Modelling Chemical & Microstructural Evolution at Dissimilar Metal Interfaces

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e·on

EPRI ELECTRIC POWER RESEARCH INSTITUTE

Scope of the Presentation

- ***Background to the problem***
- Software methods
- Efforts to simulate steel-steel interfaces
  - Construction of the model
  - Historical data for validation
- Extension to steel-nickel interfaces
- Wider applicability of software methods

Background (1)

- Power plant steam vessels are made from several different alloys depending on local temperature e.g. 2.25-Cr steel in low temperature sections, 9-Cr steel in higher temperature sections.
- These different alloys must be joined by fusion welding, a process which can negatively impact their properties.
- During long term exposure to service conditions diffusion of elements can occur across the welded interface, changing the chemical and mechanical properties of both alloys.
- With the drive to increase plant efficiency, joints will be exposed to higher temperatures and joints involving nickel-based alloys be introduced.

Background (2)

- Additionally, older power plants are being pushed beyond their designed service life.
- The consequences of long term, high temperature exposure are not necessarily well known, so predictive tools such as computational thermodynamics are of great use.
- Using these methods the interdiffusion that will occur at interfaces during welding, heat treatment and service can be predicted.
- These methods may also be used to aid in the design of new alloys, for welding and for bulk applications, that minimise diffusion or whose properties are less affected by diffusion.

Dissimilar Metal Interfaces

Increasing Temperature

Cheaper alloys used where possible

More expensive alloys used where required

Need to join dissimilar metals.

Joining Methods

- Metal pipe sections are joined together by multi-pass fusion welding.
- The weld metal is completely melted and re-solidified, as is some of the base metal.
- Adjacent parts of the base metal will have their microstructure altered by the process; these are the heat affected zones (HAZ).
- These effects must be accounted for when considering how welds will behave during service, both in terms of mechanical properties (e.g. creep resistance) and chemical behaviour.

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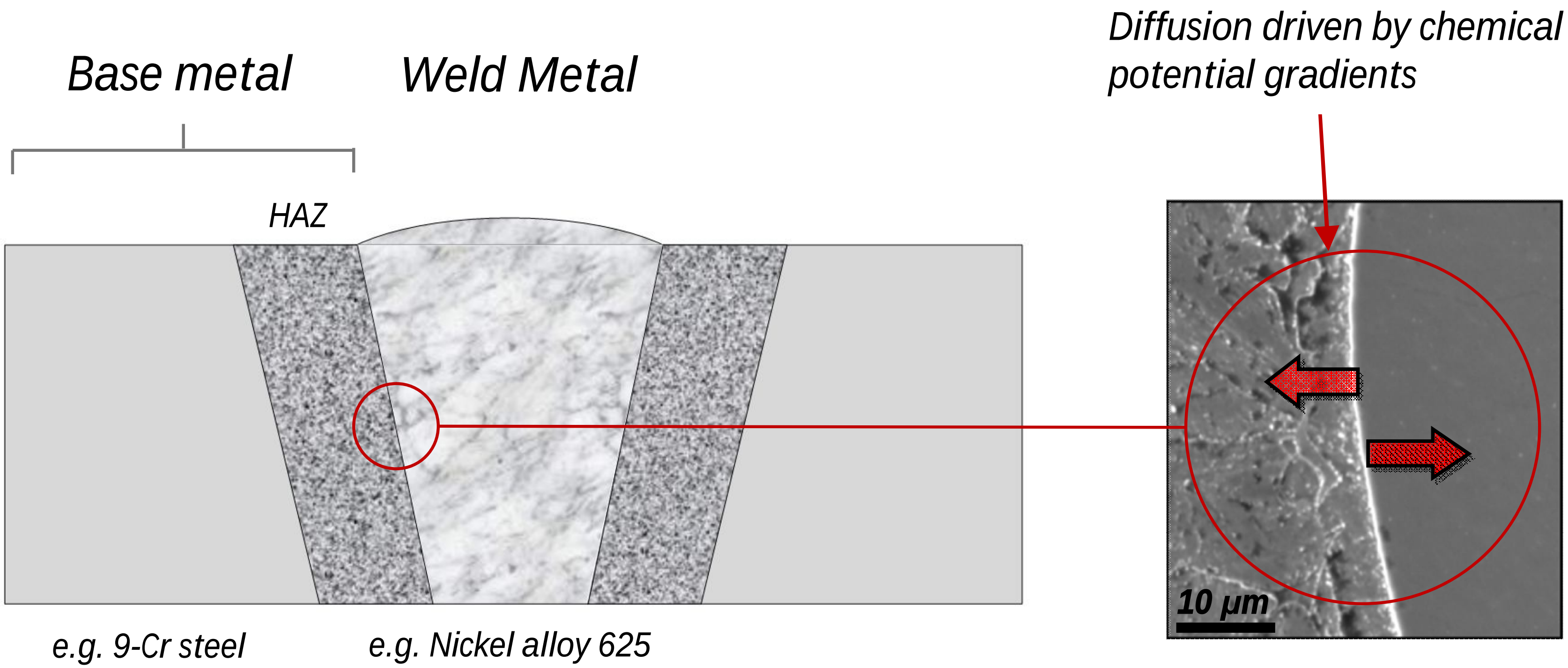
Multi-pass Fusion Welds

