Supplementary Materials for

The First-Principles Study of Interfacial Bonding Strength and Segregation Behavior of Alloyed Elements At η ($MgZn_2$)/Al Interface

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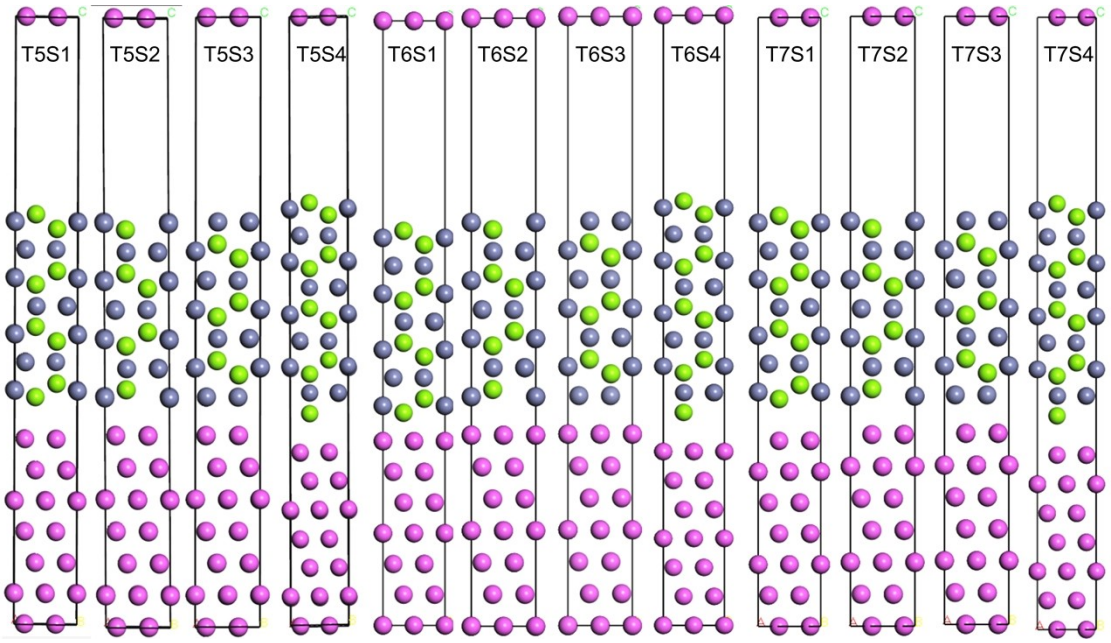

Fig.S1. Interface models of 12 different terminals projected along axis [010]

Table.S1. The charge distribution of interface atoms

Interface atoms	T5(Charge/e)				Interface atoms	T6(Charge/e)				Interface atoms	T7(Charge/e)			
	S1	S2	S3	S4		S1	S2	S3	S4		S1	S2	S3	S4
Al(5)	-0.19	-0.19	-0.12	-0.12	Al(3)	-0.06	-0.21	-0.09	-0.01	Al(7)	-0.1	-0.07	-0.04	-0.11
Al(12)	-0.19	-0.19	-0.13	-0.12	Al(10)	-0.21	-0.13	-0.06	-0.21	Al(14)	-0.36	-0.37	-0.04	-0.34
Al(19)	-0.13	-0.01	0.03	-0.09	Al(17)	-0.21	-0.13	-0.06	-0.21	Al(21)	-0.1	-0.07	-0.04	-0.11
Al(26)	-0.19	-0.19	-0.13	-0.12	Al(24)	-0.21	-0.13	-0.06	-0.21	Al(28)	-0.1	-0.07	-0.04	-0.11
Mg(1)	0.83				Mg(1)	0.75				Mg(1)	0.78			
Mg(2)		0.68			Mg(2)		0.54			Mg(2)		0.69		
Mg(3)				0.6	Mg(3)				0.51	Mg(3)				0.44
Mg(5)	0.65				Mg(5)	0.58				Mg(5)	0.83			
Zn(1)				-0.22	Zn(1)				-0.28	Zn(1)				-0.31
Zn(3)				-0.22	Zn(3)				-0.28	Zn(3)				-0.31
Zn(5)				-0.22	Zn(5)				-0.28	Zn(5)				-0.31
Zn(7)			-0.24		Zn(7)			-0.32		Zn(7)			-0.31	
Zn(9)			-0.24		Zn(9)			-0.32		Zn(9)			-0.31	
Zn(10)	-0.07				Zn(10)	-0.09				Zn(10)	-0.15			
Zn(11)			-0.24		Zn(11)			-0.32		Zn(11)			-0.31	
Zn(12)		-0.16			Zn(12)		-0.12			Zn(12)		-0.34		
Total	0.71	-0.06	-1.07	-0.51	Total	0.55	-0.18	-1.23	-0.97	Total	0.8	-0.23	-1.09	-1.16

Table.S2. Bond population, bond numbers, and bond length of interface atoms

Interface types	Population of bonds			Number of bonds			Length of bonds(Å)		
	Al-Zn	Al-Mg	Total	Al-Zn	Al-Mg	Total	Al-Zn	Al-Mg	Total
T5S1	0.91	0	0.91	3	0	3	2.8743	0	8.6232
T5S2	1.01	0	1.01	4	0	4	2.68105	0	10.7242
T5S3	2.39	0	2.39	3	0	3	2.6448	0	7.9344
T5S4	0	0.82	0.82	0	4	4	0	2.7314	10.9256
T6S1	1.09	0	1.09	1	0	1	2.60193	0	2.60193
T6S2	2.28	0	2.28	1	0	1	2.7091	0	2.7091
T6S3	0.73	0	0.73	9	0	9	2.50529	0	22.54791
T6S4	0	0.69	0.69	0	3	3	0	2.87903	8.63709
T7S1	0.92	0.29	1.21	3	1	4	2.77752	2.8949	11.22743
T7S2	1.14	0.31	1.45	3	1	4	2.67659	2.8418	10.87157
T7S3	2.28	0	2.28	9	0	9	2.77412	0	24.6708
T7S4	0	0.44	0.440	0	1	1	0	2.9995	2.9995