



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.

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

1.1 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.

1.2 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 Ferromagnetic Ordering and Lattice Diffusion –A simple model. *Zeitschrift für Metallkunde*, **83** (1992), pp. 349-355, by B. Jönsson.

1.3 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

1.4 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

1.5 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



1.6 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.

2 References with applications treated by the DICTRA

2.1 Steels:

2.1.1 Solidification and microsegregation

- 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. Neuschütz.
- Prediction of Prior Austenite Grain Size of High-phosphorous Steels through Phase Transformation Simulation. *ISIJ International*, **46** (2006), No. 6, pp. 854-858, by H.S. Kim, Y. Kobayashi and K. Nagai.
- Microsegregation Behaviour during Solidification and Homogenisation of AerMet100 Steel. *Metallurgical and Materials Transactions B*, **29B** (1998), pp. 205-210, by H.E. Lippard, C.E. Campbell, T. Björklind, U. Borggren, P. Kellgren, V.P. Dravid and G.B. Olson.
- 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.

2.1.2 Austenite→Ferrite transformation

- 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.
- Modelling microstructure development in self-shielded flux cored arc welds. *Welding Journal*, **80** (2001), pp. 91s-97s, by S.S.Babu, S.A. David, M.A. Quintana.
- Simulation of paraequilibrium growth in multicomponent systems. *Metallurgical and Materials Transactions A*, **32A** (2001), pp. 455-467, by G. Ghosh and G.B. Olson.
- 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.
- Some aspects on theoretical calculation of TTT diagram. *Solid-Solid Phase Transformations*, edited by W.C. Johnson, J.M. Howe, D.E. Laughlin and W.A. Soffa, The Minerals, Metals & Materials Society, 1994, pp. 39-44, by Z.-K. Liu.
- 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.

2.1.3 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.

2.1.4 Growth/dissolution of Carbides, Nitrides and intermetallic phases

- Design of martensitic/ferritic heat-resistant steels for application at 650 °C with supporting thermodynamic modelling *Materials Science and Engineering: A*, **477** (2008), Issues. 1-2, pp. 334-343, by V. Knezevic, J. Balun, G. Sauthoff, G. Inden and A. Schneider.
- The Cementite Spheroidization Process in High-Carbon Steels with Different Chromium Contents. *Metallurgical and Materials Transactions A*, **39** (2008), No. 3, pp. 513-521, by N.V. Luzginova, L. Zhao and J. Sietsma.
- The relationship between atomic partitioning and corrosion resistance in the weld-heat affected zone microstructures of UNS S32304 duplex stainless steel. *Journal of Materials Science*, **42** (2007), No. 21, pp. 9021-9029, by C.M. Garzón, C.A. Serna, S.D. Brandi and A.J. Ramirez.
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- Kinetics of carbide precipitation in a 2.25Cr-1Mo steel. *59th Annual ABM International Congress; Sao Paulo; Brasil; 19-22 July 2004*, by R. De Avillez, B. Marinkovic, A. L. V. Da Costa e Silva and F. Rizzo.
- Numerical and Experimental Study On The Eutectic-Carbide M₂C Decomposition Kinetics During Heat Treatment Of As Cast M₂ High-Speed Steels. *59th Annual ABM International Congress; Sao Paulo; Brasil; 19-22 July 2004*, by W. S. Da Silva, C. M. Garzon, H. Goldstein and A. P. Tschiptschin.
- Computer simulation of growth and coarsening of Laves phase in a modified 12% chromium steel. *Scandinavian Journal of Metallurgy (Denmark)*, vol. **32** (2003), pp. 94-99, by A. Bjarbo.
- Precipitation of paraequilibrium cementite: Experiments, and thermodynamic and kinetic modelling. *Acta Materialia*, **50** (2002), pp. 2099-2119, by G. Ghosh and G. B. Olson.
- Complex carbide growth, dissolution, and coarsening in a modified 12 Pct chromium steel – an experimental and theoretical study. *Metallurgical and Materials Transactions A*, **32A** (2001) pp. 19-27, by A. Bjärbo and M. Häggestrand.
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- Phase transformation in Fe-Mo-C and Fe-W-C steels – I. The structural evolution during tempering at 700°C. *Acta Materialia*, **45** (1997), pp. 2861-2878, by D.V. Shtansky and G. Inden.



2.1.5 Carbide coarsening

- Coarsening behaviour of M₂₃C₆ carbides after ageing of thermal fatigue in AISI H13 steel with niobium. *Int. J. of Fatigue*, **28** (2006), Issue. 3, pp. 175-182, by X. Hu, L. Li, X. Wu and M. Zhang.
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- Coarsening of TiC in austenitic stainless steel--experiments and simulations in comparison. *Materials Science and Engineering A*, **287**(2000), pp. 52-58, by Å. Gustafson.

2.1.6 Sigma phase formation in stainless steels

- Comparison between Quantitative Metallography and Modelling of sigma-Phase Particle Growth in AISI 347 Stainless Steel. *Metallurgical and Materials Transactions A*, **36A**, (2005), pp. 2595-2600, by J. Engman, M. Schwind, L. Nylof, J.-O. Nilsson, H.-O. Andren and J. Ågren.
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- Effects of elemental distribution on precipitation behaviour and properties of duplex stainless steel weldments. *Duplex 2000. Proceedings, 6th World Conference and Expo, Venice, Italy* (2000), pp. 693-702, by L. Karlsson, S. Rigdal and S. Pak.
- The relation between alloy composition and kinetics of intermetallic phase formation. *Duplex 2000. Proceedings, 6th World Conference and Expo, Venice, Italy* (2000), pp. 347-354, S. Hertzman, R. Pettersson, K. Frisk and T. Jerwin.