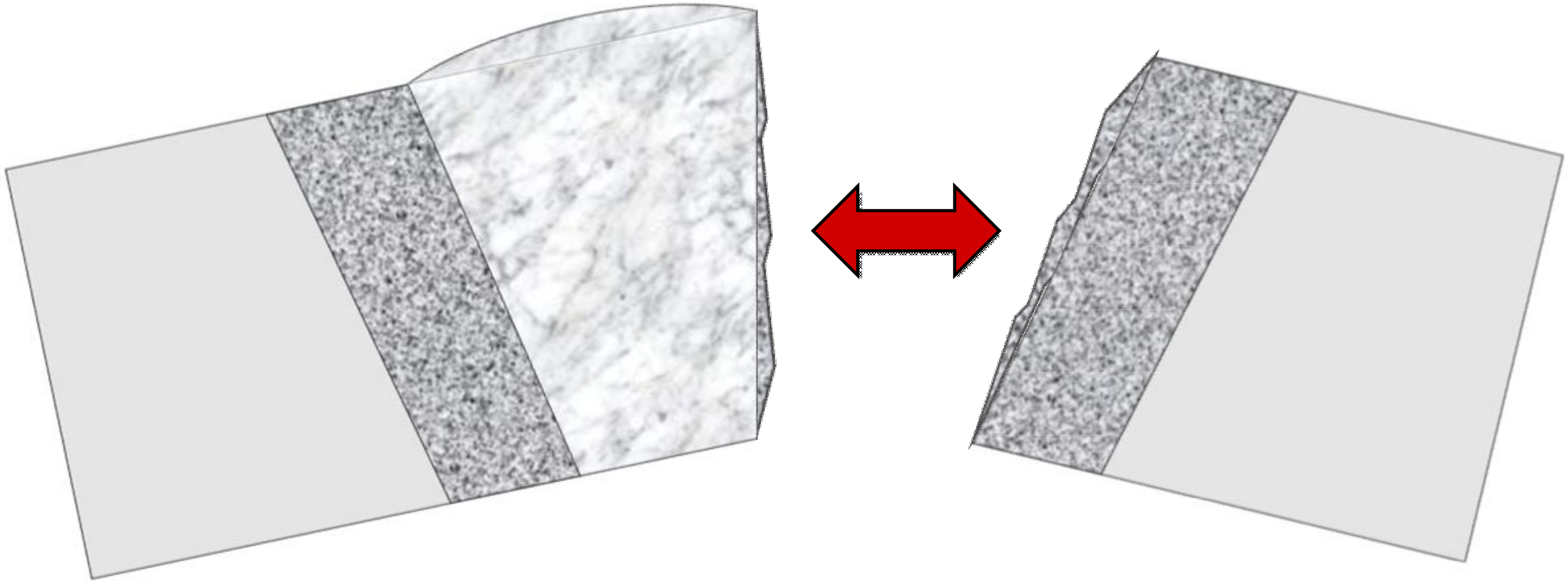


Atomic diffusion will occur across the interfaces at elevated temperature.

Failure Mechanisms at Fusion Welds

- Mismatched coefficients of thermal expansion between base and weld metals can lead to stress build-up during thermal cycling.
- The creep strength of both alloys may be lower than under ideal conditions due to the after-effects of welding.
- Diffusion across the interface leads to localised change in mechanical properties and the precipitation and dissolution of secondary phases, particularly carbides.
- Oxide particles at the surface of the weld interface can act as stress concentrators, causing a notch at the fusion line; this is exacerbated by the presence of secondary phases.

Dissimilar Metal Interfaces



Cracking can occur around the weld during service.

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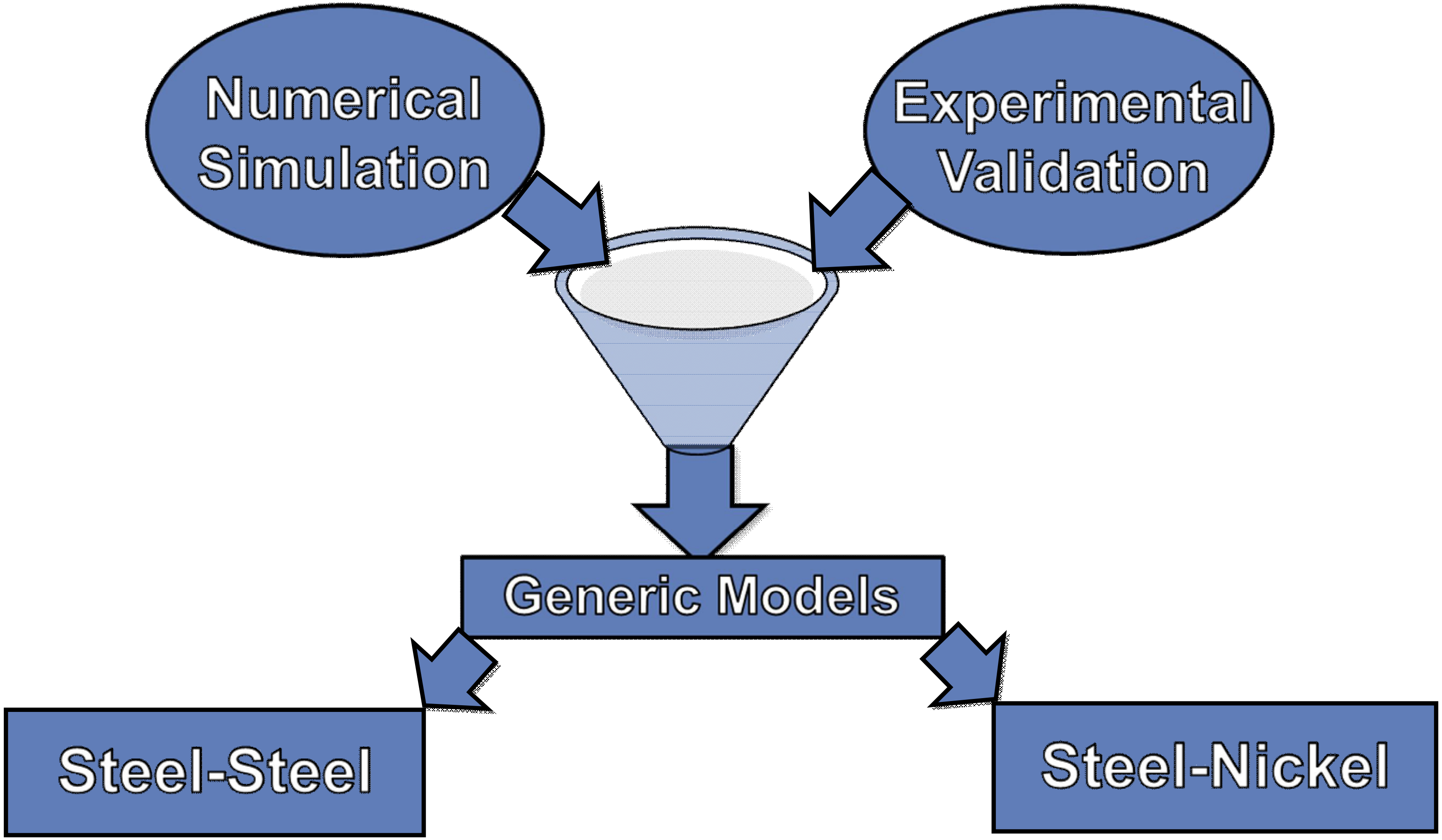
Project Overview



