Supporting information

The effect of calcination temperature on the structure and activity relationship of V/Ti catalyst for NH_3-SCR

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Methods

The reaction rate r was calculated according to the following equation:

$$r\left(mol\ s^{-1}\ m^{-2}\right) = \frac{\left(\frac{P \times V}{R \times T}\right) \times X_{NO_x}}{m_{cat} \times S_{BET}} \quad (1)$$

In the above equation, P(Pa) is the standard atmospheric pressure (1.01×10^5 Pa), V(m^3/s) is the NO flow volume, R is the proportional constant (8.314 J mol^{-1} K^{-1}), T(K) is the reaction temperature (298.15 K), X_{NO_x} is the NO_x conversion, m_{cat}(g) is the mass of the catalysts, and S_{BET} is the BET specific surface area.

Figure S1

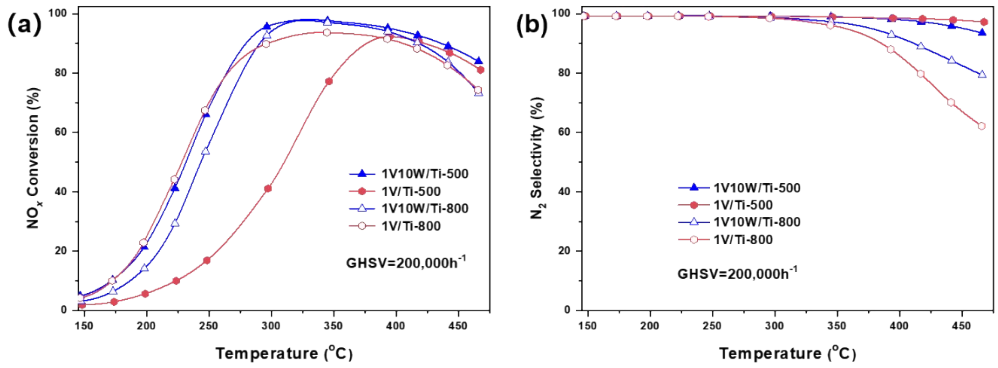

Figure S1 NH_3-SCR activity (a) and N_2 selectivity (b) over 1wt% V_2O_5/TiO_2 and 1wt% V_2O_5-10%WO_3-TiO_2 catalysts under the calcination temperature of 500 °C and 800 °C. Reaction conditions: [NO] = [NH_3] = 500 ppm, [O_2] =5%, GHSV=200,000 h^{-1}.

Figure S2

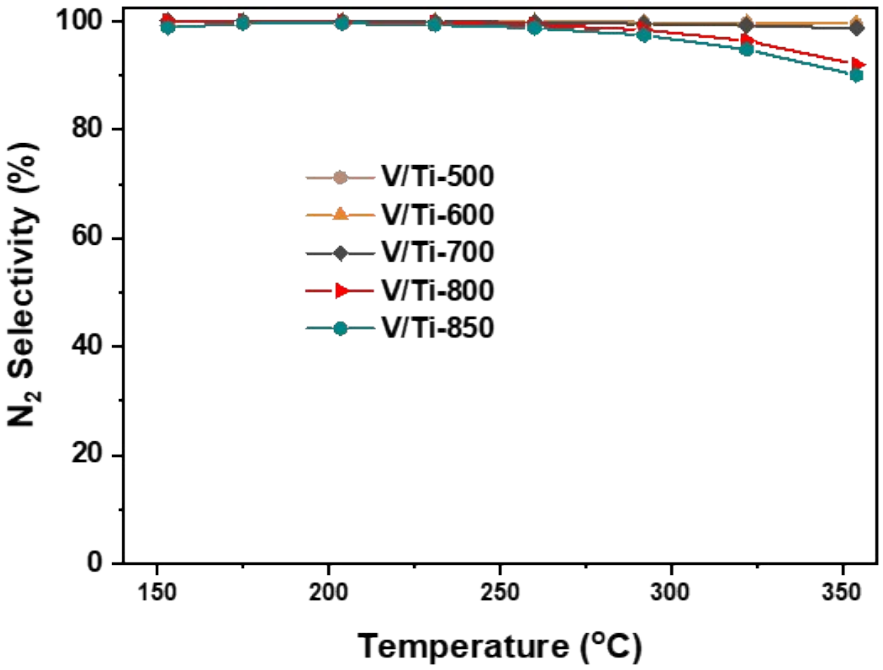

Figure S2 N_2 selectivity in NH_3-SCR reaction as function of temperature in the feed gas of 500 ml·min^{-1} total rate over the V/Ti catalysts. Reaction conditions: [NO] = [NH_3] = 500 ppm, [O_2] =5%, GHSV=100,000 h^{-1}.

