Supporting Information for

Nitriding effect on the stability and mechanical properties of the Iron Titan phase: First-principles investigation

A. D. Ishkildin[1], A. A. Kistanov[1,*], A.A. Izosimov[2], E. A. Korznikova[1,3]

[1]Research Laboratory for Metals and Alloys under Extreme Impacts, Ufa University of Science and Technology, Ufa 450076, Russia

[2]Bashkir State Medical University, Ufa 450077 Russia

[3]Institute for Metals Superplasticity Problems, Ufa 450001, Russia

*Corresponding author: andrei.kistanov.ufa@gmail.com

*Corresponding author: andrei.kistanov.ufa@gmail.com

Table S1. The elastic constants of FeTi, where X is the concentration of the nitrogen (* - clustered nitrogen).

$C_{i,j}$, GPa	X=0%	X=1.8%	X=3.7%	X=5.5%	X=7.4%	X=3.7%*	X=5.5%*	X=7.4%*
C_{11}	434.04	423.19	405.61	424.74	369.06	411.61	415.53	382.19
C_{12}	88.83	97.12	105.45	96.35	115.37	100.05	93.16	114.93
C_{13}	88.83	94.20	103.58	80.05	62.81	78.04	87.57	114.80
C_{21}	88.83	97.12	105.45	96.35	115.37	100.05	93.16	114.93
C_{22}	434.03	411.64	386.79	407.25	373.28	401.98	416.37	380.99
C_{23}	88.83	97.11	105.47	97.07	118.97	100.15	95.11	107.95
C_{31}	88.83	94.20	103.58	80.05	62.81	78.04	87.57	114.80
C_{32}	88.83	97.11	105.47	97.07	118.97	100.15	95.11	107.95
C_{33}	434.03	423.18	405.64	423.01	365.90	411.52	409.13	381.03
C_{44}	55.73	57.44	62.02	61.68	62.29	58.36	58.69	71.13
C_{55}	55.53	59.20	65.06	64.23	64.18	59.18	60.49	73.24
C_{66}	55.52	61.37	69.92	70.48	70.64	63.31	62.71	72.84

Table S2. K_v and K_R bulk moduli and G_v and G_R shear moduli of nitrogen-containing TiFe.

	$K_{V,}$ GPa	$K_{R,}$ GPa	$G_{V,}$ GPa	$G_{R,}$ GPa
		Uniformly distributed N		
FeTi	203.90	203.90	102.36	76.207
FeTi-N$_{1.8\%}$	203.88	203.86	100.24	79.40
FeTi-N$_{3.7\%}$	203.01	202.93	98.305	84.192
FeTi-N$_{5.5\%}$	200.22	200.22	104.71	85.869
FeTi-N$_{7.4\%}$	189.18	187.95	93.496	81.984
		Clustered N		
FeTi-N$_{3.7\%}$	197.96	197.92	99.296	79.926
FeTi-N$_{5.5\%}$	199.19	199.12	100.73	80.647
FeTi-N$_{7.4\%}$	202.18	202.16	97.212	88.774

Table S3. The calculated anisotropic index of nitrogen-containing FeTi.