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Mathematics of Interdiffusion

- Across a dissimilar interface diffusion of elements will occur to attain equilibrium.
- In a simple 1D binary system this follows Fick's law:

$$\frac{\partial c}{\partial t} = D \frac{\partial^2 c}{\partial x^2}$$

- In a multicomponent system, however, diffusion of each species is driven by chemical potential gradients of all species.
- A coupled set of differential equations is required to solve the problem, necessitating the use of numerical methods.

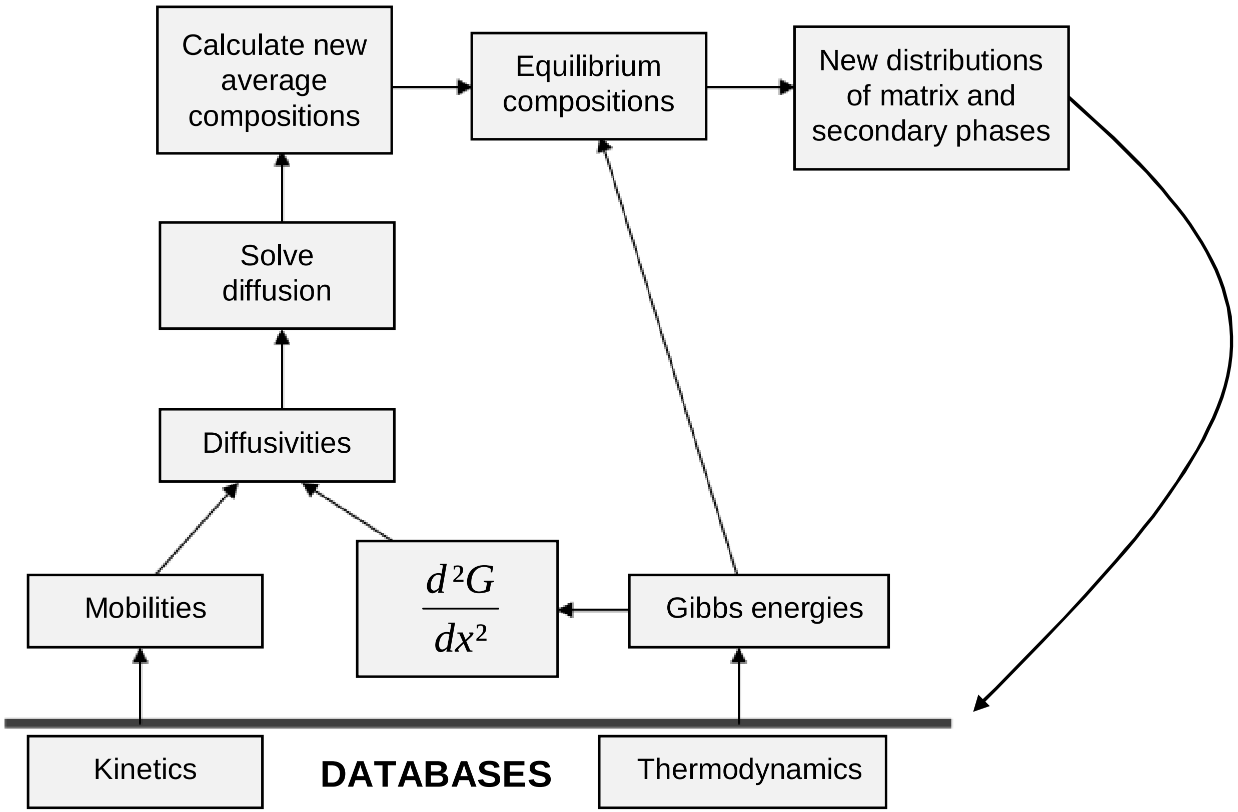
Mathematics of Interdiffusion: DICTRA

- The *DICTRA* software is used to solve these equations.

$$D_{jk} = -\sum_{i=1}^{n} \overbrace{L_{ki}}^{\text{Kinetics}} \frac{\partial \mu_i}{\underbrace{\partial c_j}_{\text{Thermodynamics}}}$$

- The diffusivities (D_{jk}) can be split into a thermodynamic term and a kinetic term.
- These are calculated separately, using data from empirical databases and combined to solve the diffusion problem in 1D between cells.
- ThermoCalc, a closely related software tool, is called as a subroutine to solve the thermodynamics.

