# Supplementary material: Relation between core polarization curvature and Peierls stress in screw dislocations in bcc Ta - a new criterion for materials design

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## I. SUPPLEMENTARY TABLES

The following Tables contain force field parameters used in the calculations. A detailed description of the qEAM Force Field can be found in [1].

## REFERENCES


[1] Alejandro Strachan, Tahir Çağın, Oğuz Gülseren, Sonali Mukherjee, Ronald E. Cohen, and William A. Goddard III.

## TABLES

TABLE I. qEAM1 paramters for Ta: two body term. The units of $b_i$ are eV$\AA^{-(4+i)}$.

| $r_m$ $\AA$ | $b_0$ | $b_1$ | $b_2$ | $b_3$ |
|---|---|---|---|---|
| 4.81253968 | 6.50281587 | -11.26455130 | 8.01451544 | -2.97299223 |
| $b_4$ | $b_5$ | $b_6$ | $b_7$ | - |
| 0.60004206 | -0.06222106 | 0.00258801 | -0.00000504 | - |

TABLE II. qEAM1 paramters for Ta: embedding energy

| $a_1$ | $a_2$ | $\alpha$ (1/Å) | $\beta$ | $a_0$ (Å) |
|---|---|---|---|---|
| 0.07293238 | 0.15781672 | 21.79609053 | 7.79329426 | 3.32389219 |
| $E_{coh}$(eV) | $B_T$ (GPa) | $\lambda$ | $f_3$ | $f_4$ |
| 8.15420437 | 183.035404 | 0.20782789 | -0.00717801 | -0.00112257 |

TABLE III. qEAM2 paramters for Ta: two body term. The units of $b_i$ are eV$\AA^{-(4+i)}$.

| $r_m$ $\AA$ | $b_0$ | $b_1$ | $b_2$ | $b_3$ |
|---|---|---|---|---|
| 4.79242711 | 6.52551016 | -11.30044468 | 8.01967789 | -2.96545156 |
| $b_4$ | $b_5$ | $b_6$ | $b_7$ | - |
| 0.59898785 | -0.06248460 | 0.00258681 | -0.00000507 | - |

TABLE IV. qEAM2 paramters for Ta: embedding energy

| $a_1$ | $a_2$ | $\alpha$ (1/Å) | $\beta$ | $a_0$ (Å) |
|---|---|---|---|---|
| 0.08391111 | 0.09548221 | 21.14074773 | 6.21703450 | 3.33099929 |
| $E_{coh}$(eV) | $B_T$ (GPa) | $\lambda$ | $f_3$ | $f_4$ |
| 8.56749534 | 188.279315 | 0.20937018 | -0.01288280 | -0.00142592 |

TABLE V. qEAM3 paramters for Ta: two body term. The units of $b_i$ are eV$\AA^{-(4+i)}$.

| $r_m$ $\AA$ | $b_0$ | $b_1$ | $b_2$ | $b_3$ |
|---|---|---|---|---|
| 4.85897615 | 6.50850868 | -11.27481642 | 8.00376899 | -2.96587445 |
| $b_4$ | $b_5$ | $b_6$ | $b_7$ | - |
| 0.60125545 | -0.06285189 | 0.00258051 | -0.00000506 | - |

TABLE VI. qEAM3 paramters for Ta: embedding energy

| $a_1$ | $a_2$ | $\alpha$ (1/Å) | $\beta$ | $a_0$ (Å) |
|---|---|---|---|---|
| 0.07669052 | 0.08923403 | 20.91292691 | 6.16313792 | 3.34989236 |
| $E_{coh}$(eV) | $B_T$ (GPa) | $\lambda$ | $f_3$ | $f_4$ |
| 8.41851807 | 184.020690 | 0.20815613 | -0.02619576 | -0.00164245 |

TABLE VII. qEAM4 paramters for Ta: two body term. The units of $b_i$ are eV$\AA^{-(4+i)}$.

| $r_m$ $\AA$ | $b_0$ | $b_1$ | $b_2$ | $b_3$ |
|---|---|---|---|---|
| 4.87104903 | 6.50027489 | -11.28228299 | 7.99669670 | -2.95979593 |
| $b_4$ | $b_5$ | $b_6$ | $b_7$ | - |
| 0.60004490 | -0.06281829 | 0.00257886 | -0.00000506 | - |

TABLE VIII. qEAM4 paramters for Ta: embedding energy

| $a_1$ | $a_2$ | $\alpha$ (1/Å) | $\beta$ | $a_0$ (Å) |
|---|---|---|---|---|
| 0.07700159 | 0.12682860 | 20.66912952 | 7.11561275 | 3.32366889 |
| $E_{coh}$(eV) | $B_T$ (GPa) | $\lambda$ | $f_3$ | $f_4$ |
| 8.15639422 | 184.488208 | 0.20705664 | -0.02490743 | -0.00152505 |