

Reference Lists on DICTRA Package and Applications

The references selectively listed in this part are mainly regarding the development of the DICTRA software/database/interface package, kinetic models implemented in the software, mobility databases used together with the package, and some specific applications utilizing the package.

You may find hundreds of good references available in literature, on various applications of the DICTRA software/database/interface package

A. General References with descriptions of the DICTRA software and the models used in the software

A.1 General description of the software and its applications

- Thermo-Calc and DICTRA, Computational tools for materials science. *Calphad*, **26** (2002), pp. 273-312, by J.O. Andersson, T. Helander, L. Höglund, P.F. Shi, and B. Sundman.
- DICTRA, a Tool for Simulation of Diffusional Transformations in Alloys. *Journal of Phase Equilibria*, **21** (2000), pp. 269-280, by A. Borgenstam, A Engström, L. Höglund and J. Ågren.
- Computer Simulation of Multicomponent Diffusional Transformations in Steel. *Fundamentals and Applications of Ternary Diffusion*, edited by G.R. Purdy, Pergamon Press, New York, NY, 1990, pp. 153-163, by J.-O. Andersson, L. Höglund, B. Jönsson and J. Ågren.

A.2 Models for diffusivities/mobilities in DICTRA

- A Phenomenological Treatment of Diffusion in Al-Fe and Al-Ni alloys having B2-B.C.C. Ordered Structure. *Acta Materialia*, **47** (1999), pp. 1141-1152, by T. Helander and J. Ågren.
- Ferromagnetic Ordering and Diffusion of Carbon and Nitrogen in bcc Cr-Fe-Ni Alloys. *Zeitschrift für Metallkunde*, **85** (1994), pp. 498-501, by B. Jönsson.
- Models for Numerical Treatment of Multicomponent Diffusion in Simple phases. *Journal of Applied Physics*, **72** (1992) pp. 1350-1355, by J.-O. Andersson and J. Ågren.
- On Ferrromagnetic Ordering and Lattice Diffusion –A simple model. *Zeitschrift für Metallkunde*, **83** (1992), pp. 349-355, by B. Jönsson.

A.3 Numerical method for solving the multicomponent diffusion equation

- Numerical Treatment of Diffusional Reactions in Multicomponent Alloys. *Journal of Physics and Chemistry of Solids*, **43** (1982), pp. 385-391, by J. Ågren

A.4 Numerical method for moving boundary problems

- On the Numerical Treatment of Moving Boundary Problems. *Zeitschrift für Metallkunde*, **83** (1992) pp. 673-678, by S. Crusius, G. Inden, U. Knoop, L. Höglund and J. Ågren

A.5 Numerical method for diffusion in dispersed systems

- Computer Simulation of Diffusion in Multiphase Systems. *Metallurgical and Materials Transactions A*, **25A** (1994), pp. 1127-1134, by A. Engström, L. Höglund and J. Ågren

A.6 Numerical method for coarsening of precipitates

- Simulation of carbo-nitride coarsening in multicomponent Cr steels for high temperature applications. *Conference Proceeding on Advanced Heat Resistant Steel for Power Generation*, edited by R. Viswanathan and J. Nutting, San Sebastian, Spain, 1998, pp.270-276, by Å. Gustafson, L. Höglund and J. Ågren.

A.7 Numerical method for diffusion through multiphase structures

- A Homogenization approach to diffusion simulations applied to $\alpha+\gamma$ Fe-Cr-Ni diffusion couples. *Acta Materialia*, **54** (2006), pp. 2431-2439, by H. Larsson and A. Engström.

B. References with applications treated by the DICTRA

B.1 Steels:

B.1.1 Solidification and microsegregation

- Comparison of solidification behavior between in situ observation and simulation of Fe-C-Si system. *Journal of Alloys and Compounds*, **613** (2014), pp. 132-138, by HM Henaio, A Sugiyama, K Nogita.
- On the microstructure and properties of 100Cr6 steel processed in the semi-solid state. *Acta Materialia*, **55** (2007), Issue 19, pp. 6553-6560, by W. Puttgen, B. Hallstedt, W. Bleck, J.F. Löffler and P.J. Uggowitzer.
- Modelling and Experiments of Solidification of AISI 304. *la metallurgia italiana* 2007, pp. 25-32, by D. Baldissin, M. Palumbo and L. Battezzati.
- Simulation of the influence of phosphorus on the prior austenite grain size of high-impurity steels. *Acta Materialia*, **54** (2006), Issue. 9, pp. 2441-2449, by H.S. Kim, Y. Kobayashi and K. Nagai.
- Semi-solid Processing of Alloys: Principles, Thermodynamic Selection Criteria, Applicability. *ISIJ International*, **46** (2006), No. 12, pp. 1852-1857, by B. Hallstedt, E. Balitchev, H. Shimahara and D. Neuschutz.
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- Diffusional solidification behaviour in 304 stainless steel; *Materials Transactions. JIM*, **39** (1998), pp. 633-639, by H.M. Lee, J.S. Bae, J.R. Soh, S.K. Kim and Y.D. Lee.

B.1.2 Homogenisation

- Homogenisation of 20SiMn2MoV steel ingots: thermodynamic/kinetic simulation and experimental validation, *Materials at High Temperatures*, <http://dx.doi.org/10.1179/1878641314Y.0000000032>, by Y. Zhang, W Q. Chen, L. Chen, Q Z. Yan and J. Sun.