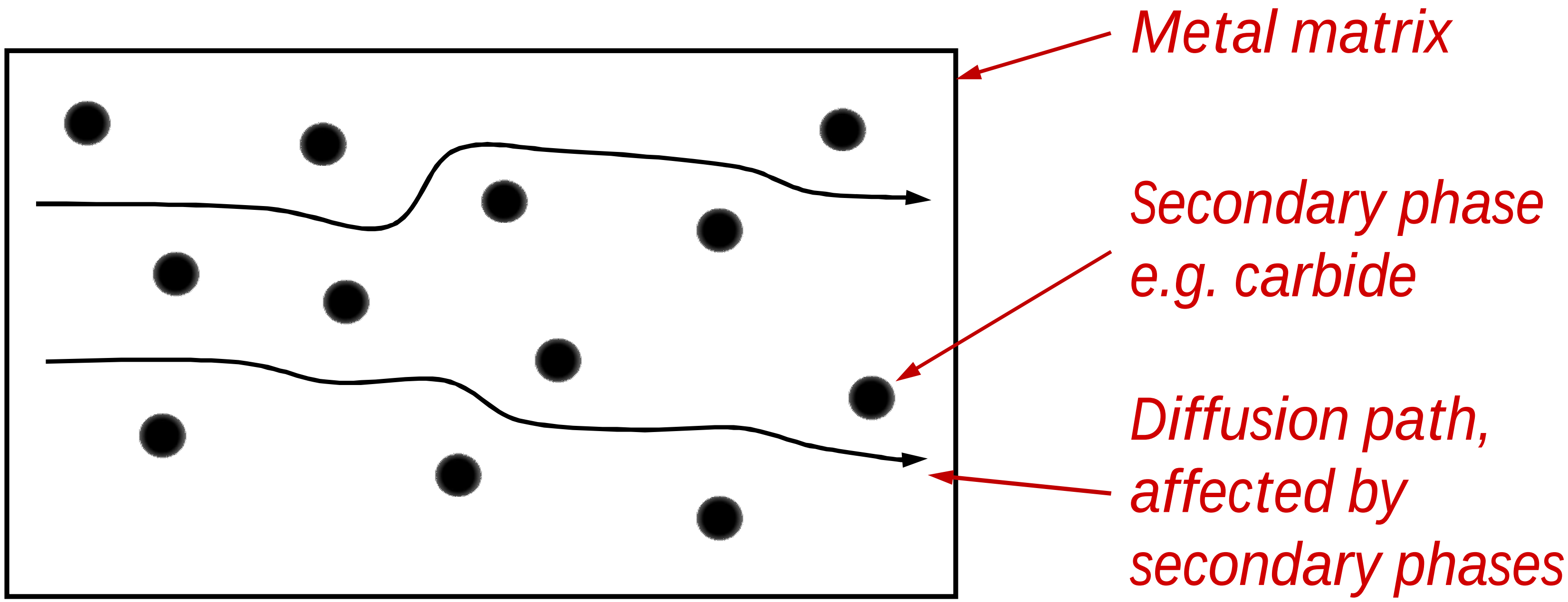
Thermokinetic Software: DICTRA



Adapted from Engstrom, 1996

The process is cycled for as much time as the user defines.

Thermokinetic Software: DICTRA



Computational methods are needed to account for secondary phases.

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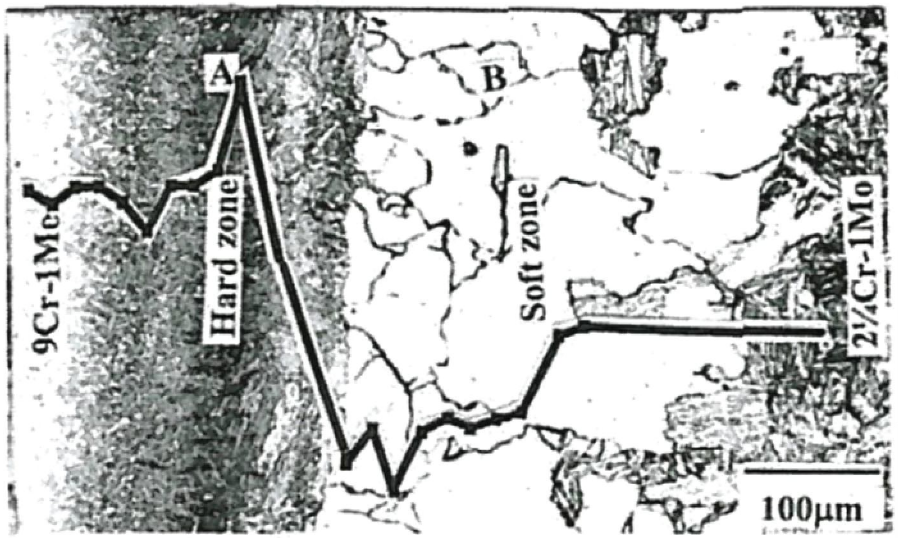
Literature Overview & Related Works

Qualitative studies

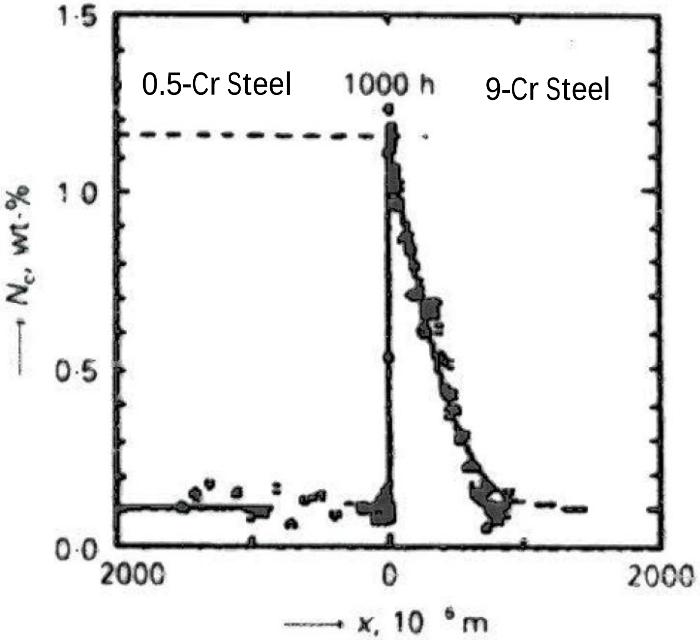
e.g. Optical micrograph & hardness profile



