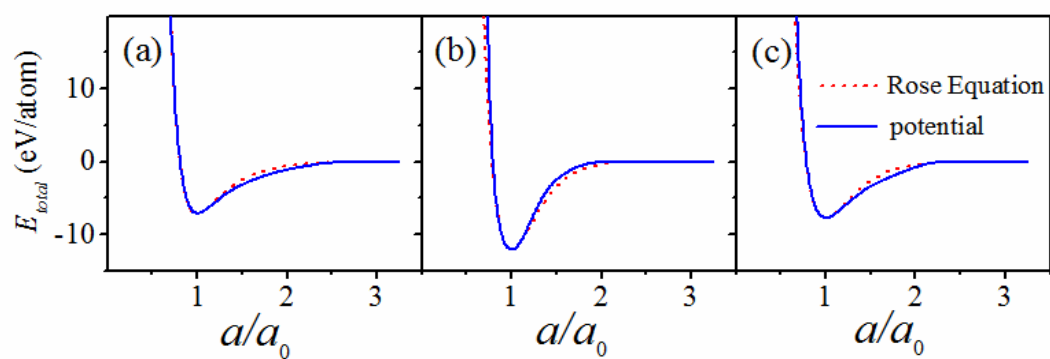


### Figure captions

**Figure S1.** Total potential energy curve with the variation of lattice constant derived from the LREP (blue solid line) and Rose Equation (red dot line) for Ni, Nb, and Ti metals.



**Figure S2.** Total potential energy curve with the variation of lattice constant derived from the LREP (blue solid line) and Rose Equation (red dot line) for B2 NiNb, L1<sub>2</sub> NiNb<sub>3</sub>, L1<sub>2</sub> Ni<sub>3</sub>Nb, B2 NiTi, L1<sub>2</sub> NiTi<sub>3</sub>, L1<sub>2</sub> Ni<sub>3</sub>Ti, B2 NbTi, L1<sub>2</sub> NbTi<sub>3</sub>, L1<sub>2</sub> Nb<sub>3</sub>Ti.