Figure S3

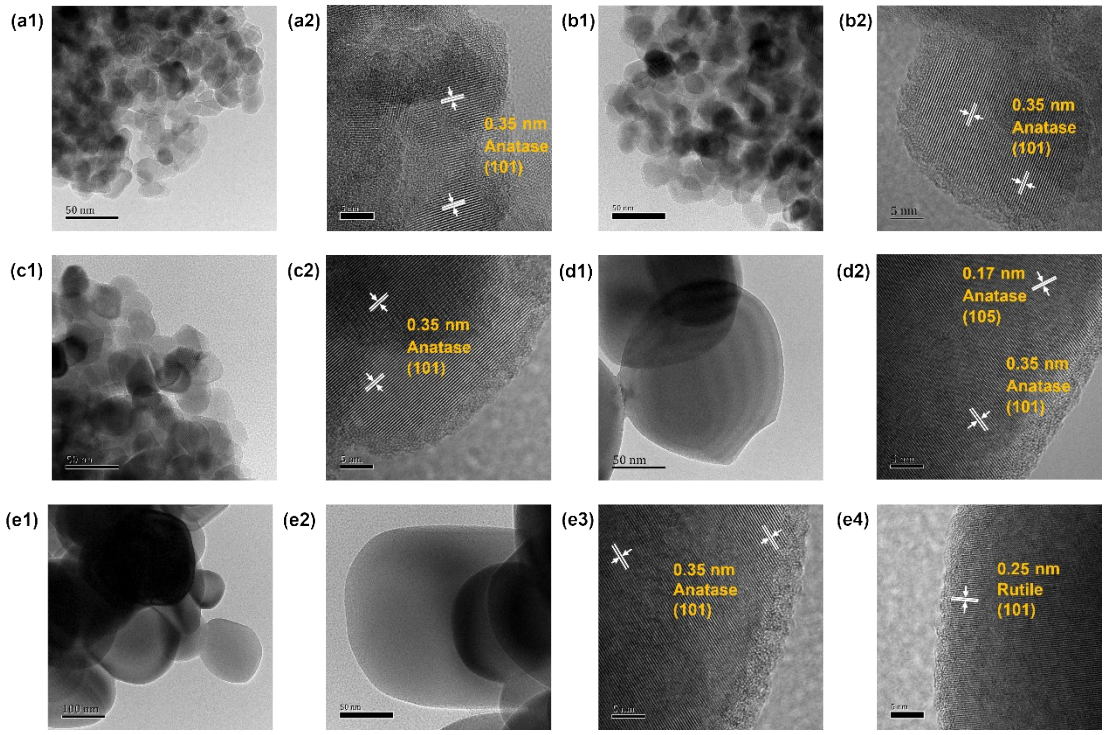

Figure S3 The TEM images (right), and HRTEM images (left) at 100nm and 5nm of catalysts. V/Ti-500 (a); V/Ti-600 (b); V/Ti-700 (c); V/Ti-800 (d); V/Ti-850 (e).

