# Modelling of Dissimilar Metal Welds

This model is developed to calculate the concentration profiles of alloying elements across the welding line of two different alloys. The purpose of this note is to give a brief description of this model, as well as to check how it performs against the work of other researchers, e.g. Campbell et al. [1,2].

The solution to the diffusion problem is in the form of error functions given below, which describe the concentration profile across the welding line, $c^{\alpha}$ and $c^{\beta}$, as a function of holding time $t$ at a given temperature:

$$\frac{c^{\alpha}-c^{\alpha\beta}}{c^{\alpha 0}-c^{\alpha\beta}} = -\mathrm{erf}\left(\frac{x}{2\sqrt{D^{\alpha}t}}\right) \quad (1a)$$

$$\frac{c^{\beta}-c^{\beta\alpha}}{c^{\beta 0}-c^{\beta\alpha}} = \mathrm{erf}\left(\frac{x}{2\sqrt{D^{\beta}t}}\right) \quad (1b)$$

where $c^{\alpha 0}$ and $c^{\beta 0}$ are the initial concentration of a given element in the two alloys, and $c^{\alpha\beta}$ and $c^{\beta\alpha}$ are the concentrations of this element at either side of the $\alpha/\beta$ interface. They are assumed equal to the mean value of $c^{\alpha 0}$ and $c^{\beta 0}$ in the current model. $D^{\alpha}$ and $D^{\beta}$ are the diffusion coefficient of this element on the two sides.

Experimental concentration profiles of four diffusion couples were reported for René-95/René-88, René-95/IN718, IN100/IN718 and IN100/René-88 in Ref. [1]. The welded assembly underwent a hot isostatic-pressing at 140 MPa, 1150°C for 4 hours and then heat-treated at 1150°C for 1000 hours. The compositions of these alloys are listed in Table 1. In addition to their nominal compositions, the measured compositions are also provided, which are the average of 10 measurements near the outer edge of each alloy, i.e. well beyond the diffusion distance.

Table 1. Nominal and measured average compositions of the four alloys (mass fraction).

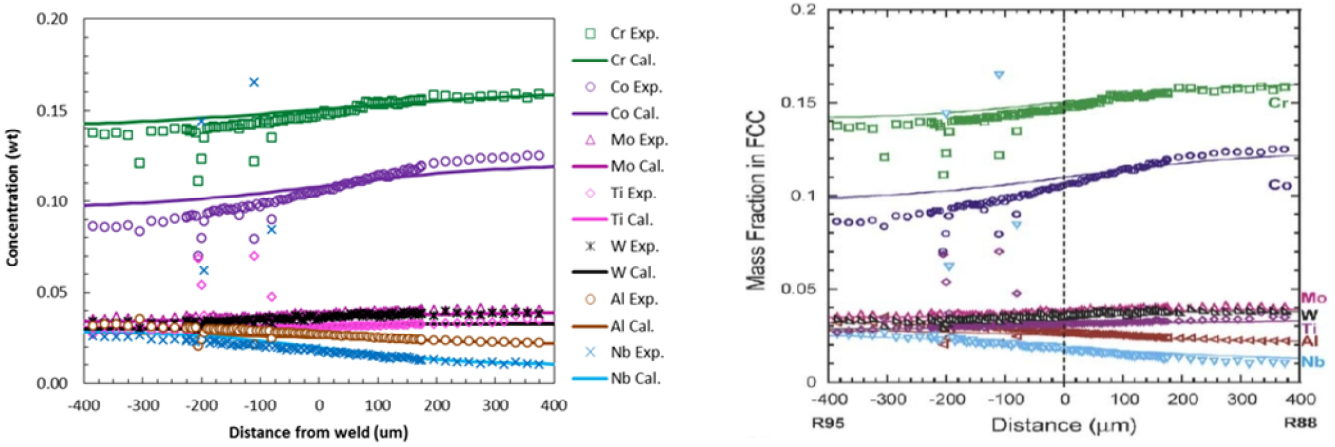
| | René-88 | | René-95 | | IN718 | | IN100 | |
|---|---|---|---|---|---|---|---|---|
| | Nominal | Measured average | Nominal | Measured average | Nominal | Measured average | Nominal | Measured average |
| Ni | 0.557 | 0.0577 | 0.624 | 0.606 | 0.53 | 0.547 | 0.604 | 0.560 |
| Al | 0.021 | 0.020 | 0.035 | 0.030 | 0.005 | 0.004 | 0.055 | 0.044 |
| Co | 0.13 | 0.12 | 0.08 | 0.096 | – | – | 0.15 | 0.184 |
| Cr | 0.16 | 0.16 | 0.13 | 0.14 | 0.19 | 0.183 | 0.10 | 0.128 |
| Fe | – | – | – | – | 0.185 | 0.181 | – | – |
| Mo | 0.04 | 0.039 | 0.035 | 0.034 | 0.035 | 0.029 | 0.03 | 0.033 |
| Nb | 0.007 | 0.011 | 0.035 | 0.030 | 0.051 | 0.046 | – | – |
| Ti | 0.037 | 0.036 | 0.037 | 0.031 | 0.009 | 0.0010 | 0.047 | 0.043 |
| V | – | – | – | – | – | – | 0.01 | 0.007 |
| W | 0.04 | 0.033 | 0.035 | 0.030 | – | – | – | – |
| C | 0.0003 | 0.00052[a] | 0.0003 | 0.00053[a] | 0.0008 | 0.00022[a] | 0.0016 | 0.00076[a] |
| B | 0.00015 | 0.00016[a] | 0.00015 | 0.0001[a] | – | – | 0.0014 | 0.0001[a] |
| Zr | 0.0003 | 0.00045[a] | 0.0003 | 0.0005[a] | – | – | 0.0006 | 0.0006[a] |

