J. Wang, Y.L. Zhou, M. Li, and Q. Hou, “A modified W-W interatomic potential based on *ab initio* calculations,” Modelling Simul. Mater. Sci. Eng. **22** (2014) 015004. doi:10.1088/0965-0393/22/1/015004

Abstract:

In this paper we have developed a Finnis–Sinclair-type interatomic potential for W–W interactions that is based on *ab initio* calculations. The modified potential is able to reproduce the correct formation energies of self-interstitial atom (SIA) defects in tungsten, offering a significant improvement over the Ackland–Thetford tungsten potential. Using the modified potential, the thermal expansion is calculated in a temperature range from 0 to 3500 K. The results are in reasonable agreement with the experimental data, thus overcoming the shortcomings of the negative thermal expansion using the Derlet–Nguyen– Manh–Dudarev tungsten potential. The W–W potential presented here is also applied to study in detail the diffusion of SIAs in tungsten. We reveal that the initial SIA initiates a sequence of tungsten atom displacements and replacements in the <1 1 1> direction. An Arrhenius fit to the diffusion data at temperatures below 550 K indicates a migration energy of 0.022 eV, which is in reasonable agreement with the experimental data.

Note that this file corrects a typo in Equations 4 and 5 of the published paper. The symbol ‘f(r)’ should be ‘V(r)’ in equation (4) and in equation (5) ‘V(r)’ should be ‘f(r)’.

The total energy of an N-atom system is given by

$$E_{tot} = \sum_{i}^{N} F\left(\rho_i\right) + \frac{1}{2}\sum_{ij, i\neq j}^{N} V\left(r_{ij}\right), \qquad (1)$$

where the embedding energy $F\left(\rho\right)$ is given by

$$F\left(\rho\right) = -A\sqrt{\rho} \quad , \qquad (2)$$

and

$$\rho_i = \sum_{j, j\neq i} f\left(r_{ij}\right) \quad . \qquad (3)$$

For the present work, the pairwise potential function and the electronic density function will be represented by a series of polynomial functions,

$$V(r)=\sum_{n=1}^{N}\left(A_n+B_n r+C_n r^2+D_n r^3+E_n r^4+F_n r^5+G_n r^6+H_n r^7\right)\Theta(r_n-r)\Theta(r-r_{n+1}),$$

$$r_1 < r \le r_{N+1} \qquad (4)$$

and

$$f(r)=\sum_{n=1}^{N'}\left(A'_n+B'_n r+C'_n r^2+D'_n r^3+E'_n r^4+F'_n r^5+G'_n r^6+H'_n r^7\right)\Theta(r'_n-r)\Theta(r-r'_{n+1}),$$

$$r'_1 < r \le r'_{N'+1} \quad , \qquad (5)$$

respectively, where $\Theta(x)$ is a Heaviside step function, defined as $\Theta(x)=1$ for $x \ge 0$ and $\Theta(x)=0$ for $x<0$.

Parameters for the present W-W potential. The units are combinations of eV and Å to have Eqs. (1) to (5) be expressed in units of eV.

A_n	B_n	C_n	D_n
836.733119131673	-1092.73723146209	570.244952195581	-149.176023687989
185.476611562764	-65.1531905705160	-144.143194717123	128.381692972279
4483.32942908444	798.771513881627	-3119.64856577141	-2188.34199479366
497.885673416326	-663.034572443750	332.677312093750	-74.4188648500000
1033.67091988025	-1124.85381286782	408.726035584526	-49.5696850121021
10782.4399433266	-13005.0298918015	5234.58604338040	-703.009068965912

E_n	F_n	G_n	H_n	r_n
19.7590956539449	-1.10929154438237	8.583068847656250E-3	0.0	4.25270034968853
-42.2614091514405	6.18967940283576	-0.329017639160156	0.0	3.18798422753811
3852.65707605729	-1773.50698078752	352.122068405151	-26.2997150421143	3.08288478612900
6.25419990000000	0.0	0.0	0.0	2.83075976371765
0.0	0.0	0.0	0.0	2.72917079940438
0.0	0.0	0.0	0.0	2.46177387237549

A'_n	B'_n	C'_n	D'_n
0.176113968245774	-4.42727651433102	6.08596367085100	-3.31627185619130
-9.01097257391517	17.7652430017672	-14.0448182382562	5.85262981750376
2941.47663526372	-4976.29995214059	3363.92566298462	-1135.68505574601
-506.899715533763	1117.19138346861	-1025.00865314071	501.406917325721
170.584208417048	-191.839109698533	72.0025483634399	-9.01365494002994
98.5798682207654	-105.456860917279	37.4588301923518	-4.40904970411985

Potential parameters.

E_n'	F_n'	G_n'	H_n'	r_n'
0.889234910474537	-0.117663809722679	6.163730456134172E-3	0.0	4.44999316573143
-1.36849120887594	0.170647289763123	-8.865704319423323E-3	0.0	3.26985955238342
191.481369497020	-12.8985156307958	0.0	0.0	3.14614844381809
-137.946827388616	20.2386766904903	-1.23706225652103	0.0	2.79194164276123
0.0	0.0	0.0	0.0	2.66148281335831
0.0	0.0	0.0	0.0	2.50066447257996

Potential parameters.

N	N'	r_{N+1}	$r_{N'+1}'$	A
6	6	0.0	0.0	10.3632760643959