-Type	Space Group Symmetry	Number of Atoms/prim-cell	ΔE^1 meV/atom	ΔE^2 meV/atom
$SiCl_4$	*P21/m*	10	53.8	-35.0
Al_4U	*Imma*	10	63.5	-25.3
$SrSn_4$	*Cmcm*	10	65.2	-23.6
$AgAu_4$	*Cmcm*	10	77.1	-11.7
$MoNi_4$	*I4/m*	5	78.6	-10.2
$AlAu_4$	*P213*	20	107.2	18.4
SQS-01	*Pm*	20	53.7	-35.1
SQS-02	*P1*	32	50.4	-39.8
SQS-03	*P1*	32	47.7	-42.4
SQS-04	*P1*	32	46.8	-43.4
SQS-05	*P1*	32	47.2	-43.0
SQS-06	*P1*	40	49.3	-39.5
SQS-07	*P1*	40	44.8	-44.0
SQS-08	*P1*	40	42.9	-45.9
SQS-09	*P1*	80	47.9	-40.9

Supplementary References

[S1] Saal, J.E., Kirklin, S., Aykol, M. et al. Materials Design and Discovery with High-Throughput Density Functional Theory: The Open Quantum Materials Database (OQMD). JOM 65, 1501–1509 (2013). https://doi.org/10.1007/s11837-013-0755-4

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