8.1 DEVELOPMENT OF INTERATOMIC POTENTIALS IN TUNGSTEN-RHENIUM SYSTEMS—W. Setyawan, G. Nandipati, and R. J. Kurtz (Pacific Northwest National Laboratory)

OBJECTIVE

The objective of this research is to develop interatomic potentials for exploring radiation damage in W in the presence of solid transmutant Re and radiation-induced precipitation of W-Re intermetallics.

SUMMARY

Reference data are generated using the ab initio method to fit interatomic potentials for the W-Re system. The reference data include single phases of W and Re, strained structures, slabs, systems containing several concentrations of vacancies, systems containing various types of interstitial defects, melt structures, structures in the σ and χ phases, and structures containing several concentrations of solid solutions of Re in bcc W and W in hcp Re. Future work will start the fitting iterations.

PROGRESS AND STATUS

This research is in the early stage. In this report, we present the reference structures that will be used to fit interatomic potentials. While experimental data may also be included, here we present the reference data that are calculated using VASP [1, 2] software within the density functional theory (DFT) framework. Core electrons are modeled with accurate projector-augmented-wave pseudopotentials [2]. Electrons in 6s and 5d states are treated as valence electrons. Perdew-Burke-Ernzerhof formulations [3] were employed for the exchange-correlation functionals. Plane wave cutoff energy is set at ENCUT = 300 eV. A Monkhorst-Pack [4] k-point grid is employed. Following the convergence study of k-points for the 3x3x3 bcc W (54 atoms), the energy converges to within 1 meV/atom with a 6x6x6 k-point grid, i.e. the number of atoms multiplied by the number of k-points is KPPRA = 54*6*6*6 = 11,664. Therefore, for all other systems, the k-point grid is set such that the KPPRA is approximately 12,000.

<u>Pure W</u>

Table 1 summarizes the reference data for pure W. For each system, the number of atoms (N_{atoms}) and the total energy (E_{total}) are given. In Table 1, universal strains refer to the universal linear-independent coupling strains (ULICS) [5]. In general, there are 6 ULICS strain vectors as the following (given in engineering notation):

u_1 = [1 2 3 4 5 6] * factor
u_2 = [-2 1 4 -3 6 -5] * factor
u_3 = [3 -5 -1 6 2 -4] * factor
u_4 = [-4 -6 5 1 -3 3] * factor
u_5 = [5 4 6 -2 -1 -3] * factor
u_6 = [-6 3 -2 5 -4 1] * factor

For a given strain vector u = [e_1 e_2 e_3 e_4 e_5 e_6], the corresponding strain tensor is

$$\varepsilon = \begin{bmatrix} e_1 & e_6/2 & e_5/2 \\ e_6/2 & e_2 & e_4/2 \\ e_5/2 & e_4/2 & e_3 \end{bmatrix}$$

The slab systems are constructed from a bcc conventional cell and include approximately 15 Å of vacuum space. To obtain the melt reference structures, classical molecular dynamics simulations are performed with LAMMPS [6] software using the W potential from Ref. [7]. Three melt structures are taken for the DFT simulations. In the DFT, for each melt structure, three different hydrostatic strains of -0.05, 0, and 0.2 are applied and the forces and energies are calculated.

Table 1. Reference data for pure W

System	N_{atoms}	E_{total} (eV)
bcc	54	-702.5819394
simple cubic	27	-312.636272
fcc	108	-1351.76693
hcp	48	-624.4633856
hydrostatic strain in bcc:		
-0.3	54	1097.254324
-0.25	54	379.5085514
-0.2	54	-112.8243529
-0.15	54	-420.0384223
-0.1	54	-594.0784846
-0.05	54	-676.6818088
-0.02	54	-695.6090639
-0.01	54	-698.0294595
0.01	54	-698.0363247
0.02	54	-695.9368593
0.05	54	-682.8022404
0.1	54	-644.4434419
0.15	54	-594.0470566
0.2	54	-538.4563672
0.25	54	-482.1371869
0.3	54	-427.9757802
0.4	54	-331.7395263
0.5	54	-255.0060816
universal strain u_1, factor = 0.01	54	-697.8249173
slab systems:		
{100} 9 layers	81	-1008.513982
{100} 10 layers	90	-1125.5968
{110} 8 layers	96	-1214.146302
{110} 9 layers	108	-1370.328137
{111} 15 layers	60	-749.6910502
{111} 16 layers	64	-802.0618372
vacancies in bcc:		
1	127	-1649.133084
8	120	-1534.820091
16	112	-1405.917881
32	96	-1174.650616
interstitial in bcc at site:		
octahedral	251	-3252.613316
tetrahedral	251	-3253.257761
melt structures:		

structure 1, strain = -0.05	128	-1416.5574
structure 1, strain = 0	128	-1525.7440
structure 1, strain = 0.2	128	-1291.6383
structure 2, strain = -0.05	128	-1413.6436
structure 2, strain = 0	128	-1525.1460
structure 2, strain = 0.2	128	-1293.8987
structure 3, strain = -0.05	128	-1407.0131
structure 3, strain = 0	128	-1519.3006
structure 3, strain = 0.2	128	-1292.5626