Figure S4

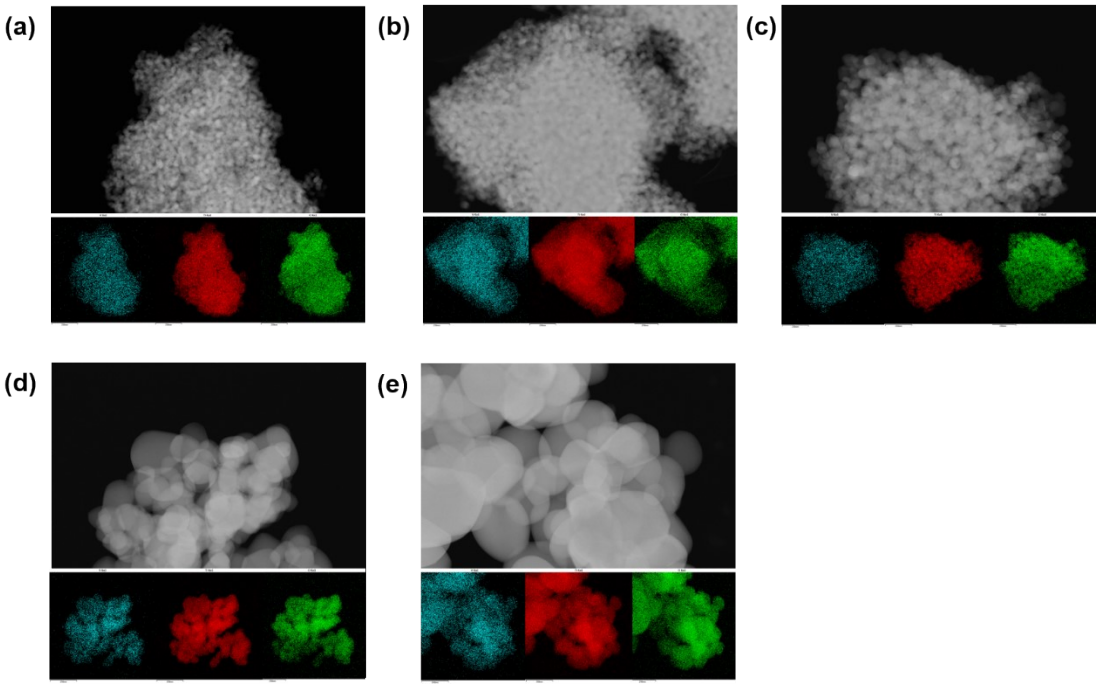

Figure S 4 The mapping images at 250nm of catalysts blue as V, green as O, and red as Ti. V/Ti-500 (a); V/Ti-600 (b); V/Ti-700 (c); V/Ti-800 (d); V/Ti-850 (e).

Figure S5

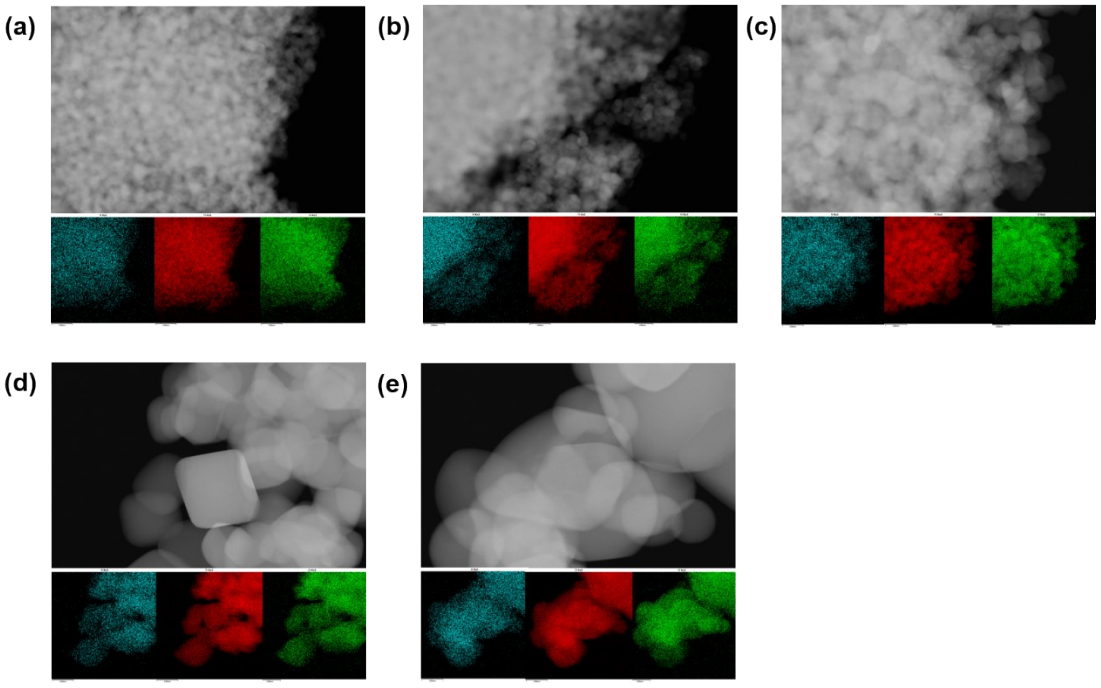

Figure S5 The mapping images at 100nm of catalysts blue as V, green as O, and red as Ti. V/Ti-500 (a); V/Ti-600 (b); V/Ti-700 (c); V/Ti-800 (d); V/Ti-850 (e).

