Metal	a (Å)	E <sub>coh</sub> (eV/atom)	E <sub>f</sub> <sup>v</sup> (eV/atom)	E <sub>f</sub> <sup>v</sup> (eV/atom)	E <sub>f</sub> (eV/atom)	C <sub>11</sub> (GPa)	C <sub>12</sub> (GPa)	C <sub>44</sub> (GPa)
			unrelaxed	relaxed				
Ag	4.085999	2.96744	1.0427	1.022	<100>: 4.077	124.06	93.44	46.13
Au	4.078000	3.78905	1.0127	0.962	<100>: 4.403	186.12	156.99	41.95
Cu	3.614999	3.51935	1.2196	1.189	<100>: 3.624	168.49	121.33	75.31
Fe	2.866500	4.31600	1.8901	1.705	<110>: 4.884	243.39	145.03	116.00
W	3.165200	8.91000	3.7754	3.676	<110>: 10.300	532.58	204.98	163.17
Ni	3.524220	4.45900	1.4599	1.424	<100>: 3.881	261.22	150.81	131.70