

References for DICTRA and its Applications

The references selectively listed in this document are 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 it. A search of the literature will also include other available references not listed here.

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

A.1 General description of DICTRA and its applications

1. Andersson, J.-O., Helander, T., Höglund, L., Shi, P. & Sundman, B. Thermo-Calc & DICTRA, computational tools for materials science. *Calphad* **26**, 273–312 (2002).
2. Andersson, J.-O., Höglund, L., Jönsson, B. & Ågren, J. in *Fundamentals and Applications of Ternary Diffusion: Proceedings of Metallurgical Society of Canadian Institute of Mining and Metallurgy* (ed. Purdy, G. R.) 153–163 (Elsevier, 1990).
3. Borgenstam, A., Höglund, L., Ågren, J. & Engström, A. DICTRA, a tool for simulation of diffusional transformations in alloys. *J. Phase Equilibria* **21**, 269–280 (2000).

A.2 Models for diffusivities/mobilities in DICTRA

1. Andersson, J.-O. & Ågren, J. Models for numerical treatment of multicomponent diffusion in simple phases. *J. Appl. Phys.* **72**, 1350–1355 (1992).
2. Helander, T. & Ågren, J. A phenomenological treatment of diffusion in Al–Fe and Al–Ni alloys having B2-b.c.c. ordered structure. *Acta Mater.* **47**, 1141–1152 (1999).
3. Jönsson, B. Ferromagnetic ordering and diffusion of carbon and nitrogen in bcc Cr–Fe–Ni alloys. *Zeitschrift für Met.* **85**, 498–501 (1994).
4. Jönsson, B. On Ferromagnetic Ordering and Lattice Diffusion: A Simple Model. *Zeitschrift für Met.* **83**, 349–355 (1992).

A.3 Numerical method for solving the multicomponent diffusion equation

- Ågren, J. Numerical treatment of diffusional reactions in multicomponent alloys. *J. Phys. Chem. Solids* **43**, 385–391 (1982).

A.4 Numerical method for moving boundary problems

- Crusius, S., Inden, G., Knoop, U., Höglund, L. & Ågren, J. On the numerical treatment of moving boundary problems. *Zeitschrift für Met.* **83**, 673–678 (1992).

A.5 Numerical method for diffusion in dispersed systems

- Engström, A., Höglund, L. & Ågren, J. Computer simulation of diffusion in multiphase systems. *Metall. Mater. Trans. A* **25**, 1127–1134 (1994).

A.6 Numerical method for coarsening of precipitates

- Gustafson, Å., Höglund, L. & Ågren, J. Simulation of carbo-nitride coarsening in multicomponent Cr-steels for high temperature applications. in *Advanced heat resistant steels for power generation. Conference (San Sebastian, Spain 27/04/1998)* (1998).

A.7 Numerical method for diffusion through multiphase structures

- Larsson, H. & Engström, A. A homogenization approach to diffusion simulations applied to $\alpha + \gamma$ Fe–Cr–Ni diffusion couples. *Acta Mater.* **54**, 2431–2439 (2006).