B.1.3 Austenite \rightarrow Ferrite transformation

- Kinetic Transition During the Growth of Proeutectoid Ferrite in Fe-C-Mn-Si Quaternary Steel, *Met. Mater. Int.* **19** (2013), No. 2, pp. 153-158, by GH Zhang, YU Heo, EJ Song, DW Suh .
- Atom probe tomography of the austenite-ferrite interphase boundary composition in a model alloy Fe-C-Mn. *Scripta Materialia*, **55** (2006), pp. 1071-1074, by O. Thuillier, F. Danoix, M. Gouné and D. Blavette.

- An assessment of interfacial dissipation effects at reconstructive ferrite-austenite interfaces. *Acta Materialia*, **53** (2005), pp. 141-149, by A. Saha, G. Ghosh and G.B. Olson.
- Modelling of phase transformation of plain carbon steels during continuous cooling. *Cailiao Kexue Yu Jishu (Journal of Materials Science & Technology) (China) (USA)*, vol. **19** (2003), pp. 262-264, by Y Zhang, C. Mo, D. Li and Y. Li.
- The influence of Ti, Nb and S on the austenite decomposition and the precipitation in if ("interstitial free") steels. *58th Annual ABM International Congress; Rio de Janeiro; Brasil; 21-24 July 2003*, by R. R. De Avillez, A. L. V. Da Costa e Silva and A. C. Rocha.
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- Computer simulations of phase transformation in steels. *Materials and Design*, **22** (2001), pp. 39-43, by J.B. Li, C. Yang and H. Dong.
- An assessment of the Si mobility and the application to phase transformations in silicon steels. *Zeitschrift für Metallkunde*, **88** (1997), pp. 795-799, by P. Franke and G. Inden.
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- On the growth of ferrite allotriomorphs in Fe-C alloys. *Zeitschrift für Metallkunde*, **83** (1992), pp. 729 - 738, by S. Crusius, L. Höglund, G. Inden, U. Knoop and J. Ågren.
- Computer simulations of the austenite/ferrite diffusional transformations in low alloyed steels. *Acta Materialia*, **30** (1982) pp. 841-851, by J. Ågren.

B.1.4 Growth of secondary austenite

- Growth kinetics of secondary austenite in the welding microstructure of a UNS S32304 duplex stainless steel. *Acta Materialia*, **54** (2006), pp. 3321-3331, by C.M. Garzón and A.J. Ramirez.

B.1.5 Annealing of austenite

- Bainite: Fragmentation of crystallographically homogeneous domains, *Int. J. of Materials Research*, **103** (2012), pp. 476-482, by Junhak Pak, DongWooSuh and H. K. D. H. Bhadeshia.

B.1.6 Growth/dissolution of Carbides, Nitrides and intermetallic phases

- Carbide Dissolution during intercritical austenitization in bearing steel. *J. of Wuhan Univ. of Technology – Mater. Sci. Ed.* **29** (2014), Issue 6, pp. 1242-1245, by X Zhang, D Tang, Y Wang.
- Dissolution of Iron-chromium Carbides during White Layer Formation Induced by Hard Turning of AISI 52100 Steel, *Procedia CIRP*, **14** (2014), pp. 107-112, by SB Hosseini, R Dahlgren, K Rytberg, U Klement.
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- Precipitation of paraequilibrium cementite: Experiments, and thermodynamic and kinetic modelling. *Acta Materialia*, **50** (2002), pp. 2099-2119, by G. Ghosh and G. B. Olson.
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- An experimental and theoretical study of cementite dissolution in an Fe-Cr-C alloy. *Metallurgical and Materials Transactions A*, **22A** (1991), pp. 1745-1752, by Z.-K. Liu, L. Höglund, B. Jönsson and J. Ågren.
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B.1.7 Carbide coarsening

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B.1.8 Sigma phase formation in stainless steels

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B.1.9 Interdiffusion in compounds and cladding steels

- Microstructural Stability of Dissimilar Weld Joint of Creep-Resistant Steels with Increased Nitrogen Content at 500-900 °C. *Defect and Diffusion Forum*, **263** (2007), pp. 195-200, by B. Zlámál, R. Foret, J. Nursik and M. Svoboda.
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B.1.10 Carburizing

- Carburisation of Fe-X (X=Si, Mo, V) diffusion couples. *Calphad, Article in Press* (2008), by R. Bernst, G. Inden and A. Schneider.
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B.1.11 Nitriding and Nitrocarburizing

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B.2 Nickel based superalloys:

B.2.1 Solidification and microsegregation

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B.2.2 Interdiffusion

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B.2.3 Precipitate Growth/Dissolution

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B.2.4 Coarsening of γ' precipitates

- Simulation of carbo-nitride coarsening in multicomponent Cr steels for high temperature applications. *Conference Proceeding on Advanced Heat Resistant Steel for Power Generation*, edited by R. Viswanathan and J. Nutting, San Sebastian, Spain, 1998, pp. 270-276, by Å. Gustafson, L. Höglund and J. Ågren.

B.2.5 Transient liquid-phase bonding

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B.3 Aluminum based alloys:

B.3.1 Solidification and microsegregation

- Computation of solidification paths in multiphase alloys with back-diffusion. *Calphad*, **31** (2007), No. 4, pp.490-504, by D. Larouche.
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B.3.2 Precipitate dissolution

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B.3.3 Precipitate growth

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B.3.4 Laser hardening and laser welding

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B.4 Cemented carbides:

B.4.1 Diffusion in the liquid Co binder

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