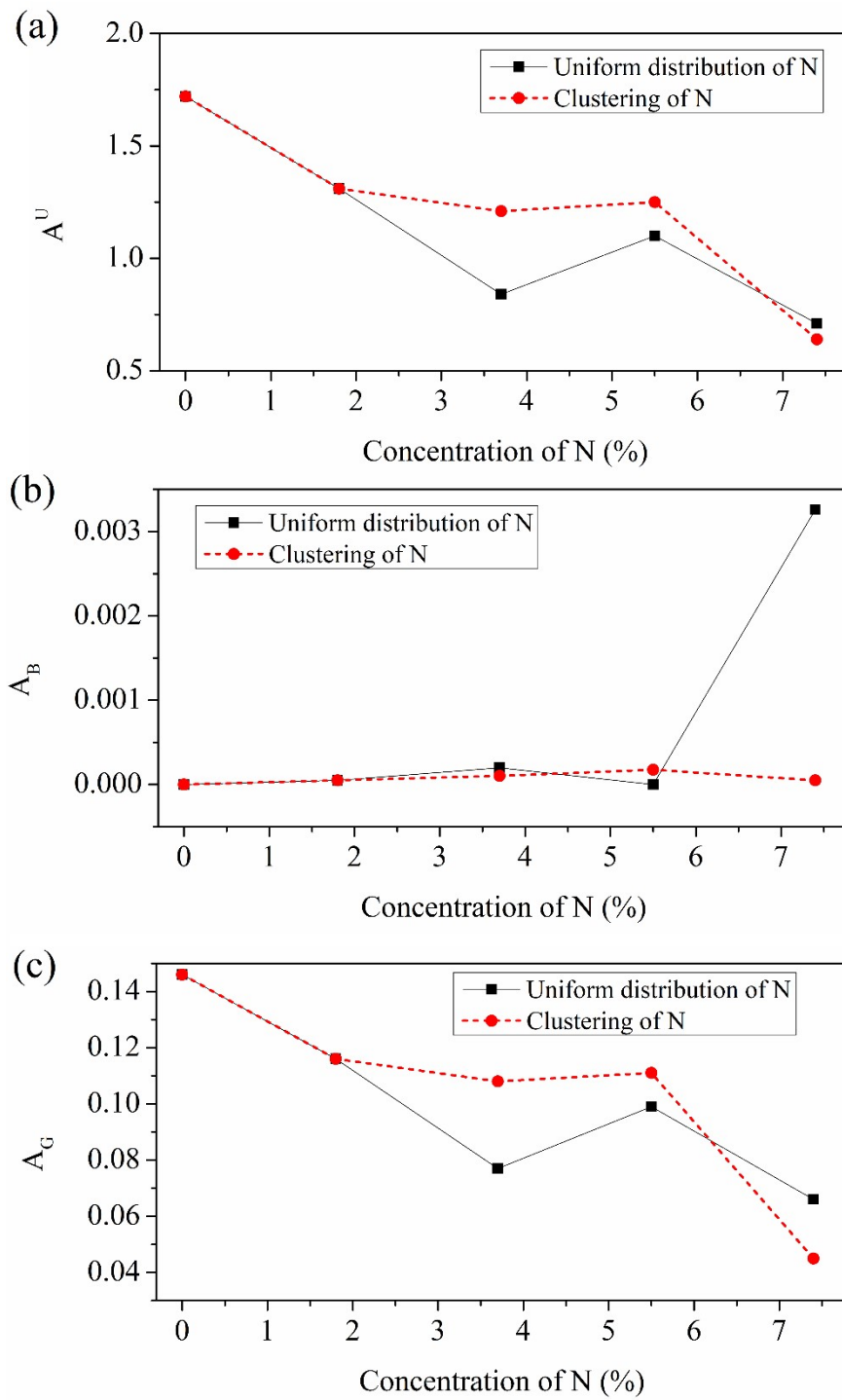|	A^U	$A_B,\%$	$A_G,\%$	$A_{\{100\}}$	$A_{\{010\}}$	$A_{\{001\}}$
			Uniformly distributed N			
FeTi	1.72	0	14.6	0.32	0.32	0.32
FeTi-N$_{1.8\%}$	1.31	0.0049	11.6	0.35	0.37	0.38
FeTi-N$_{3.7\%}$	0.84	0.0197	7.7	0.41	0.44	0.48
FeTi-N$_{5.5\%}$	1.10	0	9.9	0.36	0.40	0.44
FeTi-N$_{7.4\%}$	0.71	0.3261	6.6	0.41	0.51	0.55
			Clustered N			
FeTi-N$_{3.7\%}$	1.21	0.0101	10.8	0.35	0.39	0.41
FeTi-N$_{5.5\%}$	1.25	0.0175	11.1	0.36	0.38	0.39
FeTi-N$_{7.4\%}$	0.64	0.0049	4.5	0.53	0.54	0.55