References with applications treated by DICTRA

A.8 Steels

Solidification and microsegregation

1. Baldissin, D., Palumbo, M. & Battezzati, L. Modelling and Experiments of Solidification of AISI 304. *La Metall. Ital.* **0**, 25–32 (2007).
2. Hallstedt, B., Balitchev, E., Shimahara, H. & Neuschütz, D. Semi-solid Processing of Alloys: Principles, Thermodynamic Selection Criteria, Applicability. *ISIJ Int.* **46**, 1852–1857 (2006).
3. Heno, H. M., Sugiyama, A. & Nogita, K. Comparison of solidification behavior between in situ observation and simulation of Fe–C–Si system. *J. Alloys Compd.* **613**, 132–138 (2014).
4. Kim, H. S., Kobayashi, Y. & Nagai, K. Simulation of the influence of phosphorus on the prior austenite grain size of high-impurity steels. *Acta Mater.* **54**, 2441–2449 (2006).
5. Kim, H. S., Kobayashi, Y. & Nagai, K. Prediction of Prior Austenite Grain Size of High-phosphorous Steels through Phase Transformation Simulation. *ISIJ Int.* **46**, 854–858 (2006).
6. Lee, H. M., Bae, J. S., Soh, J. R., Kim, S. K. & Lee, Y. D. Diffusional Solidification Behavior in 304 Stainless Steel. *Mater. Trans. JIM* **39**, 633–639 (1998).
7. Lippard, H. E. *et al.* Microsegregation behavior during solidification and homogenization of AerMet100 steel. *Metall. Mater. Trans. B* **29**, 205–210 (1998).
8. Püttgen, W., Hallstedt, B., Bleck, W., Löffler, J. F. & Uggowitzer, P. J. On the microstructure and properties of 100Cr6 steel processed in the semi-solid state. *Acta Mater.* **55**, 6553–6560 (2007).

Homogenisation

- Zhang, Y., Chen, W. Q., Chen, L., Yan, Q. Z. & Sun, J. Homogenisation of 20SiMn2MoV steel ingots: thermodynamic/kinetic simulation and experimental validation. *Mater. High Temp.* **32**, 412–418 (2015).

Austenite → Ferrite transformation

1. Ågren, J. Computer simulations of the austenite/ferrite diffusional transformations in low alloyed steels. *Acta Metall.* **30**, 841–851 (1982).
2. Babu, S. S., Quintana, M. A. & David, S. A. Modeling Microstructure Development in Self-Shielded Flux Cored Arc Welds. *Weld. J. (Miami, FL, United States)* **80**, 91s–97s (2001).
3. Crusius, S., Höglund, L., Knoop, U., Inden, G. & Ågren, J. On the growth of ferrite allotriomorphs in Fe–C alloys. *Zeitschrift für Met.* **83**, 729–738 (1992).

4. De Avellez, R. R., Da Costa e Silva, A. L. V. & Rocha, A. C. The influence of Ti, Nb and S on the austenite decomposition and the precipitation in if ("interstitial free") steels. in *58° Congresso Anual da ABM (58th Annual ABM International Congress) 21-24 July 2003* (2003).
5. Franke, P. & Inden, G. An assessment of the Si mobility and the application to phase transformations in silicon steels. *Zeitschrift für Met.* **88**, 795–799 (1997).
6. Ghosh, G. & Olson, G. B. Simulation of paraequilibrium growth in multicomponent systems. *Metall. Mater. Trans. A* **32**, 455–467 (2001).
7. Li, J.-B., Yang, C. & Dong, H. Computer simulations of phase transformation in steels. *Mater. Des.* **22**, 39–43 (2001).
8. Liu, Z.-K. in *The Minerals, Metals and Minerals Society* (eds. Johnson, W. C., Delany, J. M., Laughlin, D. E. & Soffa, W. A.) 39–44 (1994).
9. Saha, A., Ghosh, G. & Olson, G. B. An assessment of interfacial dissipation effects at reconstructive ferrite–austenite interfaces. *Acta Mater.* **53**, 141–149 (2005).
10. Thuillier, O., Danoix, F., Gouné, M. & Blavette, D. Atom probe tomography of the austenite–ferrite interphase boundary composition in a model alloy Fe–C–Mn. *Scr. Mater.* **55**, 1071–1074 (2006).
11. Zhang, G.-H., Heo, Y.-U., Song, E.-J. & Suh, D.-W. Kinetic transition during the growth of proeutectoid ferrite in Fe-C-Mn-Si quaternary steel. *Met. Mater. Int.* **19**, 153–158 (2013).
12. Zhang, Y., Mo, C., Li, D. & Li, Y. Modelling of Phase Transformation of Plain Carbon Steels during Continuous Cooling. *J. Mater. Sci. Technol.* **19**, 262–264 (2003).

