Electronic Supplementary Information

Chemical short-range order in Cr-Ta-Ti-V-W high entropy alloys and their derivates from the first-principles thermodynamic study

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Table S1 Structures with the lowest enthalpies of mixing in 10 different ternary subsystems in Cr-Ta-Ti-V-W system within present database. Structures marked as ground states by ATAT package, predicted by CE, are described with superscript "GS". The values of the enthalpy of mixing are given in eV/atom

Structure	Symmetry Group	DFT	CE
Cr_2TaTi	$Imm2$	-0.020	-0.024
Cr_2TaV	$P4/mmm$	-0.025	-0.028
$CrTa_2W$	$P4/mmm$	-0.048	-0.047
Cr_2TiW	$Fm\bar{3}m$	-0.057	-0.047
Cr_2VW	$Fm\bar{3}m$	-0.063	-0.064
$CrTi_2V$	$Imm2$	-0.054	-0.027
$TaTiV_2$	$Imm2$	0.012	0.018
$TaVW_2$	$Imm2$	-0.065	-0.061
$TaTi_2W_2{}^{GS}$	$R\bar{3}m$	-0.091	-0.093
$Ta_2Ti_2W^{GS}$	$R\bar{3}m$	-0.058	-0.043
$TaTi_2W^{GS}$	$Immm$	-0.069	-0.053
$TiVW_2$	$Immm$	-0.064	-0.070

Table S2 Structures with low enthalpy of mixing in each quaternary sub-system. Enthalpy of mixing values are given in eV/atom

Structure	Symmetry Group	DFT	CE
$CrTa_2Ti_2W_2$	$R\bar{3}m$	-0.061	-0.062
$CrTa_2V_2W_2$	$R\bar{3}m$	-0.045	-0.046
$Cr_2TiV_2W_2$	$R\bar{3}m$	-0.067	-0.066
$Ta_2Ti_2VW_2$	$R\bar{3}m$	-0.053	-0.059
$Cr_2TaTi_2V_2$	$R\bar{3}m$	-0.037	-0.022

Table S3 Structures with low enthalpy of mixing for each quinary com-position in our DFT database. Enthalpy of mixing values are given in eV/atom

Structure	Symmetry Group	DFT	CE
$CrTaTi_2VW$	$P3m1$	0.031	0.032
$CrTaTiVW$	$R\bar{3}m$	-0.038	-0.044
$CrTaTiV_2W$	$Amm2$	0.029	0.022

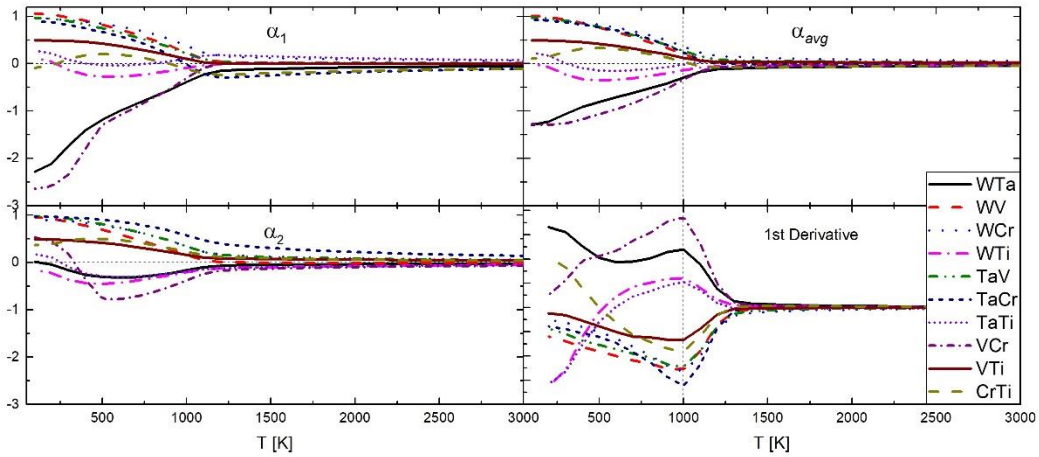

Fig. S1 Short-range order parameter for 1st and 2nd shell (left), as well as the average SRO with its derivative (right) for equiatomic quinary Cr-Ta-Ti-V-W alloy. Order-disorder transition temperature has been marked with vertical dashed line