Fig. S1. (a) A^U, (b) A_B, and (c) A_G as a function of the nitrogen concentration in FeTi.
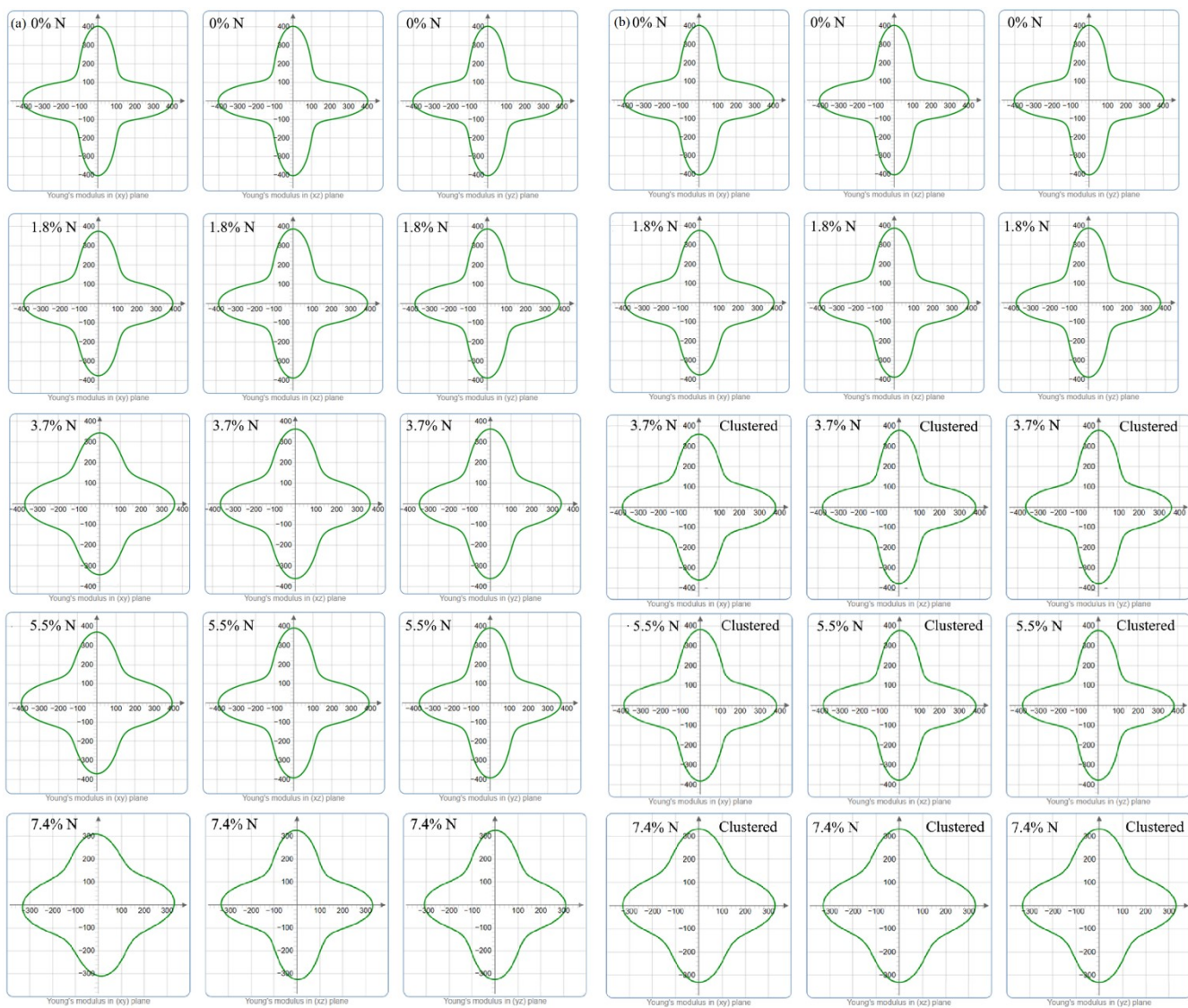
Fig. S2. The projections of linear compressibility of the FeTi