From Sudha, 2006

Quantitative Studies

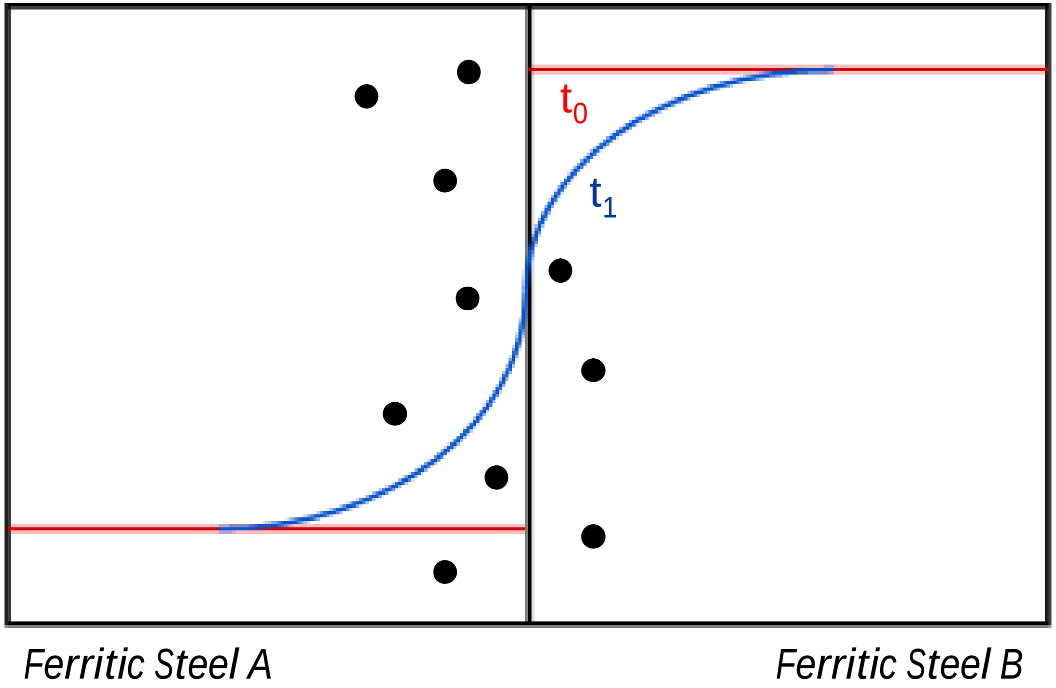
e.g. WDX (electron microprobe) data



From Million et al., 1995

Carbon enriched and denuded zones seen at interface.

Ferritic-Ferritic Interfaces



Homogenisation
+ Precipitation

Like crystal structures make simulations straightforward.

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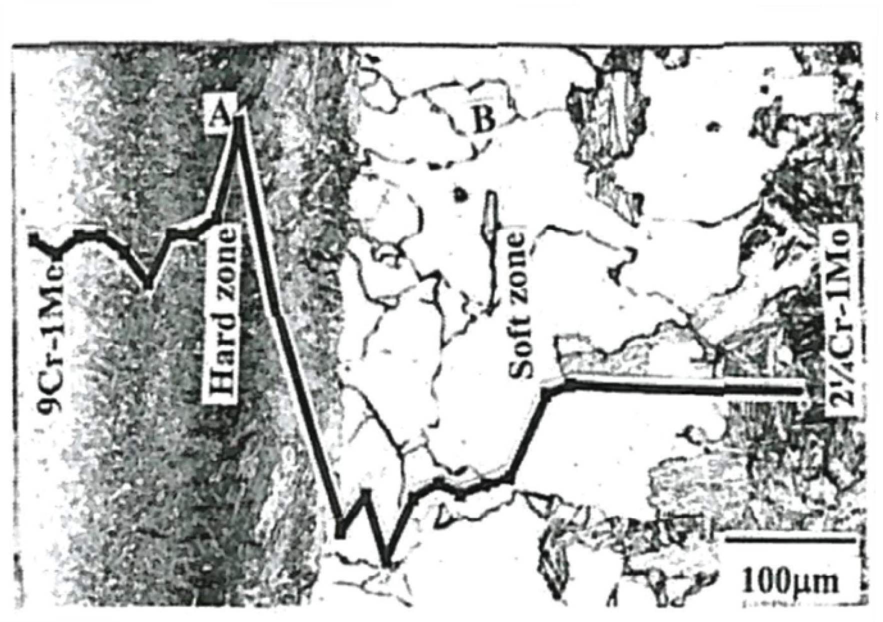
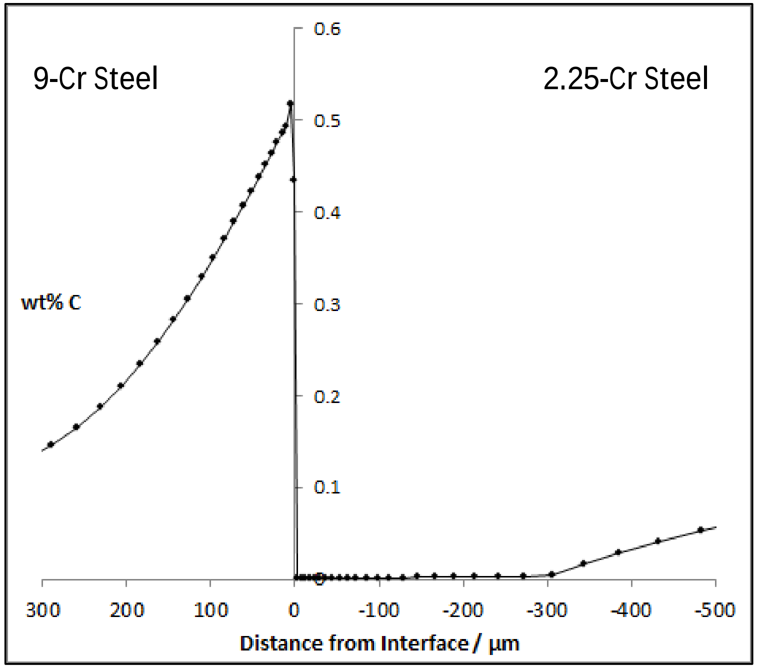
Ferritic-Ferritic Interfaces: Results