Pure Re

Table 2 summarizes the reference data for pure Re. The universal strains are applied to an hcp structure in an orthorhombic cell. In the orthorhombic cell, the x-axis is along the basal close-packed row direction, the y-axis is perpendicular to x, and the z-axis is parallel to the c-axis of the original hcp unit cell, as shown in Figure 1. Figure 2 shows interstitial sites in the hcp structure that are labeled according to Ref. [8], namely O (octahedral site), T (tetrahedral site), BO (on basal plane directly below O), BT (basal plane directly below T), BC (crowdion site in the basal close-packed row), C (midway between two atoms in the primitive hcp cell), and S (represents the position of one of the atoms in a [0001] split dumbbell). Note that Figure 2 is only for illustrating the location of the interstitial sites, while the calculations with an interstitial are performed in an hcp structure in an orthorhombic 5x3x3 supercell. The melt reference structures are generated in a similar way as in tungsten using the same ad hoc potential.

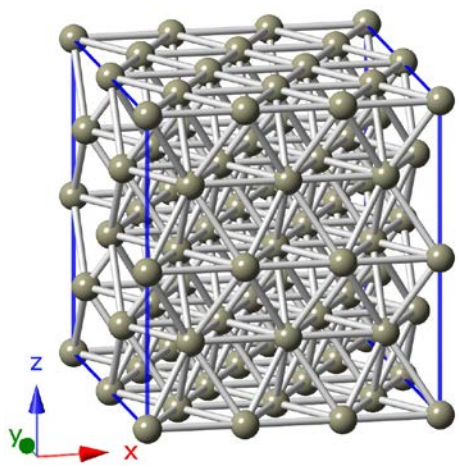

Figure 1. Hexagonal close-packed structure in an orthorhombic 3x2x2 supercell. The close-packed plane stacking is along the z axis.

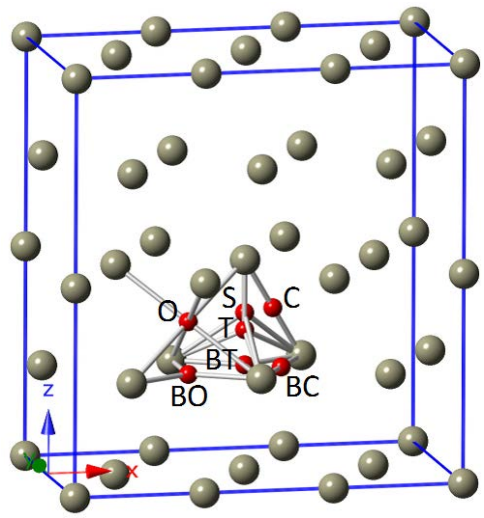

Figure 2. Schematic showing the location of interstitial sites in hcp Re.

Table 2. Reference data for pure Re

System	N_{atoms}	E_{total} (eV)
bcc	54	-650.1789284
simple cubic	27	-286.1105305
fcc	108	-1332.140438
hcp	48	-595.484282
hydrostatic strain in hcp:		
-0.3	48	1413.935322
-0.25	48	586.671512
-0.2	48	37.45553335
-0.15	48	-298.004176
-0.1	48	-484.395746
-0.05	48	-571.6722672
-0.02	48	-591.7847314
-0.01	48	-594.4713212
0.01	48	-594.9844668
0.02	48	-593.1330174
0.05	48	-580.8254842
0.1	48	-544.4645052
0.15	48	-497.0115376
0.2	48	-445.4054424
0.25	48	-394.070185
0.3	48	-345.5787228
0.4	48	-261.1465214

0.5	48	-194.5711407
universal strain u_1, factor = 0.01	48	-590.6728669
universal strain u_2, factor = 0.01	48	-591.0746809
universal strain u_3, factor = 0.01	48	-589.3892782
slab systems:		
{0001} 8 layers	96	-1165.343074
{0001} 9 layers	108	-1313.81838
{11-20} 13 layers	104	-1257.225439
{11-20} 14 layers	112	-1356.504857
{10-10} 14 layers	90	-1084.938512
{10-10} 16 layers	96	-1164.174936
vacancies in hcp:		
1	179	-2217.499345
9	171	-2095.616498
18	162	-1959.043558
36	144	-1702.973672
interstitial in hcp at site:		
O	181	-2234.04217
T	181	-2235.701694
BO	181	-2234.760093
BT	181	-2234.080058
BC	181	-2234.375194
S	181	-2235.627513
C	181	-2224.510206
melt structures:		
structure 1, strain = -0.05	144	-1473.379543
structure 1, strain = 0	144	-1636.766874
structure 1, strain = 0.2	144	-1381.390768
structure 2, strain = -0.05	144	-1469.700918
structure 2, strain = 0	144	-1635.636129
structure 2, strain = 0.2	144	-1385.244533
structure 3, strain = -0.05	144	-1488.42032
structure 3, strain = 0	144	-1646.310219
structure 3, strain = 0.2	144	-1378.614023

W-Re

Table 3 summarizes the reference data for W-Re systems. For each system, the number of W atoms (N_W) and Re atoms (N_{Re}) are presented. The crystal structure of the σ and χ phases are taken from [9]. In the σ phase, there are five unique sites labeled A, B, C, D, and E. In the χ phase, there are four sites: A, B, C, and D. In Table 3, a system in the σ phase that is labeled as WWReWRe indicates for this system the sites from A to E are occupied by W, W, Re, W, and Re, respectively.