Growth of secondary austenite

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

Annealing of austenite

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

Growth/dissolution of Carbides, Nitrides and intermetallic phases

1. Bjärbo, A. Computer simulation of growth and coarsening of Laves phase in a modified 12% chromium steel. *Scand. J. Metall.* **32**, 94–99 (2003).
2. Bjärbo, A. & Hättestrand, M. Complex carbide growth, dissolution, and coarsening in a modified 12 pct chromium steel—an experimental and theoretical study. *Metall. Mater. Trans. A* **32**, 19–27 (2001).
3. Da Silva, W. S., Garzón, C. M., Goldstein, H. & Tschiptschin, A. P. Numerical and Experimental Study on The Eutectic-Carbide M₂C Decomposition Kinetics During Heat Treatment Of As Cast M₂ High-Speed Steels. in *59° Congresso Anual da ABM / 59th Annual Congress - International* (2004). at <http://www.abmbrasil.com.br/portal-tecnologico/portal/revista_tecnologia/resumo.asp?cd=42>
4. De Avellez, R. R., Marinkovic, B., Da Costa e Silva, A. L. V. & Rizzo, F. Kinetics of carbide precipitation in a 2.25Cr-1Mo steel. in *59° Congresso Anual da ABM / 59th Annual Congress - International* (2004). at <http://www.abmbrasil.com.br/portal-tecnologico/portal/revista_tecnologia/resumo.asp?cd=42>

5. Garzón, C. M., Serna, C. A., Brandi, S. D. & Ramirez, A. J. The relationship between atomic partitioning and corrosion resistance in the weld-heat affected zone microstructures of UNS S32304 duplex stainless steel. *J. Mater. Sci.* **42**, 9021–9029 (2007).
6. Ghosh, G. & Olson, G. B. Precipitation of paraequilibrium cementite: Experiments, and thermodynamic and kinetic modeling. *Acta Mater.* **50**, 2099–2119 (2002).
7. Hosseini, S. B., Dahlgren, R., Rytberg, K. & Klement, U. Dissolution of Iron-chromium Carbides during White Layer Formation Induced by Hard Turning of AISI 52100 Steel. *Procedia CIRP* **14**, 107–112 (2014).
8. Knežević, V., Balun, J., Sauthoff, G., Inden, G. & Schneider, A. Design of martensitic/ferritic heat-resistant steels for application at 650 °C with supporting thermodynamic modelling. *Mater. Sci. Eng. A Struct. Mater. Prop. Microstruct. Process.* **477**, 334–343 (2008).
9. Li, H., Mi, Z., Zhang, X., Tang, D. & Wang, Y. Carbide dissolution during intercritical austenitization in bearing steel. *J. Wuhan Univ. Technol. Sci. Ed.* **29**, 1242–1245 (2014).
10. Liu, Z.-K., Höglund, L., Jönsson, B. & Ågren, J. An experimental and theoretical study of cementite dissolution in an Fe-Cr-C alloy. *Metall. Trans. A* **22**, 1745–1752 (1991).
11. Luzginova, N. V., Zhao, L. & Sietsma, J. The Cementite Spheroidization Process in High-Carbon Steels with Different Chromium Contents. *Metall. Mater. Trans. A* **39**, 513–521 (2008).
12. Nilsson, J.-O. Prediction of Properties in Type 347 Austenitic Stainless Steel after Long-Term Service at High Temperatures. *Mater. Sci. Forum* **539-543**, 4920–4925 (2007).
13. Schneider, A. & Inden, G. Simulation of the kinetics of precipitation reactions in ferritic steels. *Acta Mater.* **53**, 519–531 (2005).
14. Shtansky, D. V. & Inden, G. Phase Transformation in Fe-Mo-C And Fe-W-C Steels—I. The Structural Evolution During Tempering at 700°C. *Acta Mater.* **45**, 2861–2878 (1997).
15. Tancret, F. & Laigo, J. The Combination of Modeling Techniques to Predict the Service Behaviour of Heat Resistant Alloys. *Mater. Sci. Forum* **539-543**, 3070–3075 (2007).

