THERMODYNAMIC MODELLING OF INTERDIFFUSION

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Introduction

Nowadays, when time is money, researchers develop faster and cheaper methods to acquire new results. One of the ways how to do it resides in combining the aimed experiments with the sophisticated simulations inclusive of computational thermodynamics. Methods of computational thermodynamics have been successfully used for the investigation of various processes and the development of new technologies. Many of thermodynamic calculations may be used as a basic tool in the development and the optimization of new materials.

1 Preparation of samples

Samples used in the experiment consisted of couples of the following materials: **cobalt**, **nickel**, **interstitial free steel** (technical pure iron) and **austenitic stainless steel** (72Fe18Cr10Ni). The samples of 7x7x20 mm were rectangular in shape. The functional surface was grided and polished. To localize the Kirkendall interface, Al_2O_3 whiskers were placed between the samples at the mirror surface.

2 Heat treatment

The samples were diffusion bounded in a vacuum furnace at temperatures about 1100° C for 20 hours

Afterwards the samples were separated into four groups: the reference state and the states annealed at **700℃** , **800℃** and **1000℃** . The samples selected to be annealed were placed into the evacuated glass tubes and then annealed for **1000 hours** .

3 Diffusion profiles

- For the interdiffusion simulations the DICTRA (**DI**ffusion **C**ontrolled **TRA**nsformations) software was used.
- Diffusion profiles of the investigated samples were determined by **EDX** (energy-dispersive X-ray spectroscopy) .
- The measured and the calculated profiles were compared with each other.

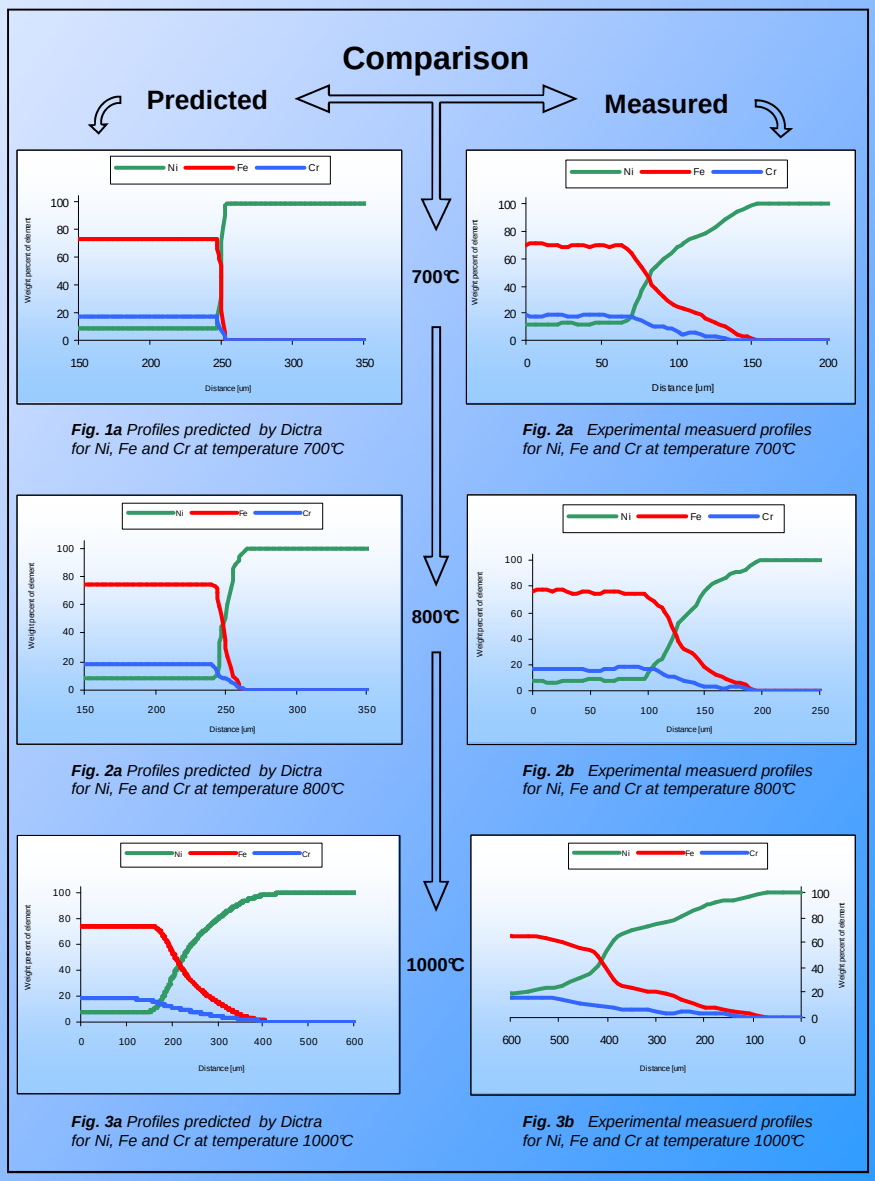

Fig. 1a *Profiles predicted by Dictra for Ni, Fe and Cr at temperature 700℃*

Fig. 2a *Experimental measuerd profiles for Ni, Fe and Cr at temperature 700℃*

Fig. 2a *Profiles predicted by Dictra for Ni, Fe and Cr at temperature 800℃*

Fig. 2b *Experimental measuerd profiles for Ni, Fe and Cr at temperature 800℃*

Fig. 3a *Profiles predicted by Dictra for Ni, Fe and Cr at temperature 1000℃*

Fig. 3b *Experimental measuerd profiles for Ni, Fe and Cr at temperature 1000℃*

Conclusion

The simulations in Materials Science was found to be faster and cheaper choice to acquire correct results. The comparison of the **predicted** diffusion profiles (Figs. 1a, 1b, 1c) with the experimentally **measured** results (Figs. 2a, 2b, 2c) shows small differences only. To look for a proportional coefficient between the both profiles, starting conditions of the experiment will be analyzed.