Optical micrograph & hardness profile



From Sudha, 2006

Simulation in DICTRA



Clark, 2013

Simulation agrees well with experiment.

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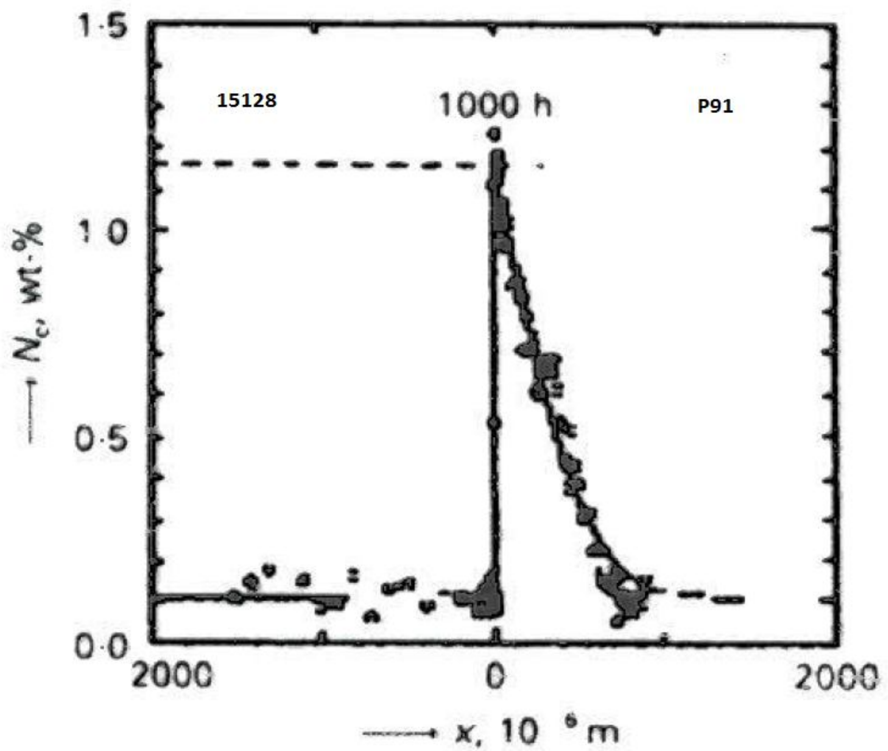
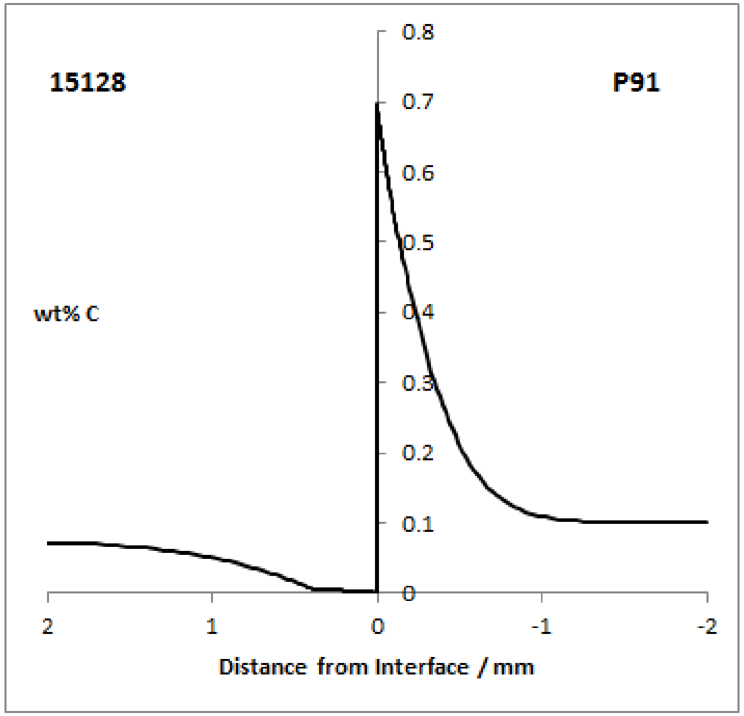
Ferritic-Ferritic Interfaces: Results (2)

