Supporting Information

Probing nano-scale phase separation at atomic resolution within β-type Ti - Mn alloy; a potential candidate for biomedical implants

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Table S1: Tensile properties of different grade of biomaterials

Sample	Yield strength (MPa)	Ultimate tensile strength (MPa)
CP-Ti (Grade 4) [1]	485	550
Co-Cr-Mo [2]	315	670
SS 316 [2]	750	965
Ti-64 ELI [1]	875	965
TNZT [1]	864	911
Ti-Mo [3]	375	690
Ti-14Mn (cold rolled)	1800	1858

Table S2: Change in lattice parameter with Mn concentration; and relation between energy of the system with minimum interatomic Mn-Mn atom distance in supercell.

Sl.No.	Composition	Mn atoms fractional coordinates in (2 x 2 x 2) supercell	Lattice Parameter (Å)	Minimum Mn-Mn atom distance (Å)	Energy (eV)
1.	Ti – 7 wt % Mn	(0.5,0.5,0.5)	3.226	6.452	-125.53467
2.	Ti – 14 wt % Mn	(0,0,0) (0.5,0.5,0.5)	3.177	2.751	-125.9538
		(0,0,0) (0,0,0.5)	3.196	1.598	-127.41873
		(0,0,0) (0.25,0.25,0.25)	3.179	1.376	-126.1603
		(0,0,0) (0,0.5,0.5)	3.199	2.262	-126.28727
3.	Ti – 21 wt % Mn	(0,0,0) (0.5,0.5,0.5) (0,0,0.5)	3.164	1.582	-128.22182
		(0,0,0) (0.5,0.5,0.5) (0.25,0.25,0.25)	3.146	1.362	-128.04161
		(0,0,0) (0.5,0.5,0.5) (0,0.5,0.5)	3.153	1.576	-128.09458
		(0.25,0.25,0.25) (0.5,0,0) (0.5,0,0.5)	3.145	1.361	-127.76723
		(0.25,0.25,0.25) (0.25,0.25,0.75) (0.5,0.5,0.5)	3.17	1.372	-128.55645
		(0.25,0.25,0.25) (0.25,0.25,0.75) (0.75,0.75,0.25)	3.155	1.372	-128.6875
		(0.25,0.25,0.25) (0.25,0.25,0.75) (0.5,0,0.5)	3.153	1.365	-128.68893

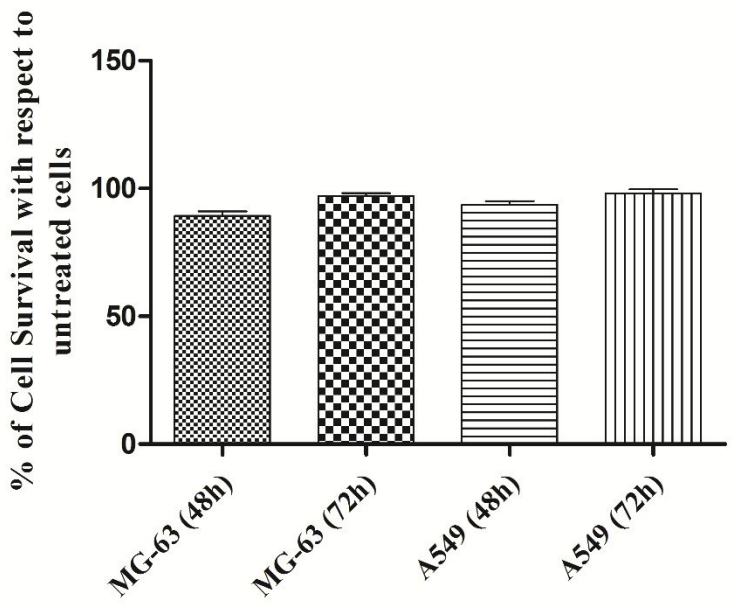

Figure S1: Cytotoxicity test of CP-Ti alloy on different cell lines at different intervals of time.

References

(1) Mitsuo, N. Mechanical Properties of Biomedical Titanium Alloys. *Mater. Sci. Eng. A* **1998**, *243* (1–2), 231–236.

(2) Long, M.; Rack, H. J. Titanium Alloys in Total Joint Replacement - a Medical Perspective. *Biomaterials* **2006**, *19*, 1621–1639.

(3) Zhao, X.; Niinomi, M.; Nakai, M.; Hieda, J. Beta Type Ti-Mo Alloys with Changeable Young's Modulus for Spinal Fixation Applications. *Acta Biomater.* **2012**, *8* (5), 1990–1997. https://doi.org/10.1016/j.actbio.2012.02.004.