

Table I. Properties calculated with EAM potentials developed in the present study.

Property	MCu1	MCu2	MCu3	MCu4	MCu5	MCu6	MCu7
a (fcc) (Å)	3.639	3.639	3.639	3.639	3.639	3.638	3.638
$E_{\text{coh}}$ (fcc) (eV/atom)	-3.425	-3.416	-3.423	-3.429	-3.428	-3.410	-3.427
$E_{\text{f}}^{\text{v}}$ (fcc) (eV/atom)	1.11	1.12	1.11	1.10	1.07	1.05	1.03
$E_{\text{f}}^{\text{m}}$ (fcc) (eV/atom)	0.91	0.91	0.92	0.93	0.95	0.98	1.00
$E_{\text{D}}$ (fcc) (eV/atom)	2.01	2.03	2.02	2.02	2.02	2.03	2.02
$C_{11}$ (GPa)	173	174	174	175	175	177	178
$C_{12}$ (GPa)	128	127	127	127	127	126	125
$C_{44}$ (GPa)	84	84	84	84	84	83	83
$E_{\text{f}}^{\text{i}} (<100> \text{fcc})$ (eV/atom)	2.82	2.81	2.81	2.82	2.82	2.82	2.81
$\gamma (<100> \text{fcc})$ (meV/Å <sup>2</sup> )	79	78	75	72	66	58	53
$\gamma (<110> \text{fcc})$ (meV/Å <sup>2</sup> )	83	82	80	77	72	65	60
$\gamma (<111> \text{fcc})$ (meV/Å <sup>2</sup> )	68	67	64	61	55	47	41
$E^{\text{SF}}$ (meV/Å <sup>2</sup> )	0.91	1.55	2.76	3.85	5.91	9.35	11.65
$E^{\text{CTB}}$ energy (meV/Å <sup>2</sup> )	0.46	0.78	1.38	1.92	2.96	4.68	5.82
$\Delta E_{\text{fcc} \rightarrow \text{bcc}}$ (eV/atom)	0.040	0.041	0.041	0.042	0.043	0.045	0.046
$\Delta E_{\text{fcc} \rightarrow \text{hcp}}$ (eV/atom)	0.0026	0.0044	0.0080	0.0109	0.0168	0.0266	0.0331
$T_{\text{m}}$ (fcc, K)	1349	1352	1353	1355	1356	1353	1351
$\Delta H_{\text{m}}$ (fcc) (eV/atom)	0.130	0.130	0.130	0.129	0.129	0.127	0.127
$\Delta V_{\text{m}}$ (fcc) (%)	3.5	3.4	3.4	3.4	3.5	3.5	3.5