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.

![Graph showing potential energy curves for Ni, Nb, and Ti]
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, L12 NiNb3, L12 Ni3Nb, B2 NiTi, L12 NiTi3, L12 Ni3Ti, B2 NbTi, L12 NbTi3, L12 Nb3Ti.