Nathalie Dupin

Ingénieur-Docteur matériaux

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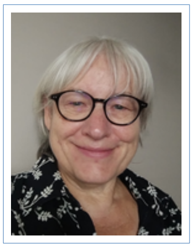

Compétences

Qualités: rigeur, pragmatisme, logique, curiosité, réactivité, créativité, gestion de projets, sens du contact, de la communication, de l'interaction.

Matériaux: fusion, ségrégation, interaction entre matériaux, équilibres impliquant la phase gazeuse, transformations de phases, états hors équilibre, microstructures, traitements thermiques, ATD, crystallographie, ...

Informatique: calcul thermodynamique, html, javascript, python, linux

Langues: anglais, espagnol

Participation à des projets de recherche

2013-2018 **TAF-ID**, *OCDE-AEN*, Thermodynamics of Advanced Fuels International Database

2011-2013 **ARMIDE**, *ANR*, Alliages de Rhénium : Modélisation, Intermétalliques et Diagrammes de phasEs

2008-2013 **F-BRIDGE**, *EC - FP7*, Basic research for innovative fuels design for GEN IV systems

2003-2007 **THALU**, *COST 535*, