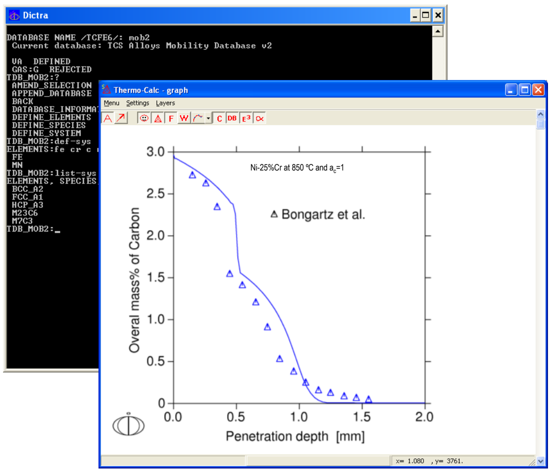
DICTRA



DICTRA is a unique general software package for simulation of DIffusion Controlled TRAnsformations in multicomponent alloys. The DICTRA software is based on a numerical solution of the multicomponent diffusion equations.

DICTRA is interfaced with *Thermo-Calc*, which performs all necessary thermodynamic calculations. The diffusion simulations are based on assessed kinetic and thermodynamic data, which have been stored in databases. Up to 10 components may be treated simultaneously in a simulation, provided that the necessary kinetic and thermodynamic data is available.

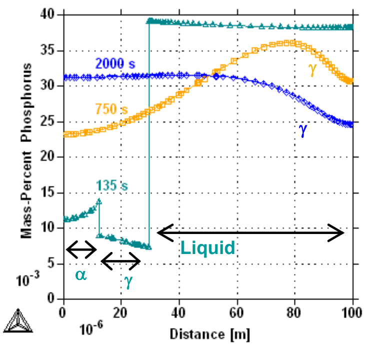
In the development of DICTRA, emphasis has been placed on linking fundamental methods to critically assessed thermodynamic and kinetic data, allowing simulations to be performed with realistic conditions on alloys of practical importance. The simulations are one-dimensional and three different geometries, cylindrical, spherical and planar can be used. This is sufficient to model many cases of interest. The cylindrical geometry can for example be used both for modeling of diffusion through a tube wall, as well as the dissolution of a rod-shaped precipitate.

Powerful & Flexible User-Interface with Specialized Modules

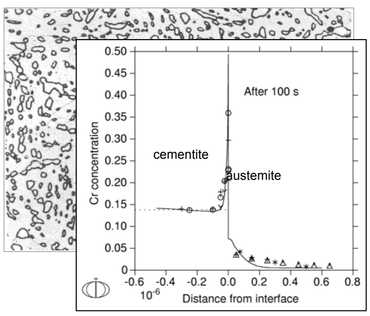
DICTRA contains several different modules for performing specialized tasks e.g. retrieving data, performing a calculation or plotting the results. The user interface consists of a command line interface where commands are typed. All commands can be abbreviated for convenience. The use of MACRO files makes it possible to save complicated command sequences and repeat them many times for different cases at different times.

Examples of DICTRA Applications:

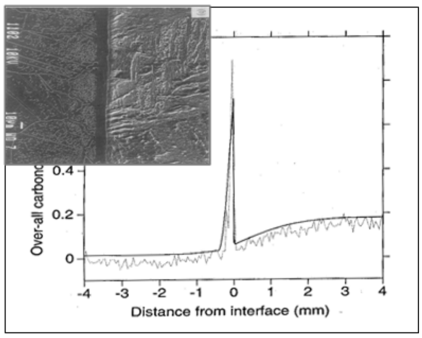
- Homogenization of alloys
- Carburization and decarburization of steel
- Nitriding of steel
- Nitrocarburization of steel
- Austenite to ferrite transformations in steel
- Growth of pearlite in alloyed steels
- Growth or dissolution of precipitates
- Microsegregation during solidification
- TLP bonding of alloys
- Sintering of cemented carbides
- Carburization of high-temperature alloys
- Interdiffusion in compounds, e.g. coating systems
- Coarsening of precipitates



