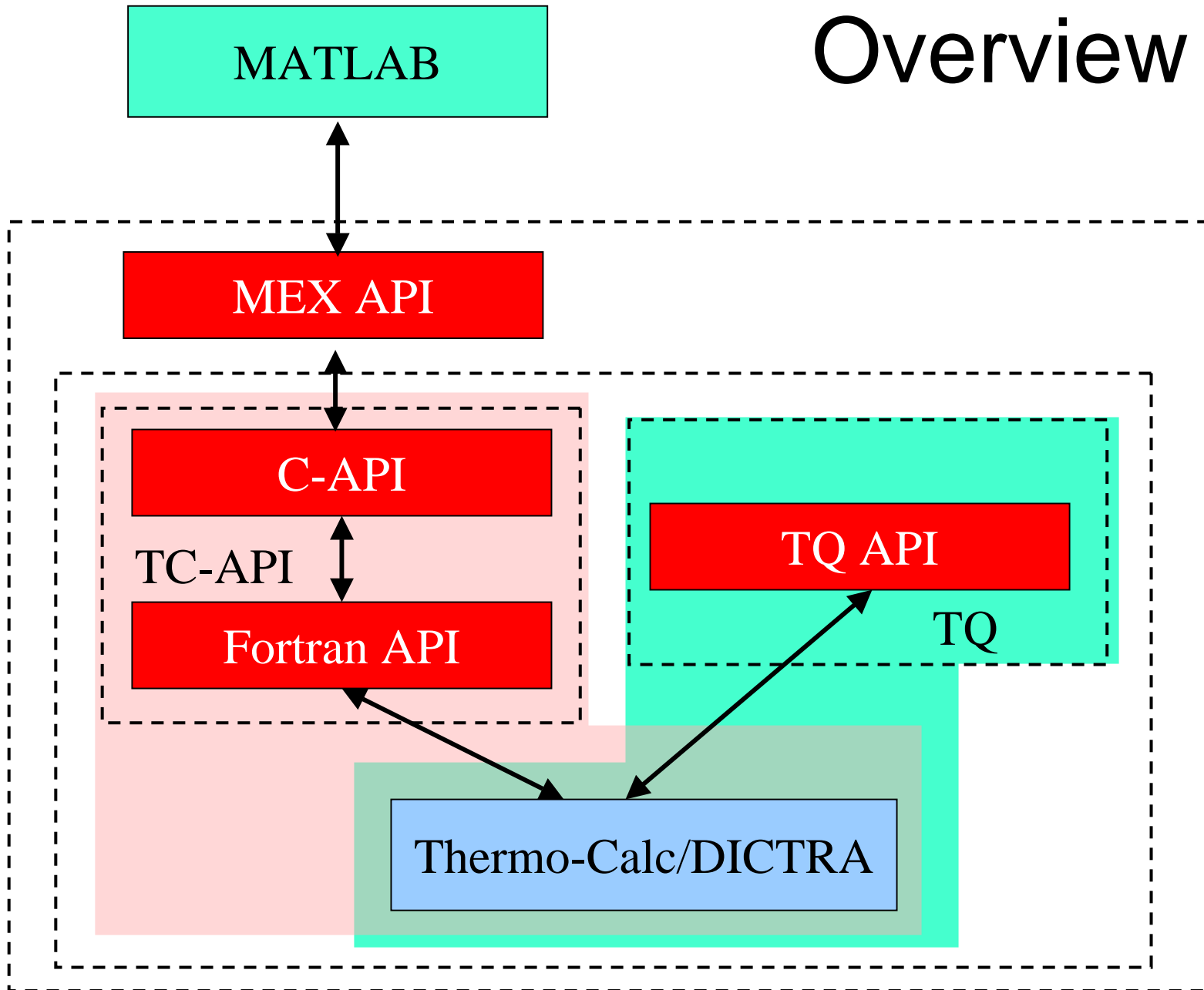


Overview



Optimization

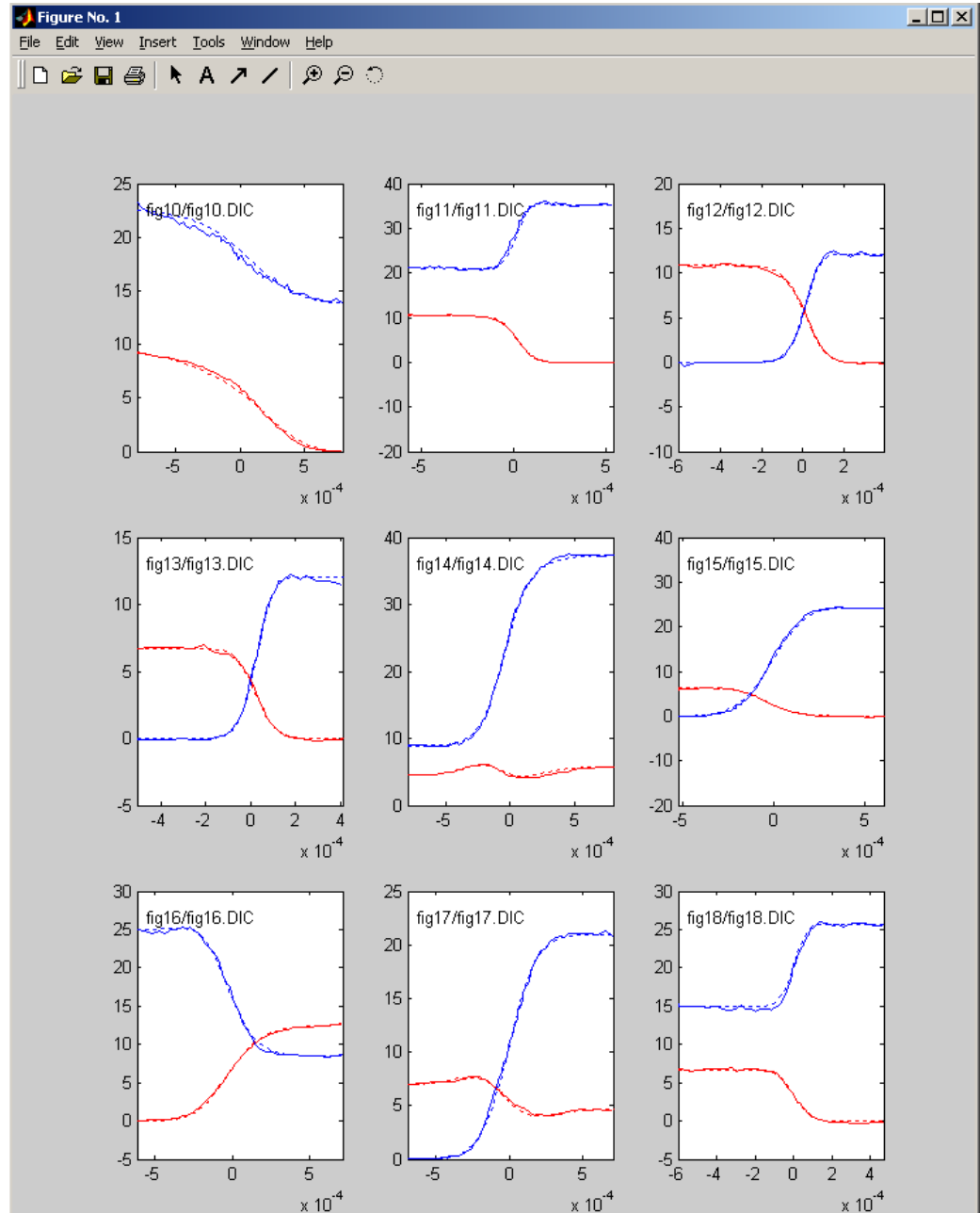
Reassessment of the interactions in Al-Cr-Ni
from the work Enström et. al