[a] Measured by wet chemical analysis.

These researchers also carried out simulations using DICTRA [3] coupled with the Ni-data thermodynamic database of Thermotech (the same database as that of JMatPro) and their own Ni diffusion mobility database [2]. We managed to get hold of the measured concentration profiles for the René-95/René-88 diffusion couple, which merits a detailed comparison, Figs. 1 and 2. As can be seen from Fig. 1 that calculations from the two models are rather similar, and both show good agreement with the measured profiles, except for the

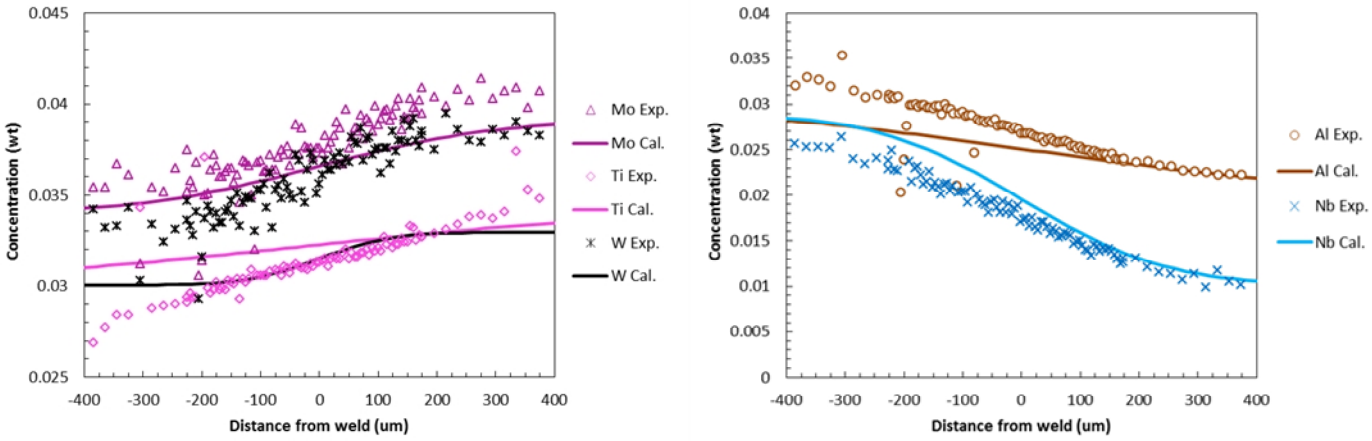
[1] C.E. Campbell, J.C. Zhao and M.F. Henry, Examination of Ni-base superalloy diffusion couples containing multiphase regions, Materials Science and Engineering A 407 (2005) 135–146.
[2] C.E. Campbell, J.C. Zhao and M.F. Henry, Comparison of experimental and simulated multicomponent Ni-base superalloy diffusion couples, Journal of Phase Equilibria and Diffusion 25(1) (2004) 6–15.
[3] A. Borgenstam, A. Engström, L. Höglund and J. Ågren, DICTRA, a tool for simulation of diffusional transformations in alloys, Journal of phase equilibria 21(3) (2000) 269–280.