supercell containing uniformly distributed and clustered N.
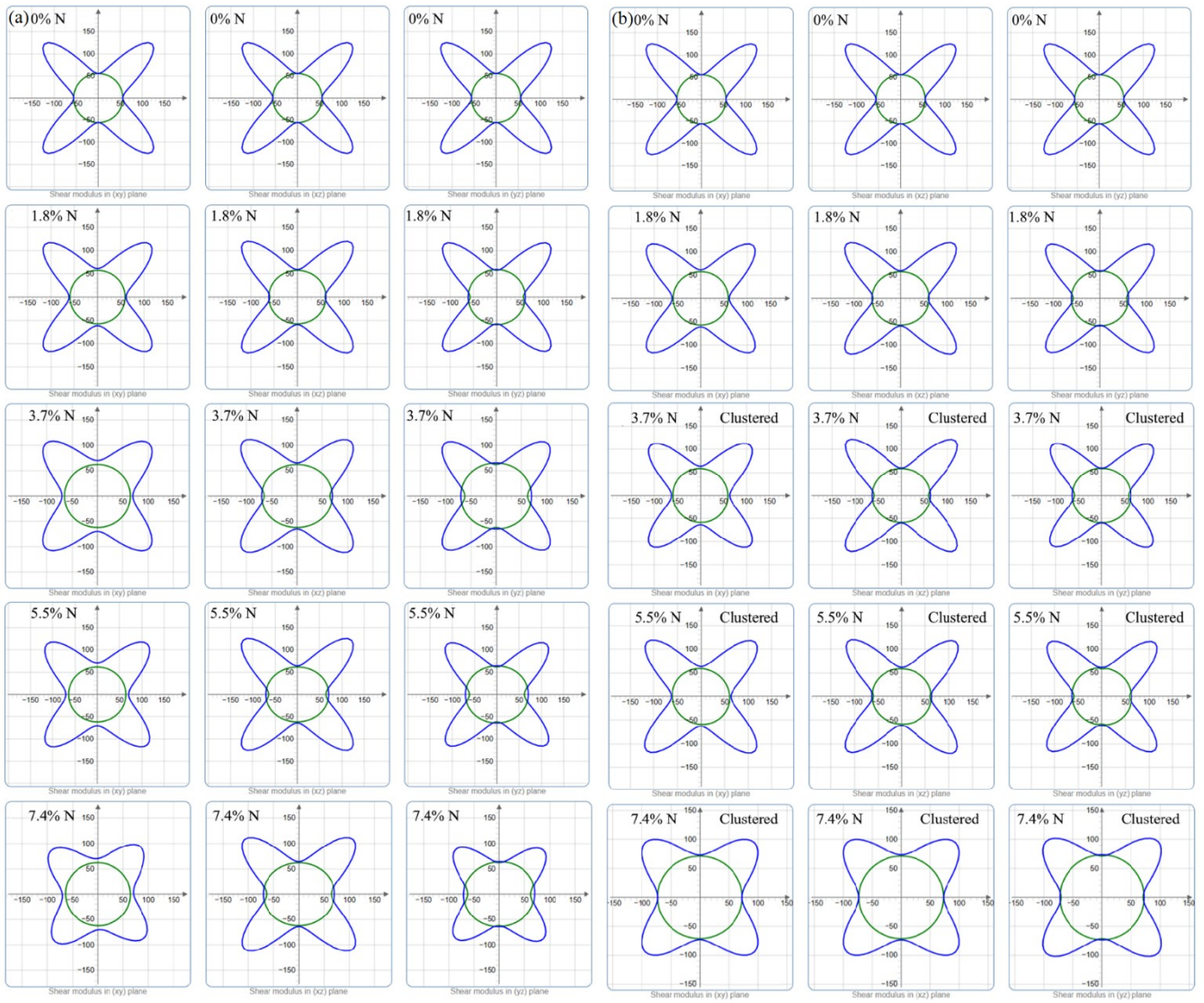
Fig. S3. The projections of Young's modulus of FeTi containing (a) uniformly distributed and (b) clustered N.