Carbide coarsening

1. Gustafson, Å. Coarsening of TiC in austenitic stainless steel — experiments and simulations in comparison. *Mater. Sci. Eng. A Struct. Mater. Prop. Microstruct. Process.* **287**, 52–58 (2000).
2. Gustafson, Å. & Hättstrand, M. Coarsening of precipitates in an advanced creep resistant 9% chromium steel—quantitative microscopy and simulations. *Mater. Sci. Eng. A Struct. Mater. Prop. Microstruct. Process.* **333**, 279–286 (2002).
3. Hu, X., Li, L., Wu, X. & Zhang, M. Coarsening behavior of M23C6 carbides after ageing or thermal fatigue in AISI H13 steel with niobium. *Int. J. Fatigue* **28**, 175–182 (2006).
4. Hu, X., Zhang, M., Wu, X. & Li, L. Simulations of Coarsening Behaviour for M23C6 Carbides in AISI H13 Steel. *J. Mater. Sci. Technol.* **22**, 153–158 (2006).
5. Xiao, X. & Liu, G. Coarsening behavior for M23C6 carbide in 12 %Cr-reduced activation ferrite/martensite steel: experimental study combined with DICTRA simulation. *J. Mater. Sci.* **48**, 5410–5419 (2013).

Sigma phase formation in stainless steels

1. Erneman, J. *et al.* Comparison between quantitative metallography and modeling of σ -phase particle growth in AISI 347 stainless steel. *Metall. Mater. Trans. A* **36**, 2595–2600 (2005).
2. Hertzman, S., Pettersson, R., Frisk, K. & Jerwin, T. The relation between alloy composition and kinetics of intermetallic phase formation. in *Duplex 2000: Proceedings, 6th World Conference and Expo* 347–354 (2000).
3. Karlsson, L., Rigdal, S. & Pak, S. Effects of elemental distribution on precipitation behaviour and properties of duplex stainless steel weldments. in *Duplex 2000: Proceedings, 6th World Conference and Expo* 693–702 (2000).
4. Schwind, M., Källqvist, J., Nilsson, J.-O., Ågren, J. & Andrén, H.-O. σ -Phase Precipitation in Stabilized Austenitic Stainless Steels. *Acta Mater.* **48**, 2473–2481 (2000).

Interdiffusion in compounds and cladding steels

1. Engström, A., Höglund, L. & Ågren, J. Computer simulation of diffusion in multiphase systems. *Metall. Mater. Trans. A* **25**, 1127–1134 (1994).
2. Foret, R., Zlamal, B. & Sopoušek, J. Structural stability of dissimilar weld between two Cr-Mo-V steels. *Weld. J.* **85**, (2006).
3. Helander, T., Ågren, J. & Nilsson, J.-O. An Experimental and Theoretical Investigation of Diffusion across a Joint of Two Multicomponent Steels. *ISIJ Int.* **37**, 1139–1145 (1997).
4. Helander, T., Andersson, H. C. M. & Oskarsson, M. Structural changes in 12–2.25% Cr weldments – an experimental and theoretical approach. *Mater. High Temp.* **17**, 389–396 (2000).
5. Omichi, M., Sato, M., Tokunaga, T., Ohtani, H. & Hasebe, M. Diffusion behavior at the interface of cladding steels. *Nippon Kinzoku Gakkaishi* **68**, 1013–1019 (2004).
6. Sopoušek, J. & Foret, R. Carbon and nitrogen redistribution in weld joint of ion nitrided 15CrMoV 2-5-3 and advanced P91 heat-resistant steels. *J. Phase Equilibria Diffus.* **27**, 363–369 (2006).
7. Zlámal, B., Foret, R., Buršík, J. & Svoboda, M. Microstructural Stability of Dissimilar Weld Joint of Creep-Resistant Steels with Increased Nitrogen Content at 500 – 900 °C. *Defect Diffus. Forum* **263**, 195–200 (2007).