Co profile on the René-95 side. The lower than predicted Co concentration on the René-95 side indicates that the actual Co concentration may be lower than the measured average composition (0.096 mass fraction) used in the calculation. If the nominal Co amount (0.08 in Table 1) is used, a much better agreement would be achieved. The observed experimental scatter is due to the fact that the measured composition is for a mixture of gamma and gamma prime.




(a) (b)

Fig. 1. Comparison of measured composition profiles to calculated gamma composition profiles for René-95/René-88 from (a) the JMatPro model, and (b) the DICTRA model [1].

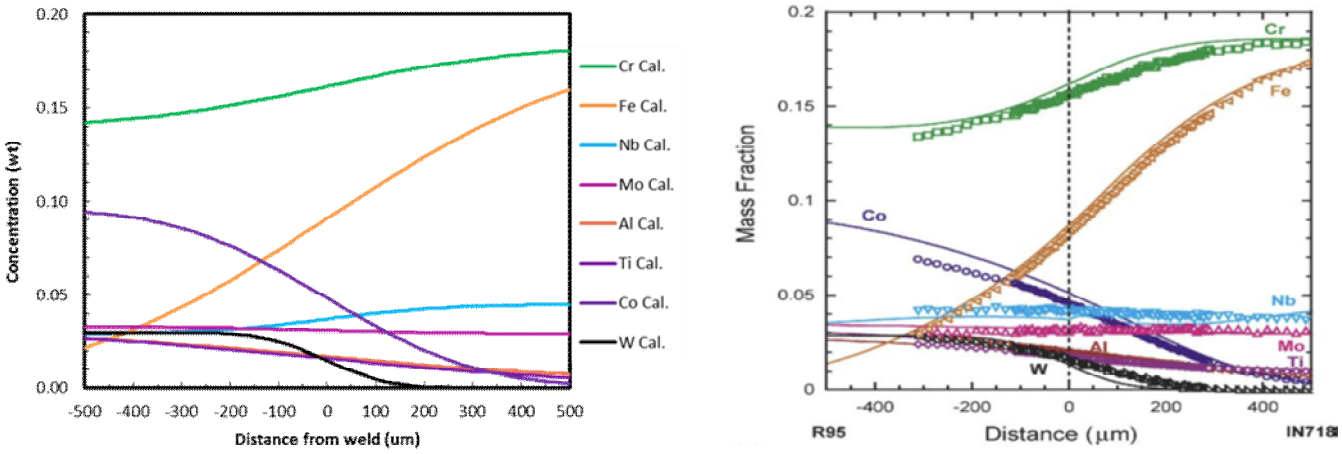



(a) (b)

Fig. 2. Comparison of measured composition profiles to calculated gamma composition profiles for René-95/René-88 from the JMatPro model for (a) Mo, Ti and W, and (b) Al and Nb.

