Output File Description

The first few slides are basically the same as your input file except the ratios are normalized.

With the “Start of Predicted Data”, the data is written in a csv manner with a column header of:

psA, psB, psC,
e1,e2,e3,e4,e5,
V_ave,b_ave,
E_ave,mu_ave,nu_ave,
sum_cnVn^2_b6,
Ty0_tensile,Delta_Eb,Delta_sigma_ss

psA/psB/psC: these three values are compositions in the pseudo-ternary diagram

e1,e2,e3,e4,e5,… are the names of your input elements, and there corresponding compositions.

V_ave: the compositionally weighted atomic volume, using the unit of Å.

$$\bar{V} = \sum_n c_n V_n$$

b_ave: the compositionally weighted burgers vector, using the unit of Å.

$$\bar{b} = \sum_n c_n b_n$$

E_ave: the compositionally weighted Young’s Modulus, using the unit of GPa.

$$\bar{E} = \sum_n c_n E_n$$

mu_ave: the compositionally weighted Shear Modulus, using the unit of GPa.

$$\bar{\mu} = \sum_n c_n \mu_n$$

nu_ave: the compositionally weighted Poisson's ratio.

$$\bar{\nu} = \sum_n c_n \nu_n$$

sum_cnVn^2_b6: a misfit parameter to describe lattice distortion

$$\frac{\sum_n c_n V_n^2}{\bar{b}^6}$$

Ty0_tensile: predicted solid solution strengthening at 0K

$$\tau_{y0} = 0.01785\alpha^{-1/3}\bar{\mu}(\frac{1+\bar{\nu}}{1-\bar{\nu}})^{4/3}[\frac{\sum_n c_n \Delta V_n^2}{b^6}]^{2/3}$$

Delta_Eb: ΔE_b, predicted thermal activation energy barriers of dislocation glide

$$\Delta E_b = 1.5618\alpha^{1/3}\bar{\mu}b^3(\frac{1+\bar{\nu}}{1-\bar{\nu}})^{2/3}[\frac{\sum_n c_n \Delta V_n^2}{b^6}]^{1/3}$$

Delta_sigma_ss: $\Delta\sigma_{ss}$, predicted solid solution strengthening at finite temperature

$$\tau_y(T,\dot{\varepsilon}) = \tau_{y0}[1-(\frac{kT}{\Delta E_b} ln\frac{\dot{\varepsilon}_0}{\dot{\varepsilon}})^{\frac{2}{3}}]$$

$$\Delta\sigma_{ss} = 3.06\tau_y(T,\dot{\varepsilon})$$