Carburizing

1. Bernst, R., Inden, G. & Schneider, A. Carburisation of Fe–X (X=Si, Mo, V) diffusion couples. *Calphad* **32**, 207–216 (2008).
2. Engström, A., Höglund, L. & Ågren, J. Computer simulation of diffusion in multiphase systems. *Metall. Mater. Trans. A* **25**, 1127–1134 (1994).
3. Kuehmann, C. J., Wise, J. P., Olson, G. B. & Campbell, C. E. Simulation of Carburization in Secondary Hardening Steels - Heat Treating Society. in *Proceedings of the 17th Conference: 1997 Induction Heat Treating Symposium* 313–319 (ASM International, 1998).
4. Sproge, L. & Ågren, J. Experimental and theoretical studies of gas consumption in the gas carburizing process. *J. Heat Treat.* **6**, 9–19 (1988).
5. Tanaka, K., Ikehata, H., Nakanishi, K. & Nishikawa, T. Growth Simulation of Spheroidized Carbide in the Carbide-Dispersed Carburizing Process. *Metall. Mater. Trans. A* **39**, 1248–1257 (2008).
6. TMS. Process design and optimization for high-temperature vacuum carburizing. in *Materials Science & Technology 2003 Conference, Modeling, Control, and Optimization in Ferrous and Non-Ferrous Industry* 381–395 (2003).

7. Turpin, T., Dulcy, J. & Gantois, M. Carbon diffusion and phase transformations during gas carburizing of high-alloyed stainless steels: Experimental study and theoretical modeling. *Metall. Mater. Trans. A* **36**, 2751–2760 (2005).
8. Yamashita, T., Tosaka, A., Aratani, M. & Narutani, T. Kinetic Analysis of Decarburizing during Continuous Annealing in Extra Low Carbon Steel. *Tetsu-to-Hagane* **85**, 821–826 (1999).

Nitriding and Nitrocarburizing

1. Du, H. & Ågren, J. Gaseous nitriding iron - evaluation of diffusion data of N in gamma' and epsilon phases. *Zeitschrift für Met.* **86**, 522–529 (1995).
2. Du, H., Lange, N. & Ågren, J. Formation of compound layers on iron during gas nitriding. *Surf. Eng.* **11**, 301–307 (1995).
3. Du, H. & Ågren, J. Theoretical treatment of nitriding and nitrocarburizing of iron. *Metall. Mater. Trans. A* **27**, 1073–1080 (1996).
4. Franco, A. R., Garzón, C. M. & Tschiptschin, A. P. Numerical and experimental study on plasma nitriding kinetics of tool steels (Análise numérica e experimental da cinética de nitretação a plasma de aços-ferramenta). in *58° Congresso Anual da ABM (58th Annual ABM International Congress) 21-24 July 2003* 3324 (2003). at <http://www.abmbrasil.com.br/portal-tecnologico/portal/revista_tecnologia/resumo.asp?cd=42>
5. Garzón, C. M. & Tschiptschin, A. P. Growth kinetics of martensitic layers during high temperature gas nitriding of a ferritic – martensitic stainless steel. *Mater. Sci. Technol.* **20**, 915–918 (2004).
6. Larsson, H. & Ågren, J. Gas nitriding of high vanadium steels—experiments and simulations. *Metall. Mater. Trans. A* **35**, 2799–2802 (2004).
7. Nakada, N. *et al.* Thermodynamics and kinetics of solution nitriding. *Calphad* **47**, 168–173 (2014).
8. Ospina, C. M. & Tschiptschin, A. P. Temperature-Pressure-Time Diagrams for Predicting Optimal Nitriding Parameters During High Temperature Gas Nitriding of Stainless Steels (Diagramas temperatura-pressão-tempo para otimizar os parâmetros de tratamento durante a nitretação gasosa em alta tem. in *59° Congresso Anual da ABM / 59th Annual Congress - International* (2004). at <http://www.abmbrasil.com.br/portal-tecnologico/portal/revista_tecnologia/resumo.asp?cd=42>