As shown in the **Figure S4** and **Figure S5**, the mapping images of V/Ti catalysts in different calcination, which indicate that the V, O, Ti distribution uniformly.

Figure S6

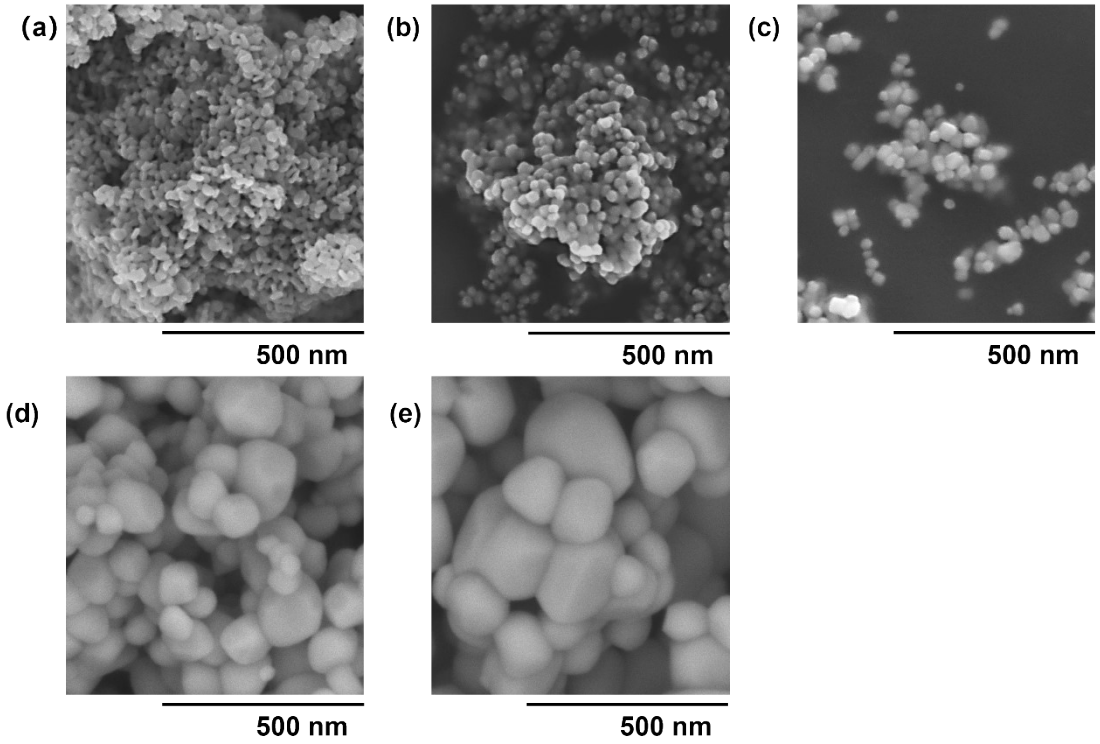

Figure S6 SEM image of V/Ti-500 (a)，V/Ti-600 (b) , V/Ti-700 (c), V/Ti-800 (d), V/Ti-850 (e).