WDX (electron microprobe) data



From Foret, 2001

Simulation in DICTRA



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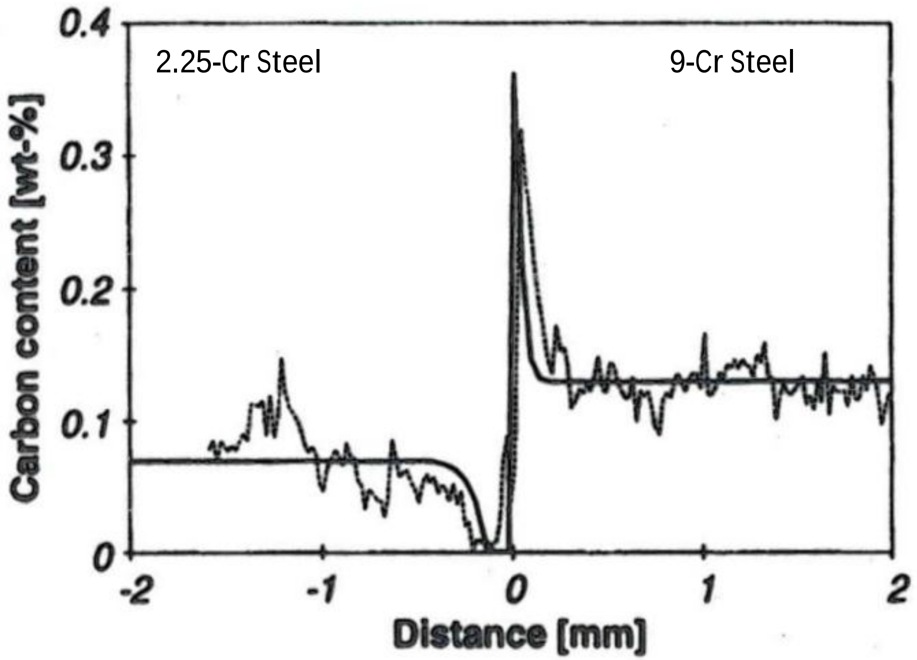
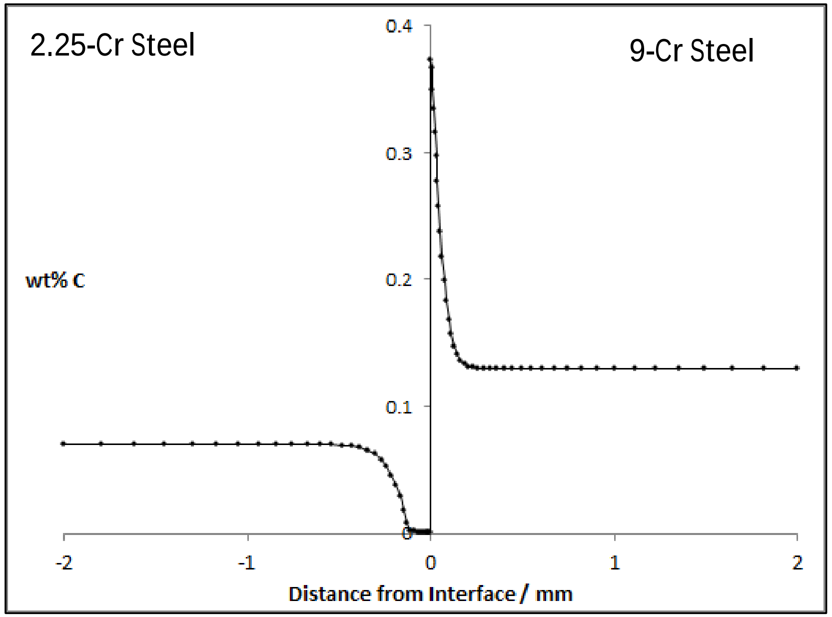
Ferritic-Ferritic Interfaces: Results (3)

WDX data & simulation in MatCalc



From Kozeschnik, 2001

Simulation in DICTRA



Clark, 2013

Simulation agrees well with experiment.

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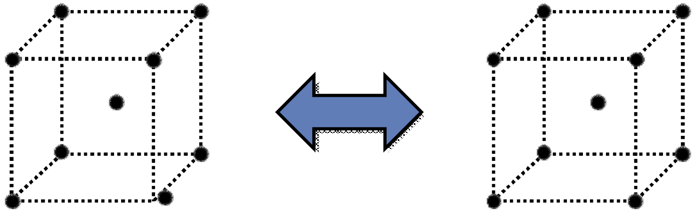
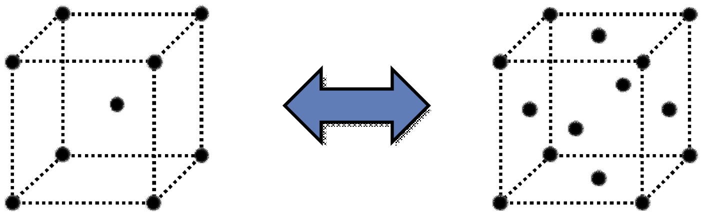
The Ferrite-Austenite Problem

- Steel-steel simulations are straightforward, as both sides have the ferritic (body-centred cubic) crystal structure.



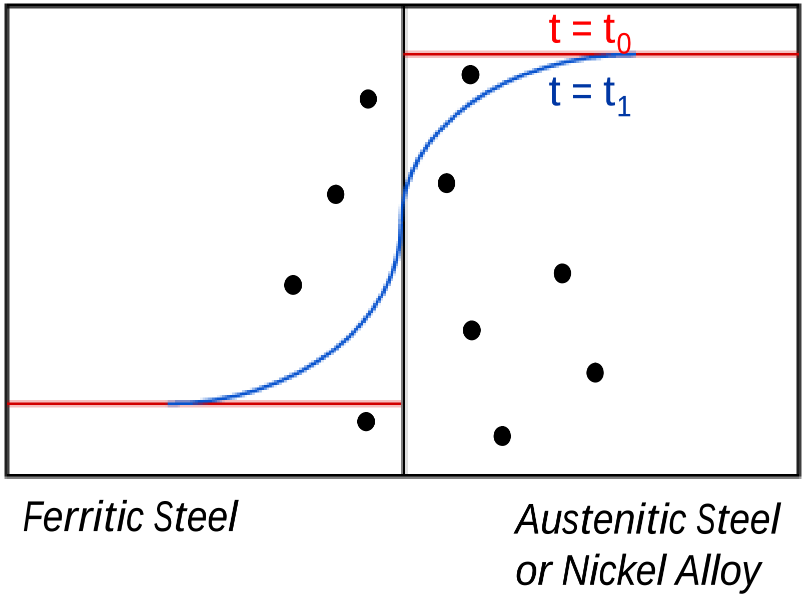
Ferritic Steel A *Ferritic Steel B*

- Stainless steels and nickel alloys are austenitic (face-centred cubic), which complicates matters; two distinct matrix phases are needed.