A.9 Nickel-based superalloys

Solidification and microsegregation

1. Meurer, B., Spencer, P. J. & Neuschütz, D. Simulation of solidification and heat treatment of nickel-base superalloy SC16. *Zeitschrift für Met.* **94**, 139–143 (2003).
2. Tancret, F. Thermo-Calc and DICTRA simulation of constitutional liquation of gamma prime (γ') during welding of Ni base superalloys. *Comput. Mater. Sci.* **41**, 13–19 (2007).
3. Walter, C., Hallstedt, B. & Warnken, N. Simulation of the solidification of CMSX-4. *Mater. Sci. Eng. A Struct. Mater. Prop. Microstruct. Process.* **397**, 385–390 (2005).

Interdiffusion

1. Baufeld, B., Bartsch, M., Brož, P. & Schmücker, M. Microstructural changes as postmortem temperature indicator in Ni–Co–Cr–Al–Y oxidation protection coatings. *Mater. Sci. Eng. A Struct. Mater. Prop. Microstruct. Process.* **384**, 162–171 (2004).
2. Campbell, C. E., Zhao, J.-C. & Henry, M. F. Examination of Ni-base superalloy diffusion couples containing multiphase regions. *Mater. Sci. Eng. A* **407**, 135–146 (2005).
3. Campbell, C. E., Zhao, J.-C. & Henry, M. F. Comparison of Experimental and Simulated Multicomponent Ni-Base Superalloy Diffusion Couples. *J. Phase Equilibria Diffus.* **25**, 6–15 (2004).
4. Chen, H., Jin, Z., Liu, C. & Zhou, K. Diffusion and phase transformation on interface between substrate and NiCrAlY in Y-PSZ thermal barrier coatings. *J. Therm. Spray Technol.* **13**, 515–520 (2004).
5. Dahl, K. V., Hald, J. & Horsewell, A. Interdiffusion Between Ni-Based Superalloy and MCrAlY Coating. *Defect Diffus. Forum* **258-260**, 73–78 (2006).
6. Du, Y. & Schuster, J. C. An effective approach to describe growth of binary intermediate phases with narrow ranges of homogeneity. *Metall. Mater. Trans. A* **32**, 2396–2400 (2001).
7. Engström, A., Morral, J. E. & Ågren, J. Computer simulations of Ni-Cr-Al multiphase diffusion couples. *Acta Mater.* **45**, 1189–1199 (1997).
8. Gómez-Acebo, T., Navarcorena, B. & Castro, F. Interdiffusion in multiphase, Al-Co-Cr-Ni-Ti diffusion couples. *J. Phase Equilibria Diffus.* **25**, 237–251 (2004).
9. Helander, T. & Ågren, J. Diffusion in the B2-BCC phase of the Al–Fe–Ni system—application of a phenomenological model. *Acta Mater.* **47**, 3291–3300 (1999).
10. Jung, A. & Schnell, A. Crack growth in a coated gas turbine superalloy under thermo-mechanical fatigue. *Int. J. Fatigue* **30**, 286–291 (2008).
11. Yao, Y. *et al.* Elements Diffusion Law of DD407/FGH95 Diffusion Bonding Under Hot Isostatic Pressing . I. Building Diffusion Bonding Model. *Acta Metall. Sin.* **49**, 1041 (2013).