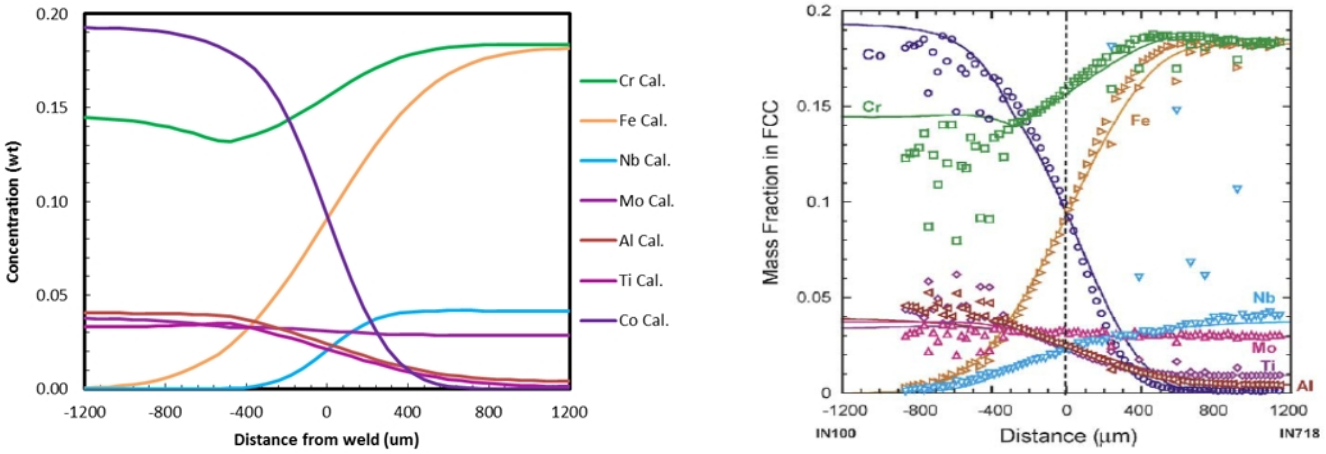
Fig. 2 shows comparisons for elements of minor amounts between the JMatPro model and the measured composition profiles. There seems to be large discrepancies for the W profile, Fig. 2(a). Again this should be primarily due to the choice of composition values used in the calculation. The mass fractions of W in alloys René-95 and René-88 are set as the "measured average" values in Table 1, i.e. 0.030 vs 0.033, respectively. If the nominal values, i.e. 0.035 vs 0.040, are used instead, the calculated W profile would be in good agreement with the measured one. Similarly the Al profile on the René-95 side can be improved if its nominal 0.035 mass fraction is used instead of the measured average 0.030. The situations with Nb and Ti are a bit different as they are both MC-carbide forming elements, so their calculations are not only affected by their amounts but also the amount of C used in the calculations.

As we do not have the exact measurements of the concentration profiles for other diffusion couples, we have put the JMatPro model calculations side by side with those plots of Campbell et al. [1], which contain experimental profiles and DICTRA simulations, for comparison, Figs. 3-5. Both models seem to give similar results, and both calculations are in reasonable agreement with the measured profiles.



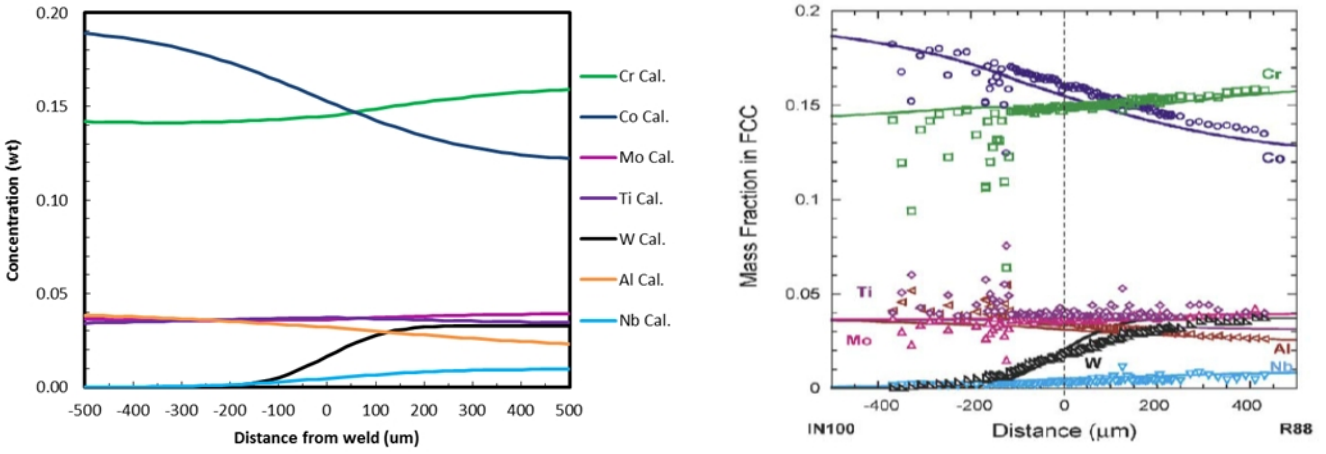

(a) (b)