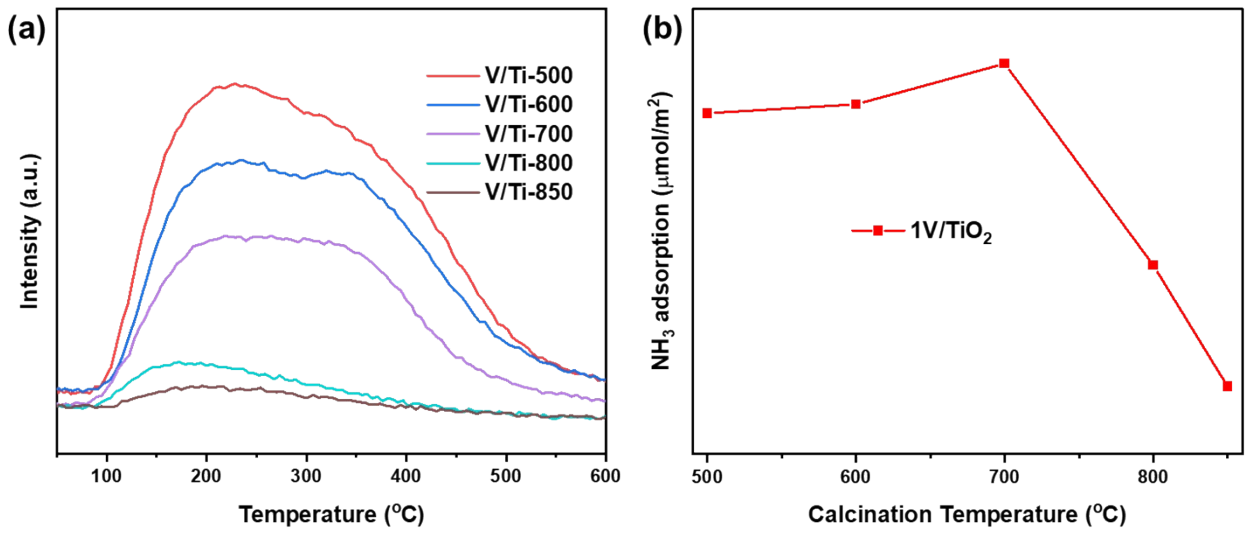

Figure S7 NH_3-TPD profiles for V/Ti catalysts (a), the NH_3 adsorption per unit specific surface area (b).

Figure S7

Figure S6 illustrates the NH_3-TPD profiles of the V/Ti catalysts. NH_3 adsorption and desorption are crucial for the catalytic cycle. It was apparent that the amount of NH_3 adsorption decreased with the calcination temperature increase. To eliminate the effect of the specific surface area, the content of NH_3 desorption per specific surface area was obtained (**Figure S6b**), which is increase with the calcination temperature increase from 500 to 700 °C, then decrease from 800 to 850 °C. V/Ti-700 catalyst reached the maximum acid amount per specific surface area, while the low-temperature NH_3-SCR activity of V/Ti-700 was poor. V/Ti-800 catalyst with the lower the amount of NH_3 adsorption, exhibited the excellent low-temperature NH_3-SCR activity. This indicated that the amount of NH_3 adsorption hardly effect the NH_3-SCR activity at low temperature.

Figure S8

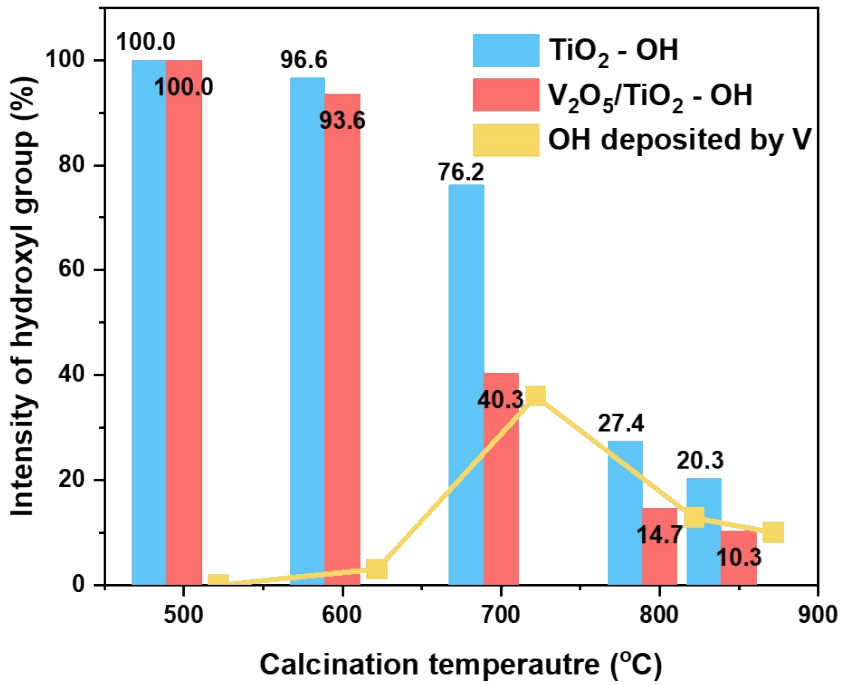

Figure S8 The intensity of the hydroxyl group over TiO_2 support and V_2O_5/TiO_2 catalysts under different calcination temperatures and the OH deposited by V species was calculated by the difference between the hydroxyl group on TiO_2 and V/Ti catalysts. The intensity of hydroxyl strength of the V/Ti-500 catalyst was set as 100%.

