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Two-side slab model

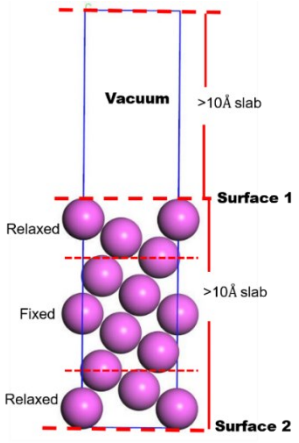

Figure 1 Diagram of a two-side slab model.

Two-side slab model: fixed several layers with the bulk structure to simulate the part which is far away from the surface, and some relaxed layers on both sides (Fig. 1) to model the part neighboring the superficies.

Calculation details

1. Ag element

(a) INCAR

ISTART=0
ICHARG = 2
ALGO = Fast
EDIFF = 0.0001
ENCUT = 400
IBRION = 2
ISIF = 2
ISPIN = 2
MAGMOM = 15*0.6
LREAL = Auto
ISMEAR = 1
NELM = 100
NSW = 99
PREC = Accurate
POTIM=0.1
SIGMA = 0.05

(b) POSCAR

Ag (100)
1.0

2.9426000118	0.0000000000	0.0000000000
0.0000000000	2.9426000118	0.0000000000
0.0000000000	0.0000000000	49.1297988892

Ag

15
Selective Dynamics
C
0.000000000 0.000000000 0.000000000 T T T
1.471300006 1.471300006 2.080646992 T T T
0.000000000 0.000000000 4.161293983 T T T
1.471300006 1.471300006 6.241940975 F F F
0.000000000 0.000000000 8.322587967 F F F
1.471300006 1.471300006 10.40372657 F F F
0.000000000 0.000000000 12.48437404 F F F
1.471300006 1.471300006 14.56502056 F F F
0.000000000 0.000000000 16.64566612 F F F
1.471300006 1.471300006 18.72631454 F F F
0.000000000 0.000000000 20.80696106 F F F
1.471300006 1.471300006 22.88760948 F F F
0.000000000 0.000000000 24.96825599 T T T
1.471300006 1.471300006 27.04890251 T T T
0.000000000 0.000000000 29.13004112 T T T

2. Cu element

(a) INCAR

ISTART=0
ICHARG = 2
ALGO = Fast
EDIFF = 0.0001
ENCUT = 400
IBRION = 2
ISIF = 2
ISPIN = 2
MAGMOM = 15*0.6
LREAL = Auto
ISMEAR = 1
NELM = 100
NSW = 99
PREC = Accurate
POTIM=0.1
SIGMA = 0.05

(b) POSCAR

Cu (100)
1.0
2.5666999817 0.0000000000 0.0000000000
0.0000000000 2.5666999817 0.0000000000
0.0000000000 0.0000000000 45.4090003967
Cu
15

Selective Dynamics
C

0.000000000	0.000000000	0.000000000	T	T	T
1.283349991	1.283349991	1.814997673	T	T	T
0.000000000	0.000000000	3.629995346	T	T	T
1.283349991	1.283349991	5.444993496	F	F	F
0.000000000	0.000000000	7.259536743	F	F	F
1.283349991	1.283349991	9.074534416	F	F	F
0.000000000	0.000000000	10.88953304	F	F	F
1.283349991	1.283349991	12.70452976	F	F	F
0.000000000	0.000000000	14.51952839	F	F	F
1.283349991	1.283349991	16.33452606	F	F	F
0.000000000	0.000000000	18.14906883	F	F	F
1.283349991	1.283349991	19.96406746	F	F	F
0.000000000	0.000000000	21.77906609	T	T	T
1.283349991	1.283349991	23.59406281	T	T	T
0.000000000	0.000000000	25.40905953	T	T	T