Fig. 3. Comparison of measured composition profiles to calculated gamma composition profiles for René-95/IN718 from (a) the current JMatPro model, and (b) the DICTRA model [1].




(a) (b)

Fig. 4. Comparison of measured composition profiles to calculated gamma composition profiles for IN100/IN718 from (a) the current JMatPro model, and (b) the DICTRA model [1].

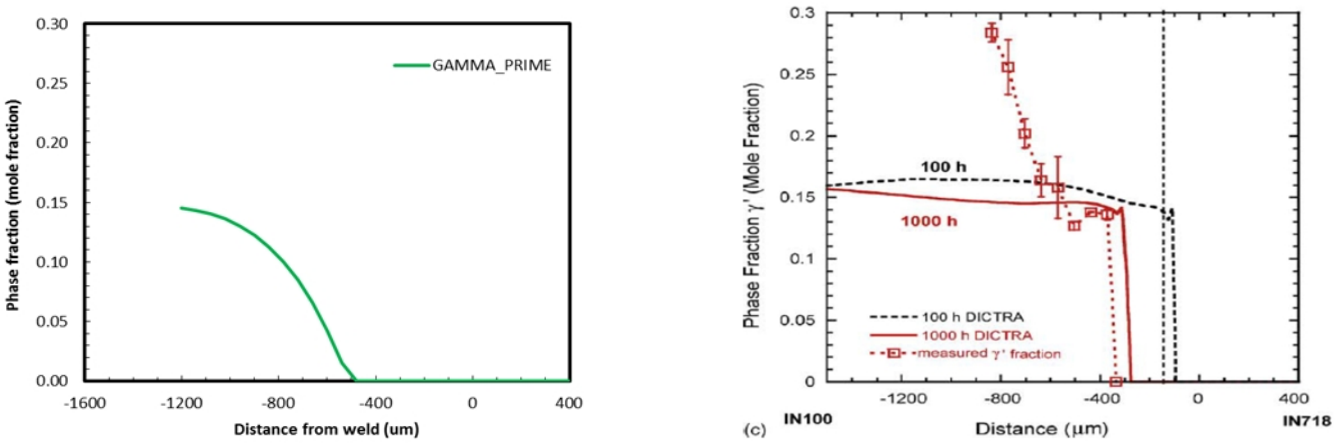



(a) (b)

Fig. 5. Comparison of measured composition profiles to calculated gamma composition profiles for IN100/René-88 from (a) the current JMatPro model, and (b) the DICTRA model [1].

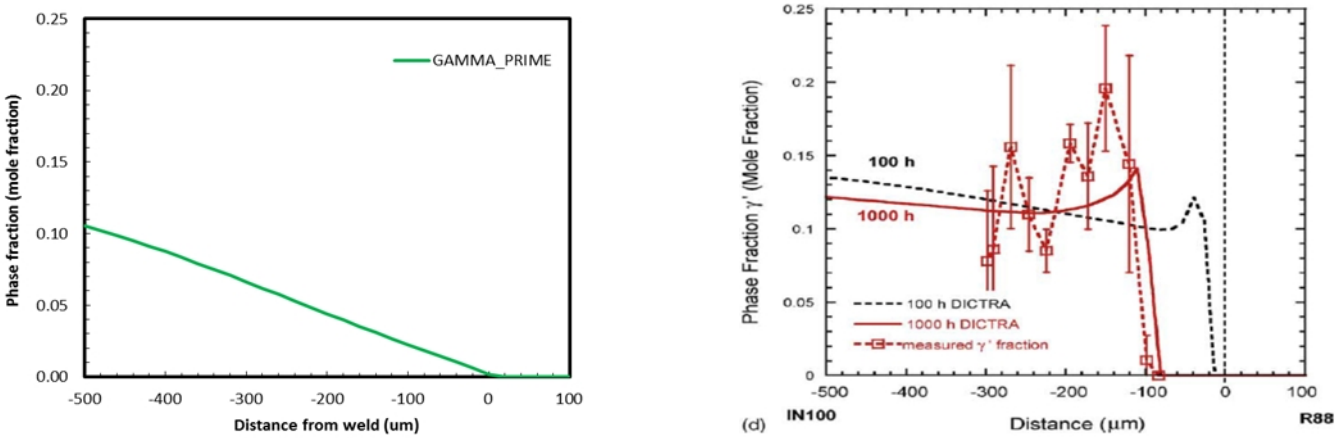
In the above JMatPro calculations, the following procedures have been observed. First each element except Ni is allowed to diffuse freely without the influence of other elements and its concentration profile at the end of the isothermal holding is calculated. This gives the composition (slice) at each distance from the welding line, with Ni being the balancing element. This composition is then allowed to reach equilibrium at this