Precipitate Growth/Dissolution

1. Bao, G. *et al.* Modeling of precipitation and Cr depletion profiles of Inconel 600 during heat treatments and LSM procedure. *J. Alloys Compd.* **419**, 118–125 (2006).
2. Bao, G., Yamamoto, M. & Shinozaki, K. Precipitation and Cr depletion profiles of Inconel 182 during heat treatments and laser surface melting. *J. Mater. Process. Technol.* **209**, 416–425 (2009).
3. Miller, M. K., Babu, S. S. & Vitek, J. M. Stability of γ' precipitates in a PWA1480 alloy. *Intermetallics* **15**, 757–766 (2007).
4. Turchi, P. E. A., Kaufman, L. & Liu, Z.-K. Modeling of Ni–Cr–Mo based alloys: Part II — Kinetics. *Calphad* **31**, 237–248 (2007).
5. Zhang, M., Dong, J., Zeng, Y. & Xie, X. A kinetic analysis on carbide growth behavior and Cr depletion region evolution near grain boundary of inconel 690 during thermal treatment processes. *Xiyou Jinshu Cailiao yu Gongcheng (Rare Met. Mater. Eng.)* **34**, 58–61 (2005).
6. Zhang, M., Cao, G., Dong, J., Zheng, L. & Yao, Z. Investigations on Dissolution Mechanism of Laves Phase in Gh4169 Alloy Ingot Based on Classical Dynamical Model. *Acta Metall. Sin.* **49**, 372 (2013).

Coarsening of γ precipitates

- Gustafson, Å., Höglund, L. & Ågren, J. Simulation of carbo-nitride coarsening in multicomponent Cr-steels for high temperature applications. in *Advanced heat resistant steels for power generation. Conference (San Sebastian, Spain 27/04/1998)* (1998).

Transient liquid-phase bonding

- Campbell, C. E. & Boettinger, W. J. Transient liquid-phase bonding in the Ni-Al-B system. *Metall. Mater. Trans. A* **31**, 2835–2847 (2000).

A.10 Aluminum based alloys**Solidification and microsegregation**

1. Larouche, D. Computation of solidification paths in multiphase alloys with back-diffusion. *Calphad* **31**, 490–504 (2007).
2. Hallstedt, B., Balitchev, E., Shimahara, H. & Neuschütz, D. Semi-solid Processing of Alloys: Principles, Thermodynamic Selection Criteria, Applicability. *ISIJ Int.* **46**, 1852–1857 (2006).
3. Battezzati, L. *et al.* Amorphisation and Devitrification of Al-Transition Metal- Rare Earth Alloys. in *Symposium MM – Amorphous and Nanocrystalline Metals* **806**, 21–32 (2003).
4. Balitchev, E., Meuser, H., Neuschütz, D. & Bleck, W. Experimental Investigation and Computer Simulation of the Liquid Fraction Evolution during the Solidification of Alloys Suitable for Semi-Solid Processing. *Steel Res. Int.* **75**, 13–19 (2004).

Precipitate dissolution

1. Thompson, R. G. & Malam, C. A DICTRA Simulation of theta-Phase Dissolution in Al-Cu Alloys. in *Nucleation and growth processes in materials Symposium, Nucleation and growth processes in materials (Materials Research Society Symposium Proceedings)* **580**, 27–34 (Materials Research Society, 2000).
2. Samaras, S. N. & Haidemenopoulos, G. N. Modelling of microsegregation and homogenization of 6061 extrudable Al-alloy. *J. Mater. Process. Technol.* **194**, 63–73 (2007).

Precipitate growth

- Hurtado, I. *et al.* Combined thermodynamic and kinetic computational simulation of heat treatments: precipitation of metastable phases in Al alloys. in *Third ASM International Europe Heat Treatment and Surface Engineering Conference in Europe (Proceedings of the 10th Congress of the IFHT)* 577–588 (1999).

Laser hardening and laser welding

1. Zervaki, A. D. & Haidemenopoulos, G. N. Computational Kinetics Simulation of the Dissolution and Coarsening in the HAZ during Laser Welding of 6061-T6 Al-Alloy. *Weld. J. (Miami, FL, United States)* **86**, 211–s (2007).
2. Haidemenopoulos, G. N. Coupled thermodynamic/kinetic analysis of diffusional transformations during laser hardening and laser welding. *J. Alloys Compd.* **320**, 302–307 (2001).

