Table 1. The 2NN MEAM parameters for Nb, Mo, T, W, and V atoms.

| | $E_C$ | $r_e$ | $B$ | $A$ | $\beta^{(0)}$ | $\beta^{(1)}$ | $\beta^{(2)}$ | $\beta^{(3)}$ | $t^{(1)}$ | $t^{(2)}$ | $t^{(3)}$ | $C_{max}$ | $C_{min}$ | d |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Nb | 7.47 | 2.860 | 1.73 | 0.72 | 5.08 | 1.0 | 2.5 | 1.0 | 1.7 | 2.8 | -1.6 | 2.80 | 0.36 | 0.00 |
| Mo | 6.81 | 2.725 | 2.65 | 0.46 | 7.03 | 1.0 | 1.0 | 1.0 | 0.5 | 3.1 | -7.5 | 2.80 | 0.64 | 0.00 |
| Ta | 8.09 | 2.860 | 1.94 | 0.67 | 4.49 | 1.0 | 1.0 | 1.0 | 1.7 | 2.1 | -3.2 | 2.80 | 0.25 | 0.00 |
| W | 8.66 | 2.740 | 3.14 | 0.40 | 6.54 | 1.0 | 1.0 | 1.0 | -0.6 | 0.3 | -8.7 | 2.80 | 0.49 | 0.00 |
| V | 5.30 | 2.625 | 1.57 | 0.73 | 4.74 | 1.0 | 2.5 | 1.0 | 3.3 | 3.2 | -2.0 | 2.80 | 0.49 | 0.00 |

Table 2. The cross-element parameters of 2NN MEAM potential for Nb, Mo, T, W, and V atoms in the LAMMPS format.

| | NbMo | NbW | NbTa | NbV | MoW | MoTa | MoV | WTa | WV | TaV |
|---|---|---|---|---|---|---|---|---|---|---|
| Reference | B2 | B2 | B2 | B2 | B2 | B2 | B2 | B2 | B2 | B2 |
| Ec | 7.201 | 8.082 | 7.758 | 6.274 | 7.737 | 7.380 | 6.076 | 8.277 | 7.001 | 6.616 |
| $r_e$ | 2.806 | 2.816 | 2.904 | 2.761 | 2.752 | 2.831 | 2.673 | 2.839 | 2.682 | 2.781 |
| α | 5.760 | 5.576 | 5.222 | 4.890 | 5.715 | 6.087 | 5.870 | 5.696 | 5.508 | 5.251 |
| attract | -0.100 | -0.100 | -0.007 | -0.100 | -0.050 | -0.100 | -0.100 | -0.100 | 0.100 | -0.100 |
| repuls | 0.011 | 0.010 | 0.062 | 0.035 | 0.080 | 0.005 | 0.002 | 0.025 | 0.100 | 0.054 |
| $\rho_0^A/\rho_0^B$ | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 | 1.000 |
| $C_{min}$(A-B-A) | 0.102 | 0.809 | 0.933 | 0.281 | 0.100 | 0.990 | 0.455 | 0.737 | 0.100 | 0.630 |
| $C_{min}$(B-B-A) | 0.100 | 0.125 | 0.100 | 0.211 | 0.651 | 0.455 | 0.578 | 0.639 | 0.629 | 0.583 |
| $C_{min}$(A-A-B) | 0.100 | 0.753 | 0.217 | 0.625 | 0.408 | 0.411 | 0.528 | 0.269 | 0.100 | 0.100 |
| $C_{min}$(A-B-B) | 0.990 | 0.434 | 0.153 | 0.990 | 0.100 | 0.990 | 0.254 | 0.990 | 0.100 | 0.955 |
| $C_{max}$(A-B-A) | 2.000 | 2.438 | 2.463 | 2.454 | 2.000 | 2.800 | 2.634 | 2.799 | 2.000 | 2.190 |
| $C_{max}$(B-B-A) | 2.102 | 2.231 | 2.130 | 2.507 | 2.154 | 2.205 | 2.245 | 2.107 | 2.230 | 2.228 |
| $C_{max}$(A-A-B) | 2.272 | 2.257 | 2.355 | 2.033 | 2.199 | 2.234 | 2.162 | 2.072 | 2.000 | 2.272 |

Table 3. The parameter sets of $C_{min}$ and $C_{max}$ for ternary elements in the LAMMPS format.

| | | $C_{min}$ | $C_{max}$ |
|---|---|---|---|
| Nb-Mo-W | (Nb-Mo-W) | 0.652 | 2.565 |
| | (Nb-W-Mo) | 0.584 | 2.192 |
| | (Mo-W-Nb) | 0.990 | 2.800 |
| Nb-Mo-Ta | (Nb-Mo-Ta) | 0.425 | 2.303 |
| | (Nb-Ta-Mo) | 0.990 | 2.409 |
| | (Mo-Ta-Nb) | 0.100 | 2.676 |
| Nb-Mo-V | (Nb-Mo-V) | 0.694 | 2.712 |
| | (Nb-V-Mo) | 0.561 | 2.800 |
| | (Mo-V-Nb) | 0.685 | 2.167 |
| Nb-W-Ta | (Nb-W-Ta) | 0.100 | 2.513 |
| | (Nb-Ta-W) | 0.985 | 2.487 |
| | (W-Ta-Nb) | 0.990 | 2.800 |
| Nb-W-V | (Nb-W-V) | 0.693 | 2.477 |
| | (Nb-V-W) | 0.915 | 2.633 |
| | (W-V-Nb) | 0.778 | 2.389 |
| Nb-Ta-V | (Nb-Ta-V) | 0.752 | 2.365 |
| | (Nb-V-Ta) | 0.693 | 2.233 |
| | (Ta-V-Nb) | 0.657 | 2.698 |
| Mo-W-Ta | (Mo-W-Ta) | 0.801 | 2.512 |
| | (Mo-Ta-W) | 0.257 | 2.800 |
| | (W-Ta-Mo) | 0.990 | 2.800 |
| Mo-W-V | (Mo-W-V) | 0.990 | 2.800 |
| | (Mo-V-W) | 0.858 | 2.077 |
| | (W-V-Mo) | 0.479 | 2.080 |
| Mo-Ta-V | (Mo-Ta-V) | 0.771 | 2.254 |
| | (Mo-V-Ta) | 0.368 | 2.176 |
| | (Ta-V-Mo) | 0.364 | 2.681 |
| W-Ta-V | (W-Ta-V) | 0.990 | 2.578 |
| | (W-V-Ta) | 0.785 | 2.778 |
| | (Ta-V-W) | 0.763 | 2.800 |

Table 4. The models of single crystal and polycrystalline $Nb_{20.6}Mo_{21.7}Ta_{15.6}W_{21.1}V_{21.0}$ RHEAs for the heating simulation.

| Grain size (nm) | Grain number | Atom number |
|---|---|---|
| single crystal | X | 1,024,000 |
| 25.3 | 4 | 4,113,488 |
| 20.1 | 8 | 4,112,402 |
| 15.6 | 17 | 4,113,753 |
| 10.0 | 65 | 4,113,509 |
| 5.2 | 450 | 4,113,688 |