temperature, 1150°C in this case, and other phases such as gamma prime and MC are allowed to come out. It is the concentration of the gamma phase that is being plotted in all the above comparison plots. As such, the amount of gamma prime and MC carbide can also be obtained from such calculations, e.g. Figs. 6 and 7. The reflection in the Cr profile on the IN100 side of the IN100/IN718 diffusion couple at around 500 µm, Fig. 4(a), is due to the formation of gamma prime, Fig 6(a).




(a) (b)

Fig. 6. Comparison of measured and calculated gamma prime fraction for IN100/IN718 from (a) the current JMatPro model, and (b) the DICTRA model [1].



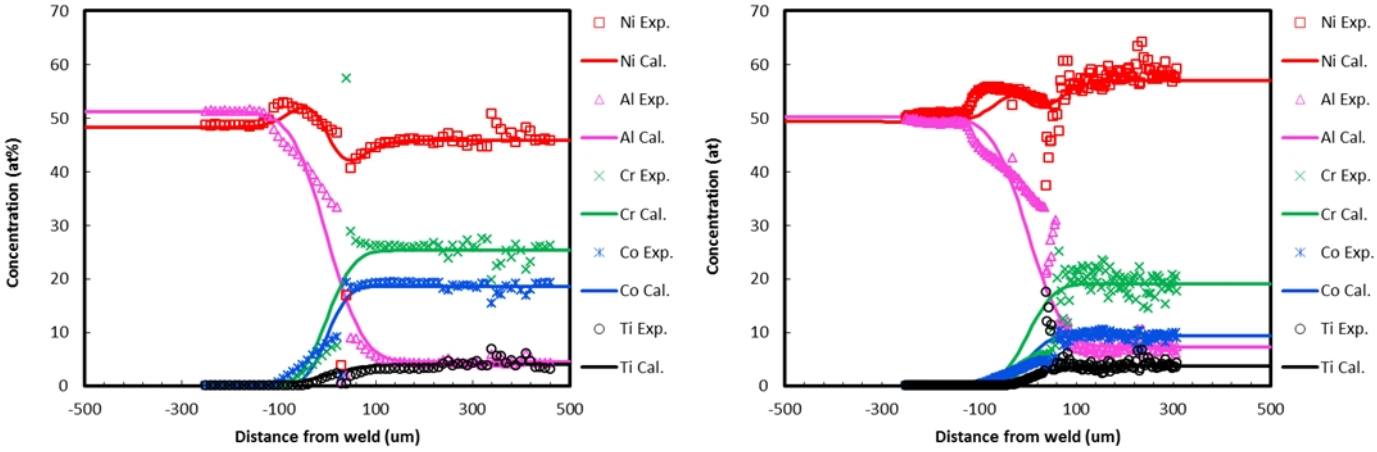

(a) (b)

Fig. 7. Comparison of measured and calculated gamma prime fraction for IN100/René-88 from (a) the current JMatPro model, and (b) the DICTRA model [1].