A.11 Cemented carbides

Diffusion in the liquid Co binder

- Walbrühl, M. Diffusion in the liquid Co binder of cemented carbides: Ab initio molecular dynamics and DICTRA simulations. (KTH Royal Institute of Technology, 2014).

Gradient sintering

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

Diffusion during sintering

1. He, Y., Li, L., Huang, S., Vleugels, J. & Van der Biest, O. Computer simulating the diffusion behavior of V and W in Co binder layer of WC–Co cemented carbide. *J. Alloys Compd.* **436**, 146–149 (2007).
2. He, Y., Li, L., Huang, S., Jef, V. & Van der Biest, O. Computer simulation of W-C-Co-V system diffusion couples. *Rare Met.* **26**, 492–497 (2007).
3. Haglund, S. & Ågren, J. W content in Co binder during sintering of WC–Co. *Acta Mater.* **46**, 2801–2807 (1998).

A.12 PM steels

Diffusion during sintering

- Shykula, P., Dudrová, E., Frykholm, R. & Bengtsson, S. Application of Computational Software for Design and Study New Types of Alloys. *Powder Metall. Prog.* **13**, 3–10 (2013).

A.13 Solders

Sn-Ag-Cu solders

- Ghosh, G. Dissolution and interfacial reactions of thin-film Ti/Ni/Ag metallizations in solder joints. *Acta Mater.* **49**, 2609–2624 (2001).

A.14 Other alloys

Au-Ni alloys

- Wang, J., Liu, L. B., Liu, H. S. & Jin, Z. P. Assessment of the diffusional mobilities in the face-centred cubic Au–Ni alloys. *Calphad* **31**, 249–255 (2007).

Al-Cu alloys

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

Al-Cu-Mn alloys

- Yin, M. & Du, Y. Diffusivities and atomic mobilities in Cu-rich fcc Al–Cu–Mn alloys. *Int. J. Mater. Res.* **103**, 807–813 (2012).

Al-Zn alloys

- Cui, Y. W., Oikawa, K., Kainuma, R. & Ishida, K. Study of Diffusion Mobility of Al–Zn Solid Solution. *J. Phase Equilibria Diffus.* **27**, 333–342 (2006).

Co-Fe and Co-Ni alloys

- Cui, Y. W. *et al.* Computational Study of Atomic Mobility for fcc Phase of Co-Fe and Co-Ni Binaries. *J. Phase Equilibria Diffus.* **29**, 2–10 (2007).

Cu-Ni alloys

1. Wang, J., Liu, H. S., Liu, L. B. & Jin, Z. P. Assessment of diffusion mobilities in FCC Cu–Ni alloys. *Calphad* **32**, 94–100 (2008).
2. Rahman, A. H. M. E. & Cavalli, M. N. Diffusion bonding of commercially pure Ni using Cu interlayer. *Mater. Charact.* **69**, 90–96 (2012).

Fe-B alloys

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

Fe-Pd and Ni-Pd diffusion couples

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

Fe-Si-Al alloys

- Barros, J., Schneider, J. & Houbaert, Y. Assessment of Si and Al diffusion for the production of high Si and high Si–Al electrical steel. *J. Magn. Magn. Mater.* **320**, e389–e392 (2008).

TiC

- Zhu, W. J. *et al.* Modeling and simulation of the TiC reaction layer growth during active brazing of diamond using DICTRA. *Comput. Mater. Sci.* **78**, 74–82 (2013).

Pu alloys

- Turchi, P. E. A., Kaufman, L., Zhou, S. & Liu, Z.-K. Thermochemical and kinetics of transformations in Pu-based alloys. *J. Alloys Compd.* **444–445**, 28–35 (2007).

Zn-Fe-Al alloy for galvanizing

- Bai, K. & Wu, P. Assessment of the Zn–Fe–Al system for kinetic study of galvanizing. *J. Alloys Compd.* **347**, 156–164 (2002).