Experimental information from Nesbitt et. al

Al-Cr-Ni

Simultaneous optimization in ternary system

9 different diffusion couples



Optimization results

AL

MQ(FCC_A1&AL,AL,CR:VA;0)	+335000	-12517
MQ(FCC_A1&AL,AL,NI:VA;0)	-41300-91.2*T	-147583
MQ(FCC_A1&AL,CR,NI:VA;0)	-53200	-54802

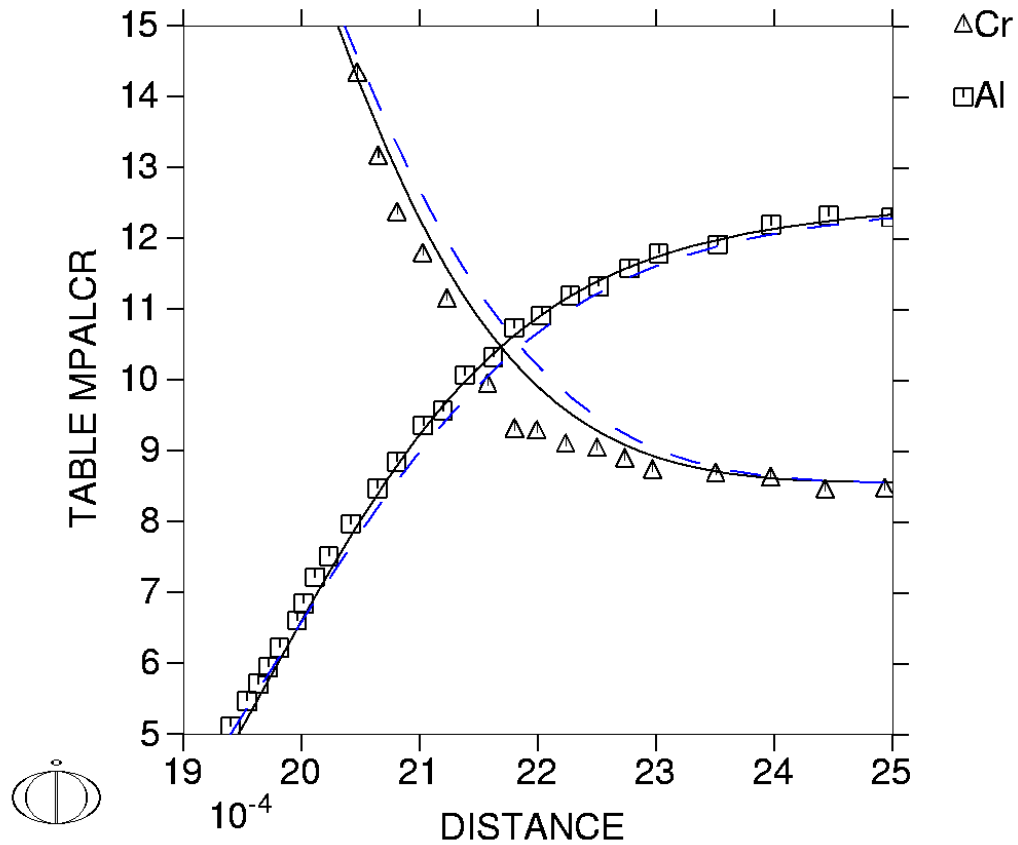
CR

MQ(FCC_A1&CR,CR,AL:VA;0)	+487000	+63451
MQ(FCC_A1&CR,CR,NI:VA;0)	-68000	-74664
MQ(FCC_A1&CR,AL,NI:VA;0)	-118000	-69668

NI

MQ(FCC_A1&NI,NI,AL:VA;0)	-113000+65.5*T	-119016
MQ(FCC_A1&NI,NI,CR:VA;0)	-81000	-21009
MQ(FCC_A1&NI,AL,CR:VA;0)	+211000	+342636

Example of fit to data



Result

- Minor improvements on fit to experimental data
- No temperature dependency on the parameters

Problems ?

- Independent mobilities
- Thermodynamic data
- Phase descriptions