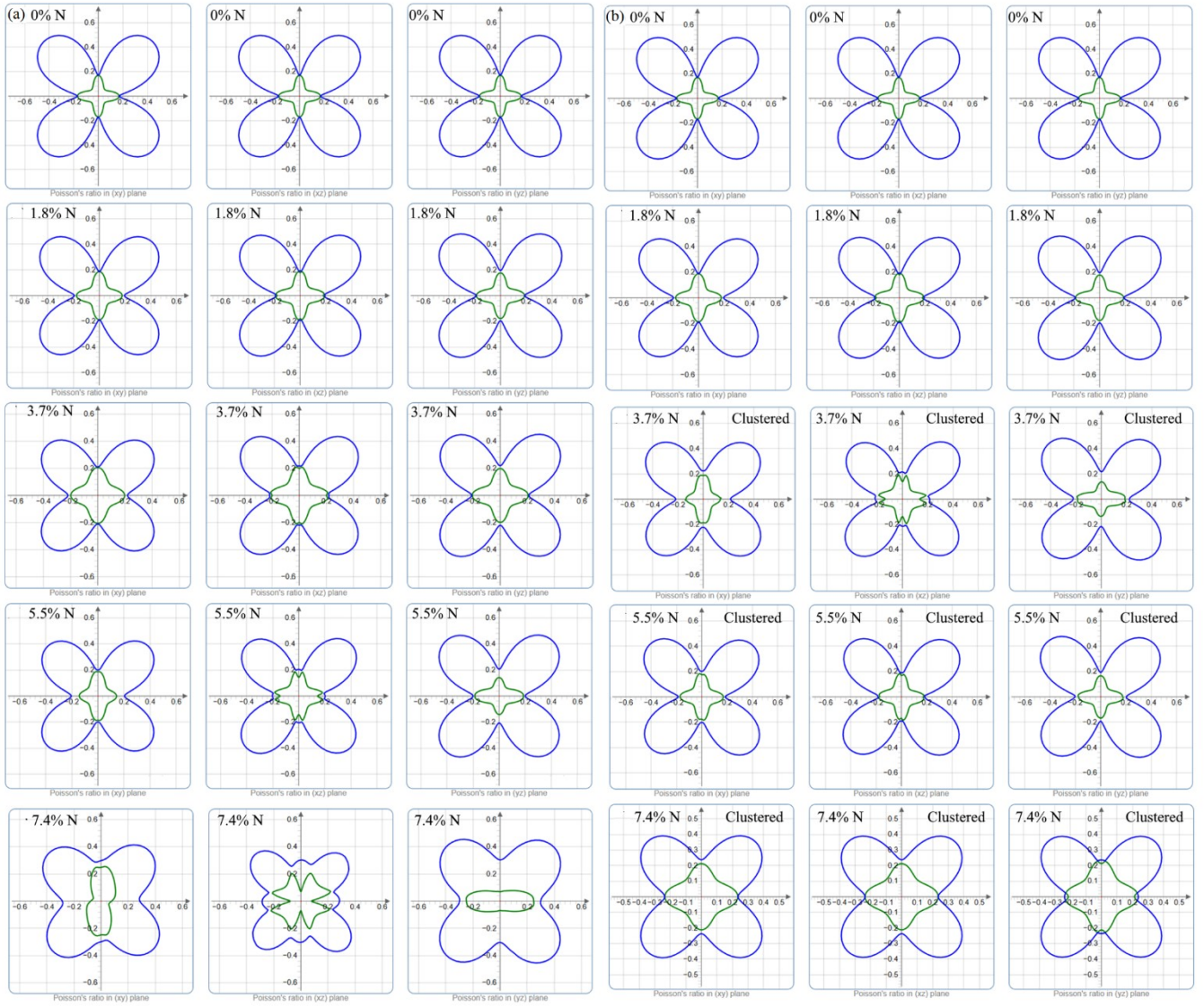
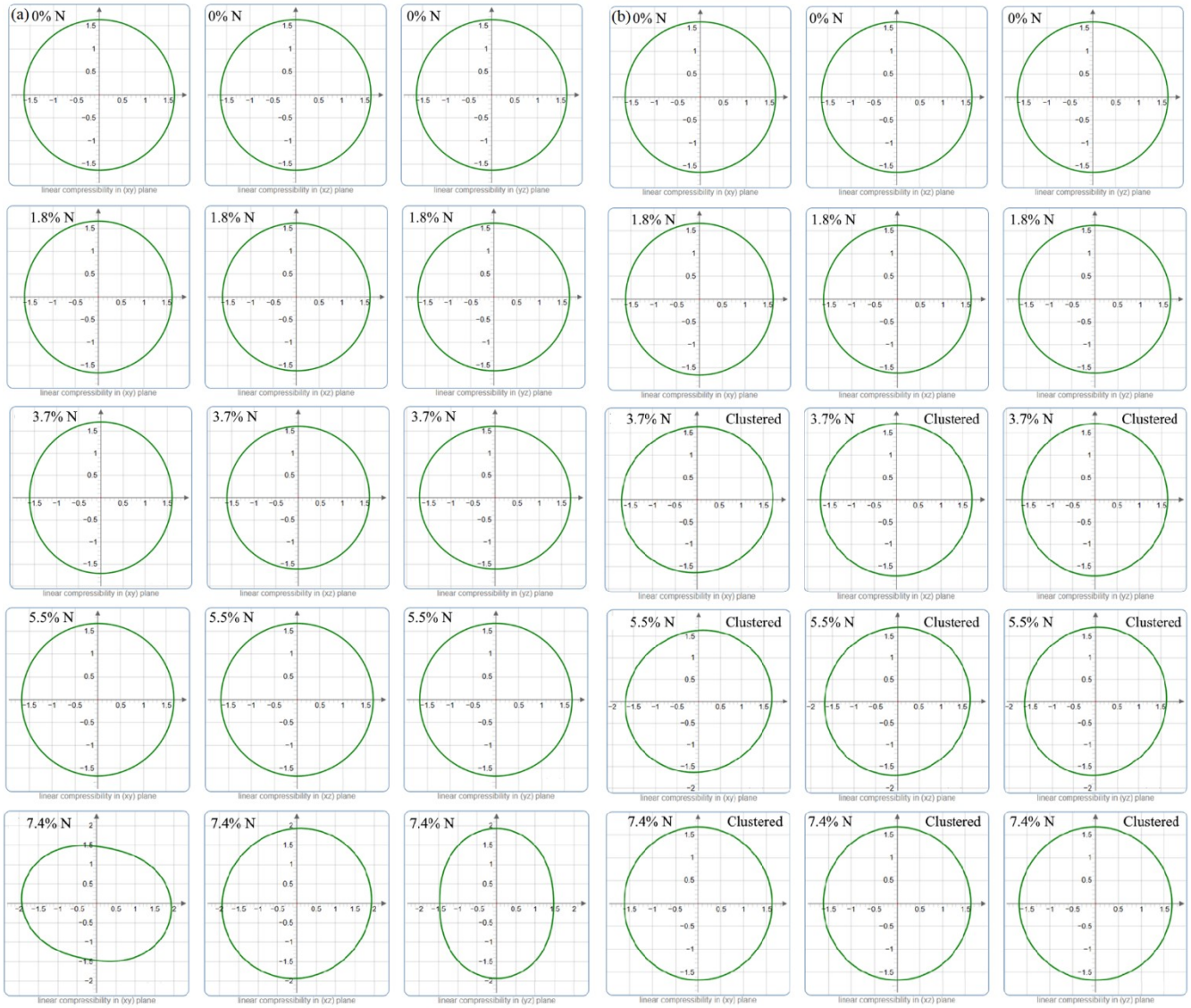**Fig. S4.** The projections of shear moduli of FeTi containing (a) uniformly distributed and (b) clustered N.

