MSE 614
Homework 04 Assignment
Stability of Surface and Subsurface Oxygen on Silver Surfaces

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In this homework, we are as a class going to examine the structure and energetic of oxidized silver surfaces using LAMMPS.

We will use the following ReaxFF potential. This has been shown to give the right structure for Ag and Ag_2O.

Title: Development of a ReaxFF potential for Ag/Zn/O and application to Ag deposition on ZnO
Authors: Lloyd, A; Cornil, D; van Duin, ACT; van Duin, D; Smith, R; Kenny, SD; Cornil, J; Beljonne, D
Journal: Surface Science
Volume: 645 Pages: 67-73
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The instructor has created 153 initial configurations and 153 corresponding LAMMPS input files varying five properties.

Property 1. Exposed Silver Surface: (111) or (110)
Property 2. Location of Oxygen Atoms: Surface, Subsurface or Both
Property 3. Type of Adsorption Site: Site geometry depends upon surface and location above.
Property 4. Fractional occupancy of sites: 0.1, 0.5 or 1.0
Property 5. Temperature: 77, 300 or 500 K.

In lecture, the instructor has emphasized that you are being trained to be a thinking computational scientist and not a technician. However, in this last homework, we shift the emphasis from getting the LAMMPS input file correct to analyzing a set of simulation results. *Therefore, you should not change either the initial configuration file or the LAMMPS input file, which have been standardized to generate consistent results.* All of the necessary input files, initial configuration files and potential file are posted on the Canvas Course Site.

Each student has two tasks.

Task 1. Run 9 simulations.
In this set of simulations you will have a constant value for Properties 1, 2 and 3. You will have a 3 by 3 grid of fractional occupancies and temperatures (Properties 4 and 5). Each simulation may take about two hours on 16 processors (1 node) on ACF, so start early. Preferably create a directory for each of your nine simulations, identified with the three digit run id number. Save all LAMMPS outputs, RDF files, MSD files and trajectory files.

Task 2. Analyze Results.
Analyze the energetics, charge distribution, radial distribution functions (RDF) and mean square displacement (MSD) files for your 9 simulations. Especially report surprising or unusual behavior that you observe. Did the particles stay in their initial positions. Did they move? If so to where? Do the energetics, charge, RDF and MSD data support what you see in the movie? Draw conclusions regarding the stability and structure of the surface and emphasize its dependence on the two variables that you have examined: fractional occupancy and temperature.

Deliverables:

The Homework 4 discussion from Task 2 will be uploaded as a pdf to the CANVAS course website.

The assignment of each student to a particular set of 9 simulations is given in the table below.

Matrix of Simulations

id #	surface	oxide layer	oxygen initial location	occupancy	T (K)	student A	student B
1	(111)	surface	top	0.1	77	mabdela1	
2	(111)	surface	top	0.1	300	mabdela1	
3	(111)	surface	top	0.1	500	mabdela1	
4	(111)	surface	top	0.5	77	mabdela1	
5	(111)	surface	top	0.5	300	mabdela1	
6	(111)	surface	top	0.5	500	mabdela1	
7	(111)	surface	top	1	77	mabdela1	
8	(111)	surface	top	1	300	mabdela1	
9	(111)	surface	top	1	500	mabdela1	
10	(111)	surface	bridge	0.1	77	bdanie36	
11	(111)	surface	bridge	0.1	300	bdanie36	
12	(111)	surface	bridge	0.1	500	bdanie36	
13	(111)	surface	bridge	0.5	77	bdanie36	
14	(111)	surface	bridge	0.5	300	bdanie36	
15	(111)	surface	bridge	0.5	500	bdanie36	
16	(111)	surface	bridge	1	77	bdanie36	
17	(111)	surface	bridge	1	300	bdanie36	
18	(111)	surface	bridge	1	500	bdanie36	
19	(111)	surface	hollow (fcc)	0.1	77	cdelamat	
20	(111)	surface	hollow (fcc)	0.1	300	cdelamat	
21	(111)	surface	hollow (fcc)	0.1	500	cdelamat	
22	(111)	surface	hollow (fcc)	0.5	77	cdelamat	
23	(111)	surface	hollow (fcc)	0.5	300	cdelamat	
24	(111)	surface	hollow (fcc)	0.5	500	cdelamat	
25	(111)	surface	hollow (fcc)	1	77	cdelamat	
26	(111)	surface	hollow (fcc)	1	300	cdelamat	
27	(111)	surface	hollow (fcc)	1	500	cdelamat	
28	(111)	surface	hollow (hcp)	0.1	77	sgodfre4	
29	(111)	surface	hollow (hcp)	0.1	300	sgodfre4	
30	(111)	surface	hollow (hcp)	0.1	500	sgodfre4	
31	(111)	surface	hollow (hcp)	0.5	77	sgodfre4	
32	(111)	surface	hollow (hcp)	0.5	300	sgodfre4	
33	(111)	surface	hollow (hcp)	0.5	500	sgodfre4	
34	(111)	surface	hollow (hcp)	1	77	sgodfre4	
35	(111)	surface	hollow (hcp)	1	300	sgodfre4	
36	(111)	surface	hollow (hcp)	1	500	sgodfre4	
37	(111)	sub-surface	tetrahedral-1	0.1	77	uigbudug	
38	(111)	sub-surface	tetrahedral-1	0.1	300	uigbudug	