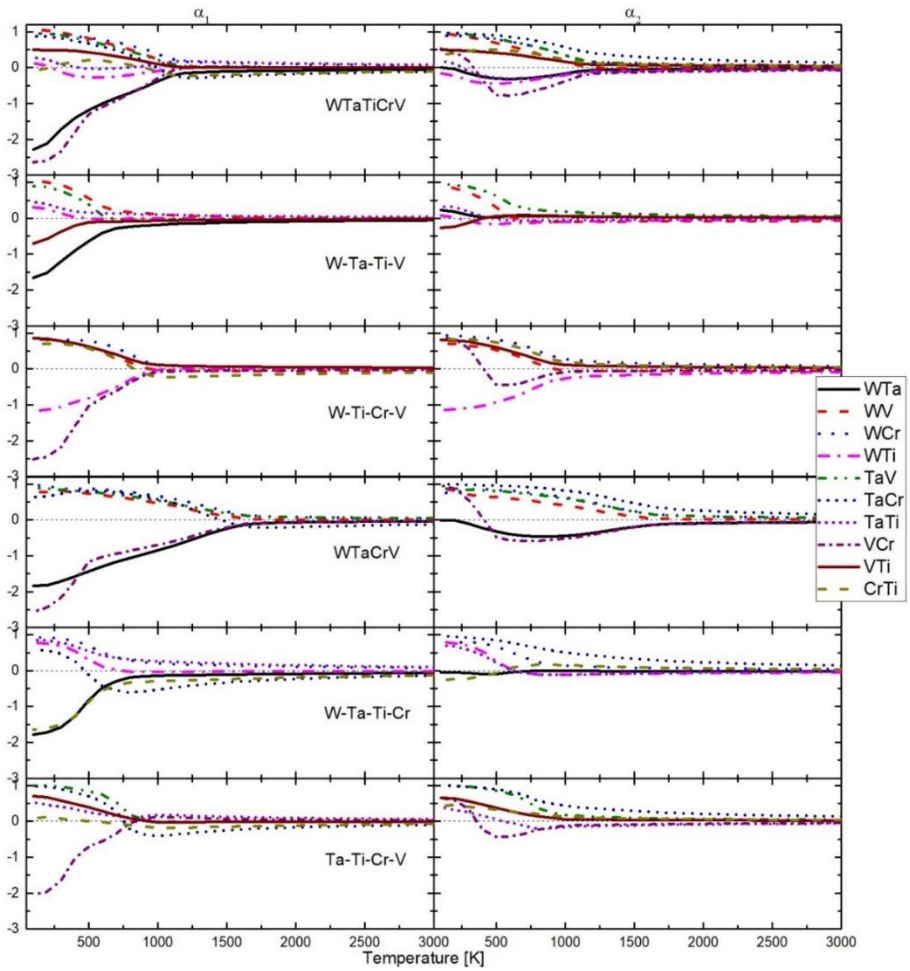

Fig. S2 Short-range order parameters for 1st (left) and 2nd (right) nearest neighbours in quaternary and quinary equiatomic alloys