Fig. S5. The projections of Poisson's ratio of the FeTi supercell containing uniformly distributed and clustered N.
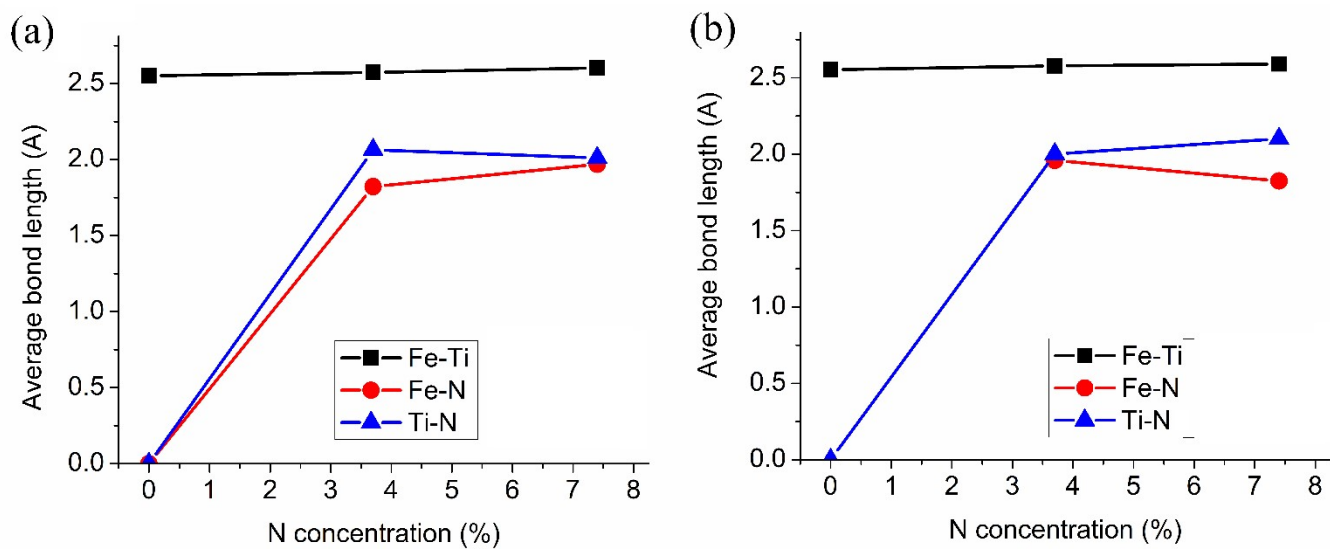
Fig. S6. The average Fe-Ti, Fe-N, and Ti-N bond length in the FeTi supercell containing (a) uniformly distributed and (b) clustered N.