39	(111)	sub-surface	tetrahedral-1	0.1	500	uigbudug	
40	(111)	sub-surface	tetrahedral-1	0.5	77	uigbudug	
41	(111)	sub-surface	tetrahedral-1	0.5	300	uigbudug	
42	(111)	sub-surface	tetrahedral-1	0.5	500	uigbudug	
43	(111)	sub-surface	tetrahedral-1	1	77	uigbudug	
44	(111)	sub-surface	tetrahedral-1	1	300	uigbudug	
45	(111)	sub-surface	tetrahedral-1	1	500	uigbudug	
46	(111)	sub-surface	tetrahedral-3	0.1	77	dli48	
47	(111)	sub-surface	tetrahedral-3	0.1	300	dli48	
48	(111)	sub-surface	tetrahedral-3	0.1	500	dli48	
49	(111)	sub-surface	tetrahedral-3	0.5	77	dli48	
50	(111)	sub-surface	tetrahedral-3	0.5	300	dli48	
51	(111)	sub-surface	tetrahedral-3	0.5	500	dli48	
52	(111)	sub-surface	tetrahedral-3	1	77	dli48	
53	(111)	sub-surface	tetrahedral-3	1	300	dli48	
54	(111)	sub-surface	tetrahedral-3	1	500	dli48	
55	(111)	sub-surface	octahedral	0.1	77	kloughl1	
56	(111)	sub-surface	octahedral	0.1	300	kloughl1	
57	(111)	sub-surface	octahedral	0.1	500	kloughl1	
58	(111)	sub-surface	octahedral	0.5	77	kloughl1	
59	(111)	sub-surface	octahedral	0.5	300	kloughl1	
60	(111)	sub-surface	octahedral	0.5	500	kloughl1	
61	(111)	sub-surface	octahedral	1	77	kloughl1	
62	(111)	sub-surface	octahedral	1	300	kloughl1	
63	(111)	sub-surface	octahedral	1	500	kloughl1	
64	(111)	both	hollow (fcc) & octahedral	0.1	77	dojedeji	
65	(111)	both	hollow (fcc) & octahedral	0.1	300	dojedeji	
66	(111)	both	hollow (fcc) & octahedral	0.1	500	dojedeji	
67	(111)	both	hollow (fcc) & octahedral	0.5	77	dojedeji	
68	(111)	both	hollow (fcc) & octahedral	0.5	300	dojedeji	
69	(111)	both	hollow (fcc) & octahedral	0.5	500	dojedeji	
70	(111)	both	hollow (fcc) & octahedral	1	77	dojedeji	
71	(111)	both	hollow (fcc) & octahedral	1	300	dojedeji	
72	(111)	both	hollow (fcc) & octahedral	1	500	dojedeji	
73	(110)	surface	top	0.1	77	eoluwas1	
74	(110)	surface	top	0.1	300	eoluwas1	
75	(110)	surface	top	0.1	500	eoluwas1	