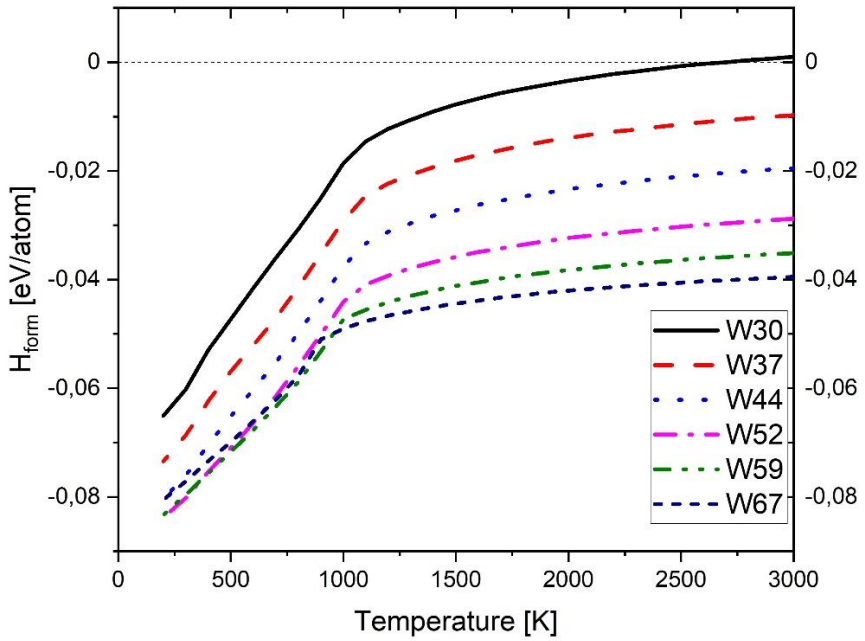

Fig. S3 Enthalpy of formation dependence on temperature for $W_x(CrTaTiV)_{1-x}$ alloys. W30, W37, W44, W52, W57 and W67 denote $W_x(CrTaTiV)_{1-x}$ alloys with W concentration equal to 30%, 37%,44%, 52%, 57% and 67%, respectively