Microsegregation



Dissolution of carbides



Interdiffusion in compounds

Method and Data

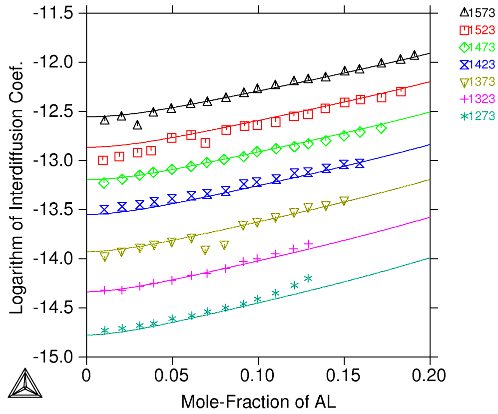
In a DICTRA simulation, the multicomponent diffusion equations:

$$J_k = -\sum_{j=1}^{n-1} \tilde{D}_{kj}^{n} \frac{\partial c_j}{\partial z}$$

are solved, using a complete, (n-1)x(n-1) temperature and concentration dependent diffusivity matrix.

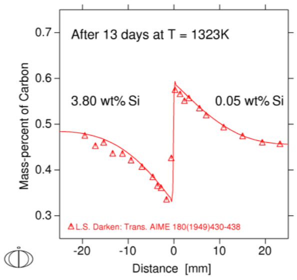
The diffusivity matrix $\tilde{D}_{kj}^{n}$ is calculated from parameters stored in a mobility database and a thermodynamic database.

The thermodynamic databases are the same as used by the Thermo-Calc software. The mobility databases are created through an assessment procedure similar to the one for thermodynamic databases. Experimental data are collected and selected from the literature. Parameters in the mobility models are optimized to give the best possible description of the experimental data (as illustrated in the left plot). The optimized parameters are then stored in a mobility database.

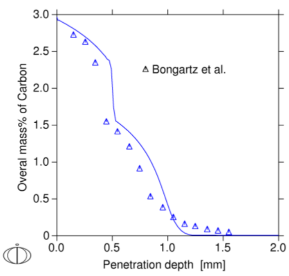


DICTRA contains a module for optimization of mobility data, PARROT. This module enables the user to expand existing mobility databases as well as creating their own databases.

Using the mobility databases it is possible to calculate e.g. tracer-, self-, intrinsic- and interdiffusion coefficients.



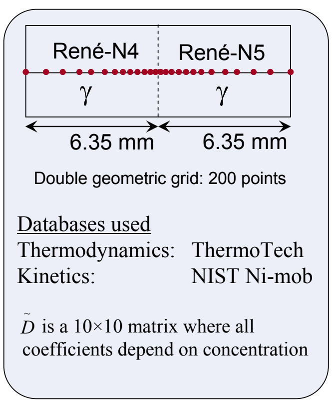
The accurate description of multicomponent diffusion in DICTRA makes it possible to account for processes such as up-hill diffusion. A simulation of the historical Darken experiment with a joint of two steels with initially similar carbon contents but different silicon contents is shown to the right. The higher silicon content in the left part of the figure increases the carbon activity, which causes carbon to diffuse to the right. A discontinuity in carbon content is seen at the gradient in silicon content.

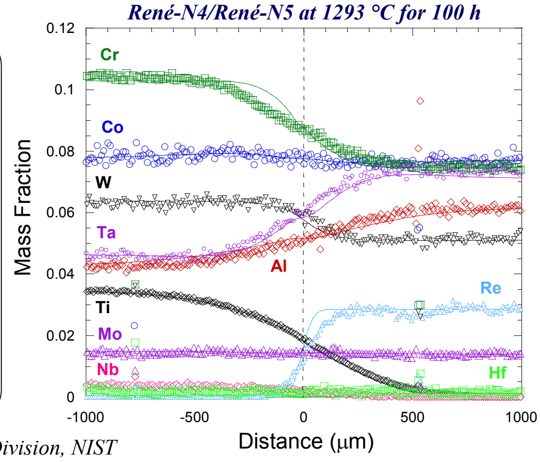


DICTRA's coupling to Thermo-Calc provides access to accurate multicomponent thermodynamics and phase equilibria making it possible to simulate e.g. diffusion in dispersed systems where precipitates act as sources and sinks of diffusing elements. The figure to the left is an example where a Ni-25Cr alloy is carburized. The carbon diffusion causes precipitation of M3C2, M7C3 carbides and the concentration profile is far from the common error-function solution that could have been expected.

The flexible post-processor in the software makes it possible to use many different axis quantities such as concentration, distance, time, activity, chemical potential and user defined functions in the plots. Illustrative diffusion paths are easily plotted as shown in the figure to the right.

Interdiffusion in complex diffusion couple





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