2.1.7 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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- Carbon and nitrogen redistribution in weld joint of ion nitrided 15CrMov 2-5-3 and advanced P91 heat-resistant steels. *J. of Phase Eq. and Diffusion*, **27** (2006), pp. 363-369, by J. Sopousek and R. Foret.
- Diffusion Behavior at the Interface of Cladding Steels. *J. of the Japan Institute of Metals*, 68 , No. 12 (2004), pp. 1013-1019, by M. Omichi, M. Sato, T. Tokunaga, H. Ohtani and M. Hasebe.
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- Computer simulation of diffusion in multiphase system. *Metallurgical and Materials Transactions A*, **25A** (1994), pp. 1127-1134, by A. Engström, L. Höglund and J. Ågren.



2.1.8 Carburizing

- Carburisation of Fe-X (X=Si, Mo, V) diffusion couples. *Calphad, Article in Press* (2008), by R. Bernst, G. Inden and A. Schneider.
- Growth Simulation of Spheroidized Carbide in the Carbide-Dispersed Carburizing Process. *Metallurgical and Materials Transactions A*, **39A** (2008), pp. 1248-1257, by K. Tanaka, H. Ikehata, K. Nakanishi and T. Nishikawa
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- Simulation of carburization in secondary hardening steels. ASM International, *Heat Treating: Proceedings of the 17th Conference: 1997 Induction Heat Treating Symposium*, (1998), pp. 313-319, by C.J. Kuehmann, J.P. Wise, G.B. Olson and C.E. Campbell.
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2.1.9 Nitriding and Nitrocarburizing

- Gas nitriding of high vanadium steels – experiments and simulations. *Metallurgical and Materials Transactions A*, **35A** (2004), pp. 2799-2802, by H. Larsson and J. Ågren.
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2.2 Nickel based superalloys:

2.2.1 Solidification and microsegregation

- Thermo-Calc and Dictra simulation of constitutional liquation of gamma prime (γ') during welding of Ni base superalloys. *Computational Materials Science*, **41** (2007), No. 1, pp. 13-19, by F. Tancret.
- Simulation of the solidification of CMSX-4. *Materials Science and Engineering A*, **397** (2005) issues 1-2, pp. 385-390, by C. Walter, B. Hallstedt and N. Warnken.
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2.2.2 Interdiffusion

- Crack growth in a coated gas turbine superalloy under thermo-mechanical fatigue. *International Journal of Fatigue*, **30** (2008), Issue 2, pp. 286-291, by A. Jung and A. Schnell.
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- Examination of Ni-base superalloy diffusion couples containing multiphase regions. *Materials Science and Engineering A*, **407** (2005), pp. 135-146, by C.E. Campbell, J.-C. Zhao and M.F. Henry.
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2.2.3 Precipitate Growth/Dissolution

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2.2.4 Coarsening of γ' precipitates

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2.2.5 Transient liquid-phase bonding

- Transient Liquid-Phase Bonding in the Ni-Al-B System. *Metallurgical and Materials Transactions A*, **31A** (2000), pp.2835-2847, by C.E. Campbell and W.J. Boettinger.



2.3 Aluminum based alloys:

2.3.1 Solidification and microsegregation

- Computation of solidification paths in multiphase alloys with back-diffusion. *Calphad*, **31** (2007), No. 4, pp.490-504, by D. Larouche.
- 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. Neuschütz.
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- Modelling of microsegregation and homogenization of 6061 extrudable Al-alloy. *Journal of Materials Processing Technology*, **194** (2007), Issues 1-3, pp. 63-73, by S.N. Samaras and G.N. Haidemenopoulos.
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2.3.3 Precipitate growth

- Combined thermodynamic and kinetic computational simulation of heat treatments: precipitation of metastable phases in Al alloys. *Proceedings of the 10th Congress of the IFHT: Incorporating the third ASM International Europe Heat Treatment and Surface Engineering Conference in Europe (UK)*, (1999), pp. 577-588, by I. Hurtado, B. Meurer, P. Spencer, D. Neuschütz, L. Lochte and J. Dunnwald.

2.3.4 Laser hardening and laser welding

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2.4 Cemented carbides:

2.4.1 Gradient sintering

- Gradient zones in WC-Ti(C,N)-Co-based cemented carbides - experimental study and computer simulations. *Acta Materialia*, **48** (2000), pp. 2177-2185, by M. Ekroth, R. Frykholm, M. Lindholm, H.-O. Andrén, and J. Ågren.

2.4.2 Diffusion during sintering

- Computer simulation of W-C-Co-V system diffusion couples. *Rare Metals*, **26** (2007), Issue 5, pp. 492-497, by Y. He, L. Li, S. Huang, J. Vleugels and O. Van der Biest.
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2.5 Solders:

2.5.1 Sn-Ag-Cu solders

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2.6 Other alloys:

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2.6.2 Al-Cu alloys

- Computational investigation of constitutional liquation in Al-Cu alloys. *Acta Materialia*, **51** (2003), 4447-4459, by C. Jiang and Z-K Liu.

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- Study of diffusion mobility of Al-Zn solid solution. *Journal of Phase Equilibria and diffusion*, **27** (2006), 333-342, by Y.W. Cui, K. Oikawa, R. Kainuma and K. Ishida.

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2.6.6 Fe-B alloys

- Modelling of primary bcc-Fe crystal growth in a Fe85B15 amorphous alloy. *Acta Materialia*, **53** (2005), 2231-2239, by M. Palumbo and M. Baricco.



2.6.7 Fe-Pd and Ni-Pd diffusion couples

- Analysis of the Kirkendall effect, marker migration and pore formation. *Acta Materialia*, **49** (2001), 1311-1317, by J Ågren and L Höglund.

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