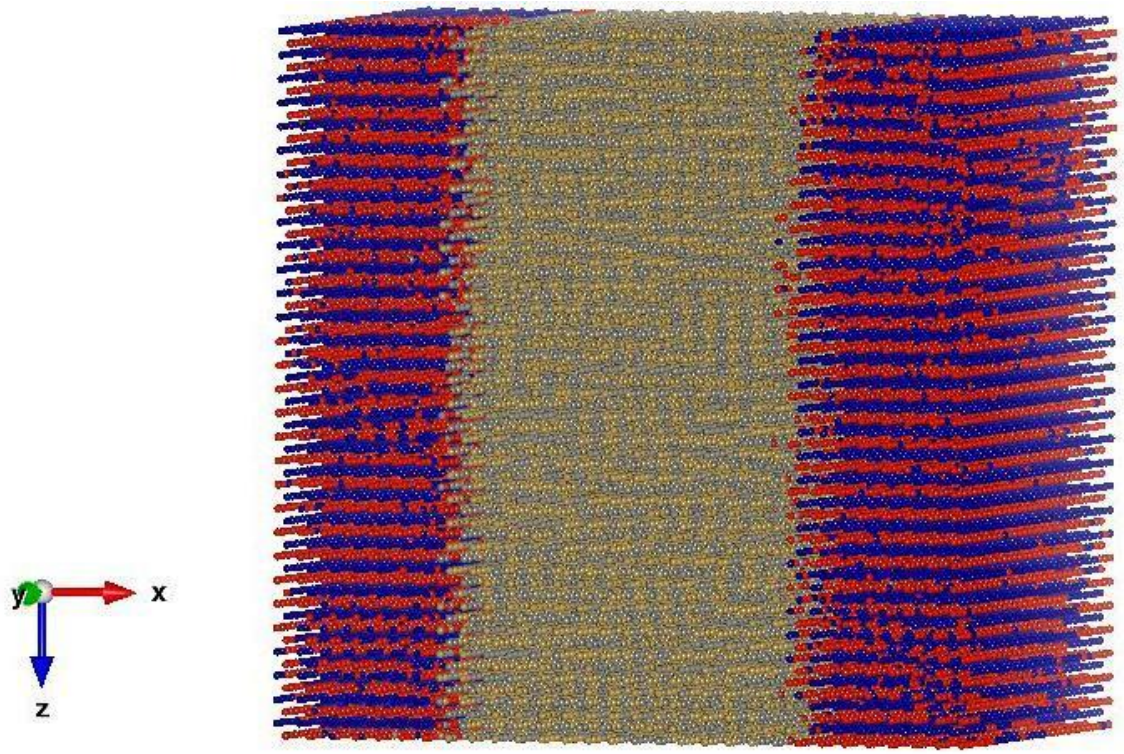

Fig. S4 30x30x30 equiatomic Cr-Ta-V-W structure at 300 K

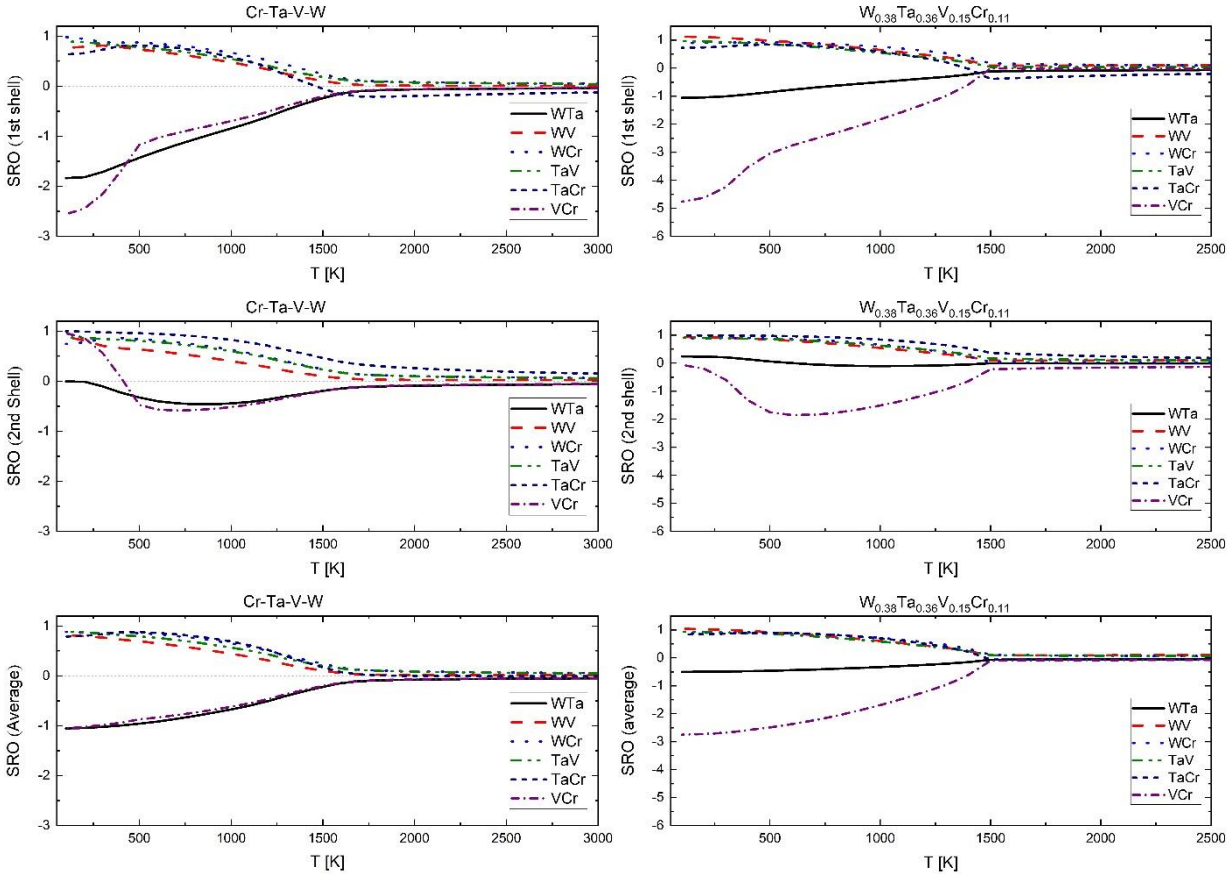

Fig. S5 The short-range order parameter as a function of temperature for 1st and 2nd shell, as well as the average SRO for equiatomic Cr-Ta-V-W (left) alloy in comparison with quaternary $W_{0.38}Ta_{0.36}Cr_{0.15}V_{0.11}$alloy (right)