3. Al element

(a) INCAR

ISTART=0
ICHARG = 2
ALGO = Fast
EDIFF = 0.0001
ENCUT = 400
IBRION = 2
ISIF = 2
ISPIN = 2
MAGMOM = 15*0.6
LREAL = Auto
ISMEAR = 1
NELM = 100
NSW = 99
PREC = Accurate
POTIM=0.1
SIGMA = 0.05

(b) POSCAR

Al (1 0 0)
1.0

2.8545000553	0.0000000000	0.0000000000
0.0000000000	2.8545000553	0.0000000000
0.0000000000	0.0000000000	49.2765998840

Al
15
Selective Dynamics

C

1.427250028	1.427250028	0.000000000	T	T	T
0.000000000	0.000000000	2.018605471	T	T	T
1.427250028	1.427250028	4.036707878	T	T	T
0.000000000	0.000000000	6.055313587	F	F	F
1.427250028	1.427250028	8.073919296	F	F	F
0.000000000	0.000000000	10.09202194	F	F	F
1.427250028	1.427250028	12.11062717	F	F	F
0.000000000	0.000000000	14.12923241	F	F	F
1.427250028	1.427250028	16.14733505	F	F	F
0.000000000	0.000000000	18.16594124	F	F	F
1.427250028	1.427250028	20.18454742	F	F	F
0.000000000	0.000000000	22.20265007	F	F	F
1.427250028	1.427250028	24.22125435	T	T	T
0.000000000	0.000000000	26.23986054	T	T	T
1.427250028	1.427250028	28.25796127	T	T	T

4. Si element

(a) INCAR

ISTART=0
ICHARG = 2
ALGO = Fast
EDIFF = 0.0001
ENCUT = 400
IBRION = 2
ISIF = 2
LREAL = Auto
ISMEAR = 0
NELM = 100
NSW = 99
PREC = Accurate
POTIM=0.1
SIGMA = 0.1

(b) POSCAR

Si (100)
1.0

7.7339491844	0.0000000000	0.0000000000
0.0000000000	3.8669745922	0.0000000000
0.0000000000	0.0000000000	41.8749122620

Si
16
Selective Dynamics
C

3.425412416	0.000000000	11.57823753	T	T	T
1.215119362	0.000000000	12.22766018	T	T	T

0.105576143	1.933487296	12.92479229	T	T	T	
3.753726244	1.933487296	12.97164822	F	F	F	
5.820376873	1.933487296	14.20565510	F	F	F	
1.947702289	1.933487296	14.50700378	F	F	F	
5.868458748	0.000000000	15.60536575	F	F	F	
1.869194984	0.000000000	15.84653664	F	F	F	
3.931267023	0.000000000	16.96583176	F	F	F	
7.665952206	0.000000000	17.20700264	F	F	F	
3.852759600	1.933487296	18.30536461	F	F	F	
7.714034557	1.933487296	18.60671234	F	F	F	
2.046735525	1.933487296	19.84072113		F	F	F
5.694885731	1.933487296	19.88757706	T	T	T	
4.585342407	0.000000000	20.58470726	T	T	T	
2.375049353	0.000000000	21.23413086	T	T	T	

Table 1 Atomic number of surface slab model for different elements.

Types	Atomic number	Types	Atomic number
Ag (100)	15	Cu (100)	15
Ag (110)	15	Cu (110)	15
Ag (111)	16	Cu (111)	15
Ag (210)	16	Cu (210)	15
Ag (211)	16	Cu (211)	15
Ag (221)	15	Cu (221)	15
Ag (311)	12	Cu (310)	15
Ag (331)	20	Cu (311)	15
Ag (511)	28	Cu (511)	15
Al (100)	15	**Si (100)**	16
Al (110)	15	**Si (110)**	16
Al (111)	15	**Si (111)**	24
Al (210)	15	Si (210)	31
Al (211)	15	Si (211)	32
Al (221)	15	Si (221)	37
Al (310)	15	Si (320)	27
Al (311)	15	Si (321)	30
Al (331)	15	Si (322)	69
Al (511)	15	Si (332)	46