

Supplementary material for

Enhancing Phase Stability in Low-Activation TiVTa-based Alloys through CALPHAD-Guided Design

Shuqing Lu^{1†}, Zhouran Zhang^{1*†}, Yu Tang, Shun Li, Shuxin Bai

1-National University of Defense Technology, Aerospace Science College, Materials Science and
Engineering Department, Hunan Province, Changsha, 410073

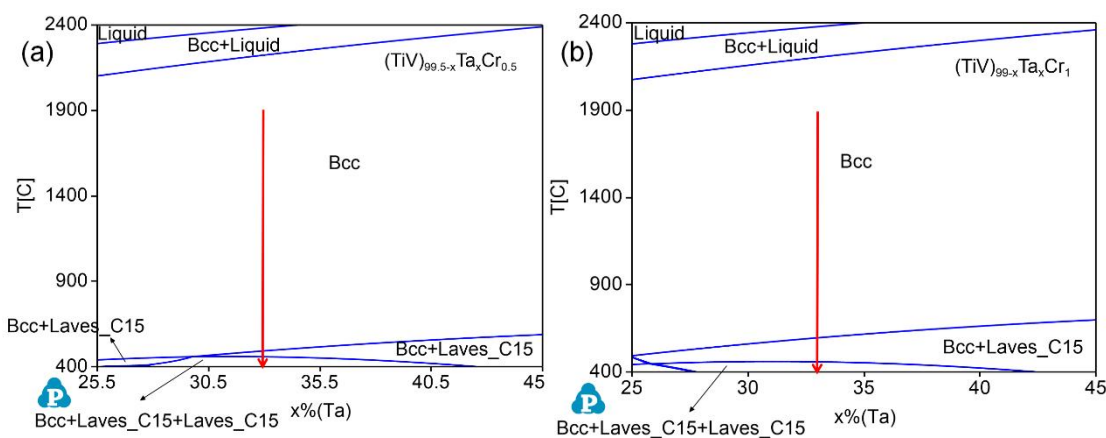


Fig. S1 The solubility regimes in (a) $(\text{TiV})_{99-x}\text{Ta}_x\text{Cr}_1$ and (b) $(\text{TiV})_{99.5-x}\text{Ta}_x\text{Cr}_{0.5}$ ($\text{Ti}_{33}\text{V}_{33}\text{Ta}_{33.5}\text{Cr}_{0.5}$ and $\text{Ti}_{33}\text{V}_{33}\text{Ta}_{33}\text{Cr}_1$ are marked by red arrows.)

Table S-I Phase composition and lattice constants of the alloys in the as-cast state and after annealing at 500°C and 700°C for 24 h, as determined by XRD.

Alloys	As-cast	Lattice	500°C 24 h	Lattice	700°C 24 h	Lattice
		constant (Å)		constant (Å)		constant (Å)
$\text{Ti}_{33}\text{V}_{33}\text{Ta}_{34}$	BCC	3.2213	BCC	3.2312	BCC	3.2299
$\text{Ti}_{29}\text{V}_{28}\text{Ta}_{43}$	BCC	3.2372	BCC	3.2394	BCC	3.2340
$\text{Ti}_{34}\text{V}_{30}\text{Ta}_{36}$	BCC	3.2310	BCC	3.2322	BCC	3.2177

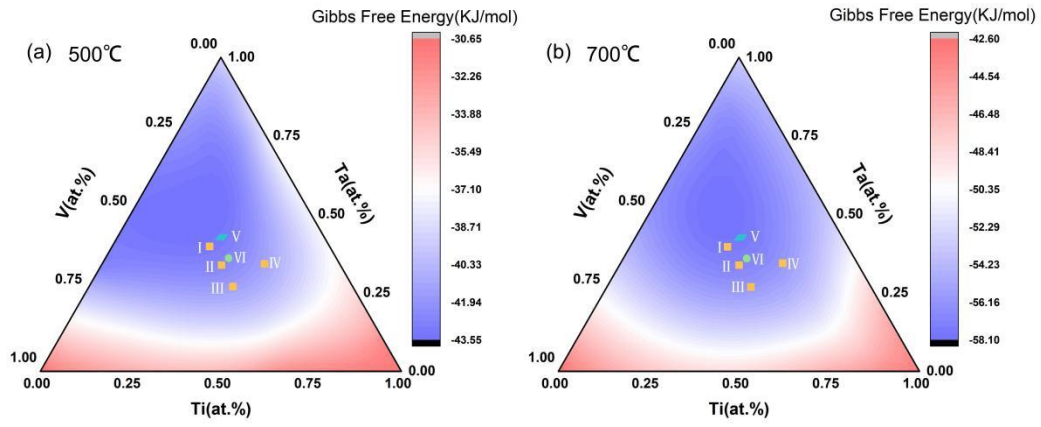


Fig. S2 (a) and (b) Calculated Gibbs free energy of TiVTa ternary alloys at 500°C and 700°C. The alloys were marked using I ($\text{Ti}_{27}\text{V}_{33}\text{Ta}_{40}$), II ($\text{Ti}_{33}\text{V}_{33}\text{Ta}_{34}$), III ($\text{Ti}_{40}\text{V}_{33}\text{Ta}_{27}$), IV ($\text{Ti}_{45}\text{V}_{20}\text{Ta}_{35}$), V ($\text{Ti}_{29}\text{V}_{28}\text{Ta}_{43}$), VI ($\text{Ti}_{34}\text{V}_{30}\text{Ta}_{36}$).