Table S1

Table S1. surface area, and the corresponding concentration ratios over different calcination temperatures V/Ti catalysts.

Sample	BET surface area (m^2/g)	Pore volume (cm^3/g) [a]	Pore size (nm) [b]	Particle size (nm)[c]	VO_x surface density (VO_x nm^{-2})	Surface concentration (at-) [d]	Bulk concentration (at-) [e]
						V/Ti	V/Ti
V/Ti-500	74.1	0.33	19.0	17.3	0.89	0.0249	0.0066
V/Ti-600	54.3	0.32	23.9	25.6	1.22	0.0341	0.0064
V/Ti-700	36.0	0.24	30.8	33.2	1.84	0.0677	0.0063
V/Ti-800	12.1	0.06	20.1	86.6	5.47	0.1279	0.0064
V/Ti-850	9.0	0.02	14.1	137.4	7.35	0.1138	0.0062

[a] BJH desorption pore volume

[b] BJH adsorption pore size

[c] measured by SEM average particle size

[d] calculated by XPS

[e] calculated by XRF

Table S2

Table S2. the corresponding concentration ratios over different calcination temperature V/Ti catalysts according to XRF results.

Sample	Bulk concentration (%) [b]							
	V_2O_5	TiO_2	P_2O_5	Al_2O_3	SiO_2	CaO	Nb_2O_5	SO_3
V/Ti-500	0.74	97.51	0.35	0.28	0.17	0.14	0.14	0.49
V/Ti-600	0.71	97.49	0.33	0.07	0.23	0.14	0.13	0.41
V/Ti-700	0.71	98.12	0.35	0.19	0.13	0.13	0.13	0.03
V/Ti-800	0.72	98.22	0.37	-	0.29	0.16	0.14	-
V/Ti-850	0.70	98.34	0.33	0.12	0.16	0.11	0.14	-

Table S3

Table S3. The XPS results of V/Ti catalysts under different calcination temperatures.

Sample	$(V^{4+}+V^{3+})/V^{5+}$	$O_\alpha/ (O_\alpha + O_\beta + O_\gamma)$	V 2p	O 1s	Ti 2p
V/Ti-500	5.90	12.5	515.9	529.9	457.6
V/Ti-600	4.71	11.7	515.9	529.9	457.7
V/Ti-700	2.07	9.2	516.2	530.1	458.3
V/Ti-800	0.88	15.7	516.6	529.8	458.5
V/Ti-850	0.57	18.8	516.8	530.0	458.8

Table S4

Table S4. The results of the characterization and SCR reaction rate.

Samples	Reaction rate	crystallite size	Monomeric	Polymeric	H_2 consumption pre unit of specific surface area (μ mol/m^2)	VO_x density	Lewis
V/Ti-500	1.6	17.0	95129.8	50850.0	7.6	0.9	5.9
V/Ti-600	3.3	25.0	148562.0	69207.0	8.1	1.2	5.2
V/Ti-700	3.3	29.0	181718.0	56969.0	4.8	1.8	8.0
V/Ti-800	31.1	48.0	165684.7	144267.0	11.3	5.5	1.7
V/Ti-850	20.7	106.0	14774.8	36517.0	10.0	7.3	0.7

Table S5

Table S5. The maximum value normalization of the characterization and SCR reaction rate.

Samples	Reaction rate	crystallite size	Monomeric	Polymeric	H_2 consumption pre unit of specific surface area (μ mol/m^2)	VO_x density	Intensity of Lewis acid
V/Ti-500	0.05	0.16	0.52	0.35	0.67	0.12	0.74
V/Ti-600	0.11	0.24	0.82	0.48	0.72	0.17	0.64
V/Ti-700	0.11	0.27	1.00	0.39	0.42	0.25	1.00
V/Ti-800	1.00	0.45	0.91	1.00	1.00	0.74	0.21
V/Ti-850	0.67	1.00	0.08	0.25	0.88	1.00	0.09