Ferritic Steel *Austenitic Steel or Nickel Alloy*

The Ferrite-Austenite Problem (2)



Options:

- Boundary conditions
- Running two simulations simultaneously
- Alternative mathematical frameworks

On-going research activity.

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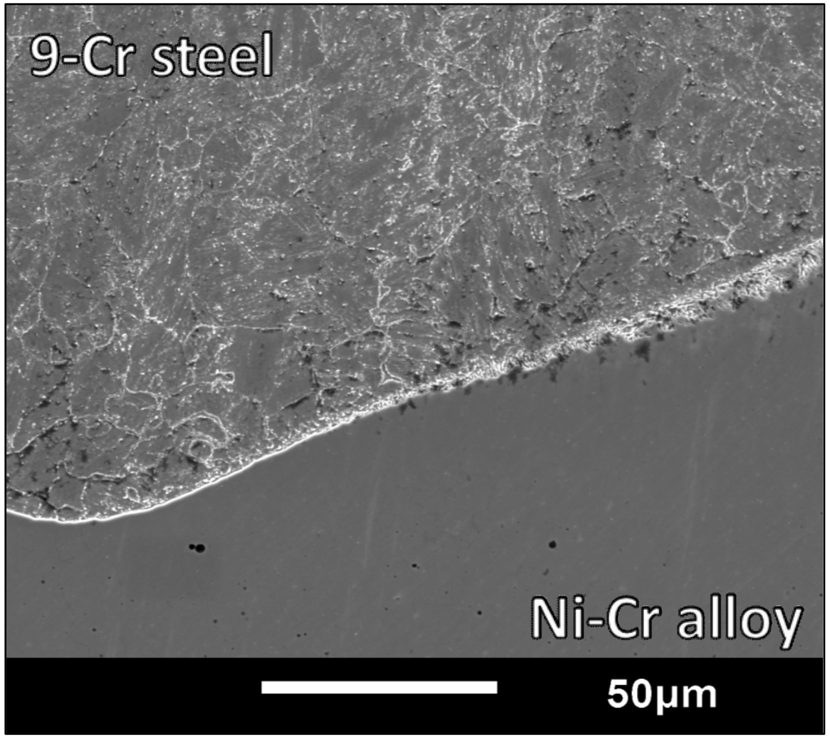
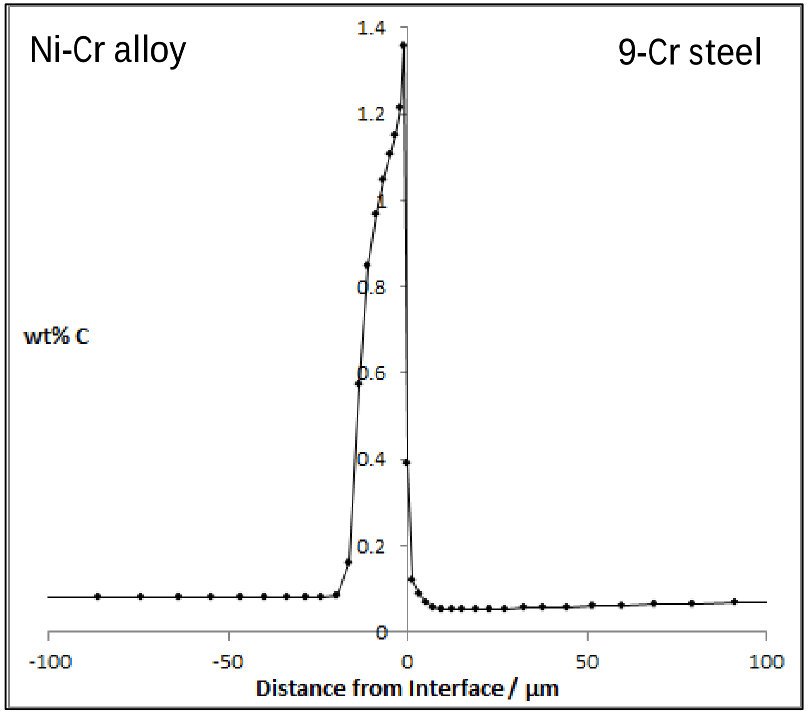
Ferrite-Austenite Simulations

SEM Image



Clark, 2013

Speculative DICTRA simulation



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Further refinement of the model is required.

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- ***Future work and wider applicability***

Research Work

Simulation	Validation
Ferritic-Ferritic Interfaces	Published data
Ferritic-Austenitic Interfaces	➢ As-welded and ex-service steel-nickel fusion weldments ➢ Steel-nickel diffusion couple

Wider Usage in Power Plant Metallurgy

- Simulation of solidification dynamics after welding dissimilar alloys.
- Alloy design (e.g. weld consumables for minimal diffusion).
- Properties of protective coatings (e.g. MCrAlY, NiCr-CrC).
- Phase stability of alloys after long term service.
- Oxidation and carburisation behaviour.
- Interfaces between other alloys, welded or otherwise.

These methods could also be extended to other industries and other sets of alloys; computational thermodynamics is a powerful and versatile toolkit.

Thank you for listening.

Any questions?

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Appendix: 4-Year Gantt Chart

Activity	Year 1				Year 2				Year 3				Year 4			
Taught Elements of EngD																
EngD Centre Summer School				*				*								
Software Training																
Task 1 Critical assessment of benchmark data																
Task 2 Modelling ferritic–ferritic interfaces																
Task 3 Modelling austenitic–ferritic interfaces																
Annual EngD progress report and presentation				*				*				*				
Preparation of EngD Thesis and final report to sponsors																