1. Molar Volume Database of High Entropy Alloys (HEAs)

PanHEA2020_MV is a molar volume database for HEA alloys, which is compatible with the PanHEA2020_TH thermodynamic database and suitable for the simulation of thermophysical properties of HEAs, such as density, thermal expansion, solidification shrinkage etc.

1.1 Components (15)

Al	C	Co	Cr	Cu	Fe	Li	Mg	Mn	Mo
Ni	Si	Ti	V	Zr					

1.2 Phases

The current molar volume database covers all 434 phases assessed in the PanHEA2020_TH database.

1.3 Database Validation

The simulated linear thermal expansion coefficient vs. temperature of the CoCrFeNi alloy is shown below to validate the current PanHEA2020_MV database.

Figure 1.1 shows the calculated linear thermal expansion coefficient (CTE) for the CoCrFeNi alloy, which is in good agreement with the experimental measurements in the literature [1]. Figure 1.2 shows calculated density contour mapping of the Co-Cr-Fe-20Mn-20Ni (at.%) at 1000°C. One can see that the stable phase regions include Fcc single phase field and Bcc+Fcc two-phase field in this isothermal section. The density of these HEAs at 1000°C will vary between 7.55~8.35 g/cm^{3}.

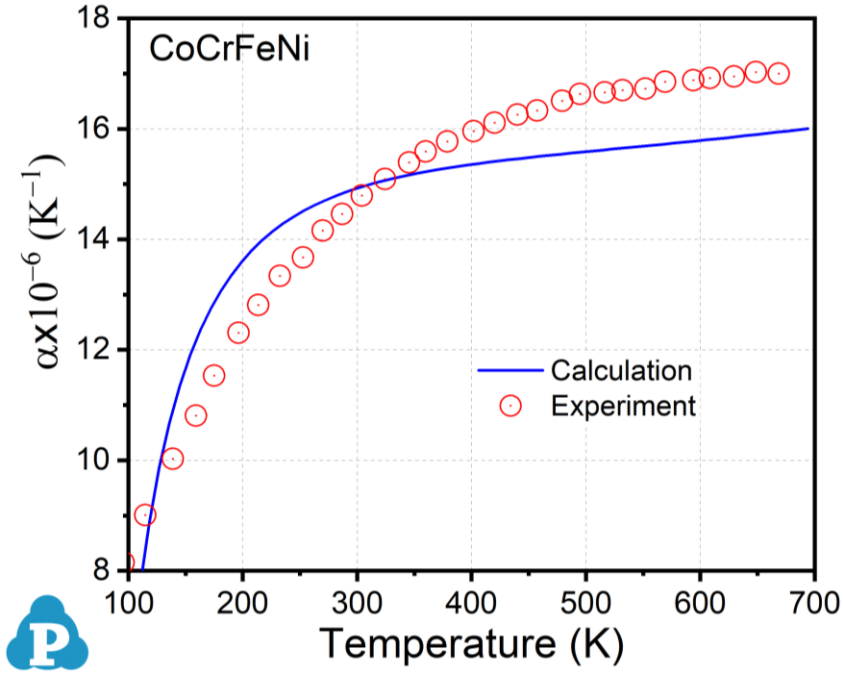

Figure 1.1: Calculated linear thermal expansion coefficient of the CoCrFeNi HEA with experimental data from ref. [1]

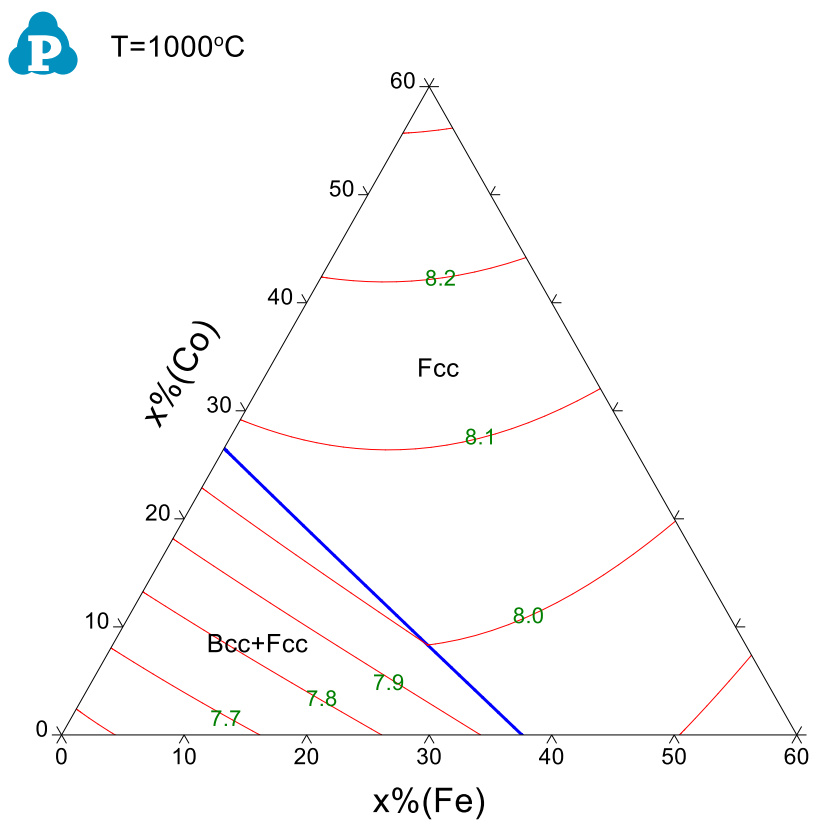

Figure 1.2: Density contour mapping of Co-Cr-Fe-20Mn-20Ni (at.%) at 1000°C

1.4 References

1. Laplanche, G., et al., *Elastic moduli and thermal expansion coefficients of medium-entropy subsystems of the CrMnFeCoNi high-entropy alloy.* Journal of Alloys and Compounds, 2018. **746**: p. 244-255.