Table 3. Reference data for W-Re systems

System	N_W	N_{Re}	N_{atoms}	N_{Re}/N_{atoms}	E_{total} (eV)
σ phase:					
dir1 WWWWW	60	0	60	0	-769.8909243
dir2 WWWWRe	44	16	60	0.266666667	-760.5954671
dir3 WWWReW	44	16	60	0.266666667	-767.0342725
dir4 WWWReRe	28	32	60	0.533333333	-757.0972315
dir5 WWReWW	44	16	60	0.266666667	-761.6438983
dir6 WWReWRe	28	32	60	0.533333333	-752.346164
dir7 WWReReW	28	32	60	0.533333333	-756.9234711
dir8 WWReReRe	12	48	60	0.8	-745.7811481
dir9 WReWWW	52	8	60	0.133333333	-763.8059406
dir10 WReWWRe	36	24	60	0.4	-755.1414963
dir11 WReWReW	36	24	60	0.4	-761.1573737
dir12 WReWReRe	20	40	60	0.666666667	-751.279495
dir13 WReReWW	36	24	60	0.4	-755.3495869
dir14 WReReWRe	20	40	60	0.666666667	-745.8949998
dir15 WReReReW	20	40	60	0.666666667	-750.2992832
dir16 WReReReRe	4	56	60	0.933333333	-739.0879598
dir17 ReWWWW	56	4	60	0.066666667	-769.2817472
dir18 ReWWWRe	40	20	60	0.333333333	-759.9939997
dir19 ReWWReW	40	20	60	0.333333333	-766.2942985
dir20 ReWWReRe	24	36	60	0.6	-755.8677306
dir21 ReWReWW	40	20	60	0.333333333	-761.1414682
dir22 ReWReWRe	24	36	60	0.6	-751.5170731
dir23 ReWReReW	24	36	60	0.6	-755.9989009
dir24 ReWReReRe	8	52	60	0.866666667	-744.1692638
dir25 ReReWWW	48	12	60	0.2	-762.9539448
dir26 ReReWWRe	32	28	60	0.466666667	-754.1006308
dir27 ReReWReW	32	28	60	0.466666667	-760.1917582
dir28 ReReWReRe	16	44	60	0.733333333	-749.7810574
dir29 ReReReWW	32	28	60	0.466666667	-754.6094754
dir30 ReReReWRe	16	44	60	0.733333333	-744.7990256
dir31 ReReReReW	16	44	60	0.733333333	-749.1253384
dir32 ReReReReRe	0	60	60	1	-737.4461744
χ phase:					
dir101 WWWW	58	0	58	0	-737.3679916
dir102 WWWRe	34	24	58	0.413793103	-735.9993855
dir103 WWReW	34	24	58	0.413793103	-731.4378711
dir104 WWReRe	10	48	58	0.827586207	-724.8259818
dir105 WReWW	50	8	58	0.137931034	-730.9013652

dir106 WReWRe	26	32	58	0.551724138	-729.1132821
dir107 WReReW	26	32	58	0.551724138	-722.8944818
dir108 WReReRe	2	56	58	0.965517241	-717.4686601
dir109 ReWWW	56	2	58	0.034482759	-735.572186
dir110 ReWWRe	32	26	58	0.448275862	-734.4248587
dir111 ReWReW	32	26	58	0.448275862	-729.3596414
dir112 ReWReRe	8	50	58	0.862068966	-723.0912448
dir113 ReReWW	48	10	58	0.172413793	-728.8281186
dir114 ReReWRe	24	34	58	0.586206897	-727.1134194
dir115 ReReReW	24	34	58	0.586206897	-720.5746825
dir116 ReReReRe	0	58	58	1	-715.5232578
Re solid solution in bcc W:					
dir201	51	3	54	0.055555556	-699.9239873
dir202	49	5	54	0.092592593	-698.2619436
dir203	40	14	54	0.259259259	-690.5199573
dir204	27	27	54	0.5	-679.4381574
dir205	14	40	54	0.740740741	-669.9094759
W solid solution in hcp Re:					
dir251	2	46	48	0.958333333	-594.7724476
dir252	5	43	48	0.895833333	-595.1800105
dir253	12	36	48	0.75	-595.7273218
dir254	24	24	48	0.5	-599.7632192
dir255	36	12	48	0.25	-614.3788765

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