Supplementary Material

First principles study of bonding mechanisms at the TiAl/TiO_2 interface

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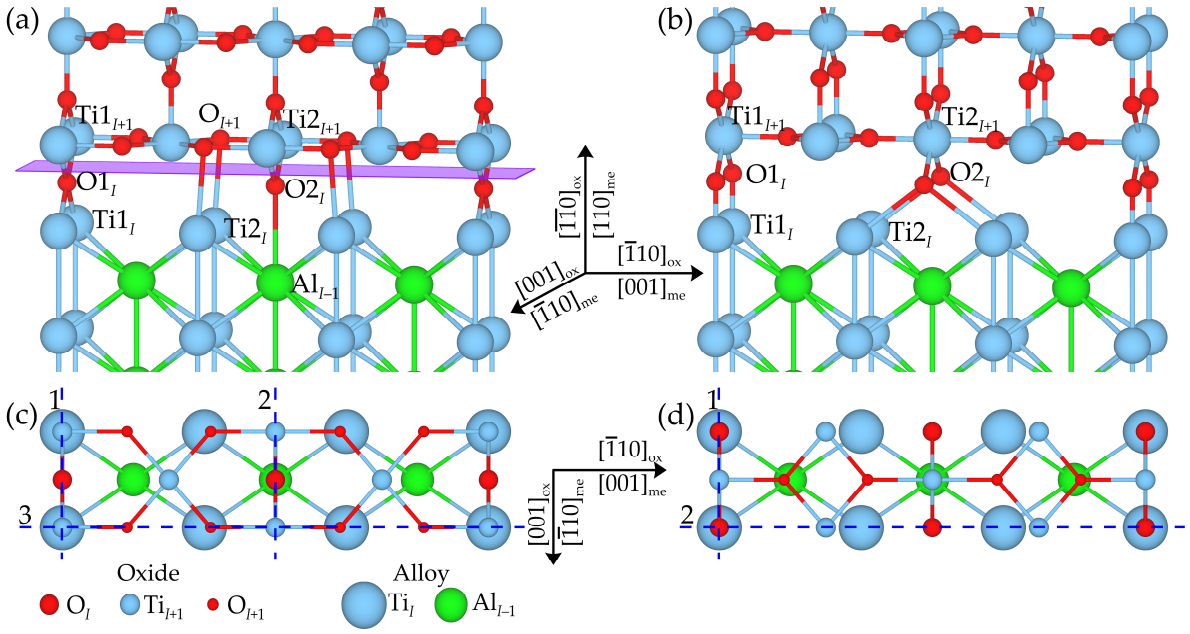

Figure S1. Atomic structures of unrelaxed interfaces with (**a**, **c**) *hollow* and (**b**, **d**) *top* configuration in case of the Ti-terminated alloy surface. Atoms which are important in interfacial bonding are marked. Symbols *I* and *I*±1 denote atoms of interfacial and subinterfacial layers.

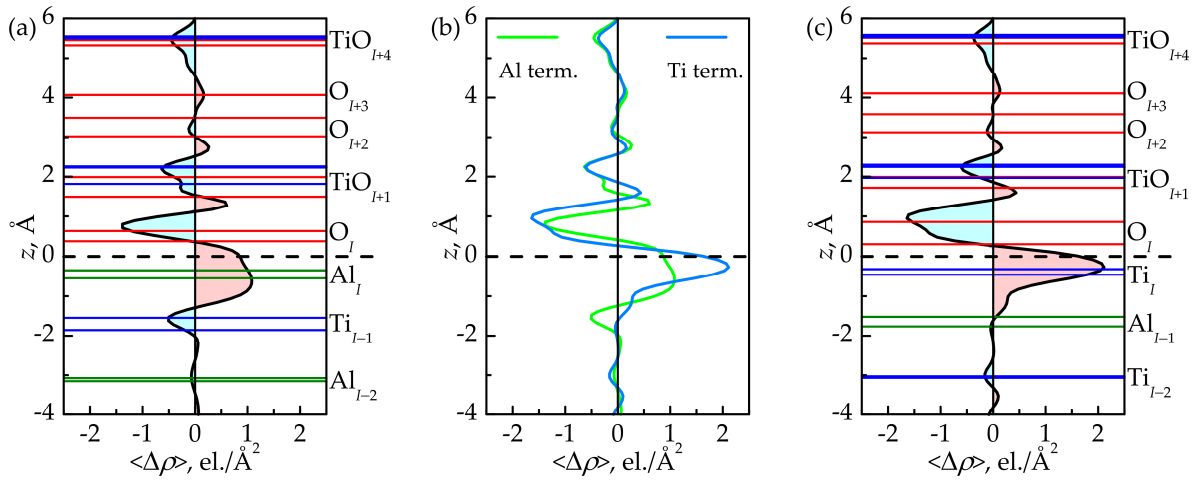

Figure S2. In-plane average charge density difference at the interface with the *hollow* configuration in case of (**a**) Al- and (**c**) Ti-terminated alloy surface with indicated atomic layer position as well as (**b**) comparison of curves for two terminations. Negative/positive values of $<\Delta\rho>$ correspond to charge accumulation/depletion. Position $z = 0$ corresponds to interface plane.

Table S1. Charge states of some interfacial and subinterfacial atoms (Q in el.), bond length between them (d in Å) and averaged overlap population (θ in el.) for pairs of the atoms in case of the *top* interface configuration.

TiAl(110)$_{Al}$/TiO$_2$(110)$_O$				**TiAl(110)$_{Ti}$/TiO$_2$(110)$_O$**			
Atom	***Q***	***d***	***θ***	**Atom**	***Q***	***d***	***θ***
Ti1$_{I+1}$	+2.13	1.99	0.280	Ti1$_{I+1}$	+2.13	1.97	0.294
O1$_I$	–0.89			O1$_I$	–0.95		
Ti2$_{I+1}$	+2.05	2.11	0.216	Ti2$_{I+1}$	+1.87	2.13	0.230
O2$_I$	–0.78			O2$_I$	-0.89		
O1$_I$	–0.89	1.78	0.671	O1$_I$	–0.95	1.84	0.668
Al1$_I$	+0.32			Ti1$_I$	+0.63		
O2$_I$	–0.78	2.02	0.440	O2$_I$	–0.89	2.09	0.387
Al2$_I$	+0.15			Ti2$_I$	+0.65		
O$_{I+1}$	–1.15	3.11	0.078	O$_{I+1}$	–1.16	2.27	0.317
Al2$_I$	+0.15			Ti2$_I$	+0.65		