76	(110)	surface	top	0.5	77	eoluwas1	
77	(110)	surface	top	0.5	300	eoluwas1	
78	(110)	surface	top	0.5	500	eoluwas1	
79	(110)	surface	top	1	77	eoluwas1	
80	(110)	surface	top	1	300	eoluwas1	
81	(110)	surface	top	1	500	eoluwas1	
82	(110)	surface	bridge (short)	0.1	77	bquebede	
83	(110)	surface	bridge (short)	0.1	300	bquebede	
84	(110)	surface	bridge (short)	0.1	500	bquebede	
85	(110)	surface	bridge (short)	0.5	77	bquebede	
86	(110)	surface	bridge (short)	0.5	300	bquebede	
87	(110)	surface	bridge (short)	0.5	500	bquebede	
88	(110)	surface	bridge (short)	1	77	bquebede	
89	(110)	surface	bridge (short)	1	300	bquebede	
90	(110)	surface	bridge (short)	1	500	bquebede	
91	(110)	surface	bridge (long)	0.1	77	msamanda	
92	(110)	surface	bridge (long)	0.1	300	msamanda	
93	(110)	surface	bridge (long)	0.1	500	msamanda	
94	(110)	surface	bridge (long)	0.5	77	msamanda	
95	(110)	surface	bridge (long)	0.5	300	msamanda	
96	(110)	surface	bridge (long)	0.5	500	msamanda	
97	(110)	surface	bridge (long)	1	77	msamanda	
98	(110)	surface	bridge (long)	1	300	msamanda	
99	(110)	surface	bridge (long)	1	500	msamanda	
100	(110)	surface	hollow	0.1	77	usuresh3	
101	(110)	surface	hollow	0.1	300	usuresh3	
102	(110)	surface	hollow	0.1	500	usuresh3	
103	(110)	surface	hollow	0.5	77	usuresh3	
104	(110)	surface	hollow	0.5	300	usuresh3	
105	(110)	surface	hollow	0.5	500	usuresh3	
106	(110)	surface	hollow	1	77	usuresh3	
107	(110)	surface	hollow	1	300	usuresh3	
108	(110)	surface	hollow	1	500	usuresh3	
109	(110)	sub-surface	square pyramidal 1	0.1	77	yyuan16	
110	(110)	sub-surface	square pyramidal 1	0.1	300	yyuan16	
111	(110)	sub-surface	square pyramidal 1	0.1	500	yyuan16	
112	(110)	sub-surface	square pyramidal 1	0.5	77	yyuan16	
113	(110)	sub-surface	square pyramidal 1	0.5	300	yyuan16	
114	(110)	sub-surface	square	0.5	500	yyuan16	

			pyramidal 1				
115	(110)	sub-surface	square pyramidal 1	1	77	yyuan16	
116	(110)	sub-surface	square pyramidal 1	1	300	yyuan16	
117	(110)	sub-surface	square pyramidal 1	1	500	yyuan16	
118	(110)	sub-surface	square pyramidal 4	0.1	77		
119	(110)	sub-surface	square pyramidal 4	0.1	300		
120	(110)	sub-surface	square pyramidal 4	0.1	500		
121	(110)	sub-surface	square pyramidal 4	0.5	77		
122	(110)	sub-surface	square pyramidal 4	0.5	300		
123	(110)	sub-surface	square pyramidal 4	0.5	500		
124	(110)	sub-surface	square pyramidal 4	1	77		
125	(110)	sub-surface	square pyramidal 4	1	300		
126	(110)	sub-surface	square pyramidal 4	1	500		
127	(110)	sub-surface	bridge (short)	0.1	77		
128	(110)	sub-surface	bridge (short)	0.1	300		
129	(110)	sub-surface	bridge (short)	0.1	500		
130	(110)	sub-surface	bridge (short)	0.5	77		
131	(110)	sub-surface	bridge (short)	0.5	300		
132	(110)	sub-surface	bridge (short)	0.5	500		
133	(110)	sub-surface	bridge (short)	1	77		
134	(110)	sub-surface	bridge (short)	1	300		
135	(110)	sub-surface	bridge (short)	1	500		
136	(110)	both	bridge (long)	0.1	77		
137	(110)	both	bridge (long)	0.1	300		
138	(110)	both	bridge (long)	0.1	500		
139	(110)	both	bridge (long)	0.5	77		
140	(110)	both	bridge (long)	0.5	300		
141	(110)	both	bridge (long)	0.5	500		
142	(110)	both	bridge (long)	1	77		
143	(110)	both	bridge (long)	1	300		
144	(110)	both	bridge (long)	1	500		
145	(110)	both	hollow & square pyramidal 1	0.1	77		
146	(110)	both	hollow & square pyramidal 1	0.1	300		

147	(110)	both	hollow & square pyramidal 1	0.1	500		
148	(110)	both	hollow & square pyramidal 1	0.5	77		
149	(110)	both	hollow & square pyramidal 1	0.5	300		
150	(110)	both	hollow & square pyramidal 1	0.5	500		
151	(110)	both	hollow & square pyramidal 1	1	77		
152	(110)	both	hollow & square pyramidal 1	1	300		
153	(110)	both	hollow & square pyramidal 1	1	500		