It should be noted that there are significant differences between the current JMatPro approach and that of DICTRA. First, this model assumes that the diffusion of one element is not affected by others, whereas diffusion coefficients are considered to be concentration dependent in DICTRA. Second, the changes in phase distributions and compositions have been considered during each time step of the diffusion simulation in DICTRA, whereas we only perform equilibrium calculations at the end of the whole diffusion process. In spite of these differences, it is remarkable to find that, generally speaking, the current JMatPro model gives very similar results to that of DICTRA simulations, and both calculations are in reasonable agreement with the measurements. The simpler approach in the current model means such calculations can be completed in typically less than a minute.

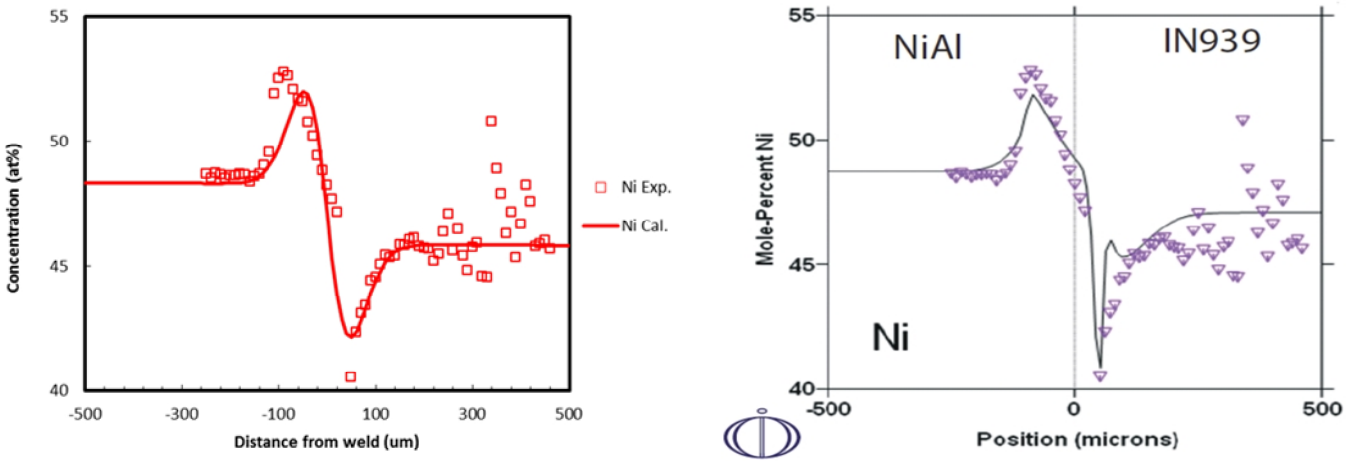
This function is applicable to all material types, as long as both alloys belong to the same alloy type, e.g. both are Ni-based superalloys or both are steels. In principle, it is possible to extend the current approach to deal with diffusion welds between different alloy types, which can happen in practice, e.g. Ni-based superalloys can be successfully welded to low-alloy steels.

Experimental concentration profiles of were also reported for diffusion couples NiAl/IN939 and NiAl/IN738 [4]. Strictly speaking the current Ni-data thermodynamic database may not be applicable to NiAl alloys, so the calculations shown in Fig. 8 should be treated with caution. The diffusion couples were heat-treated at 1050°C for 96 hours. The calculated profiles are at the end of the diffusion process, i.e. they are not the concentrations of gamma phase after further equilibrium calculations. A comparison of the JMatPro model to DICTRA calculations is shown in Fig. 9.




(a) NiAl/IN939 (b) NiAl/IN738

Fig. 8. Comparison of measured to calculated composition profiles for diffusion couples (a) NiAl/IN939, and (b) NiAl-IN738.




(a) JMatPro (b) DICTRA

Fig. 9. Comparison of measured to calculated Ni profile for diffusion couple NiAl/IN939 from (a) the current JMatPro model, and (b) the DICTRA model.

[4] E. Perez, T. Patterson and Y. Sohn, Interdiffusion analysis for NiAl versus superalloys diffusion couples, Journal of Phase Equilibria and Diffusion 27 (2006) 659-664.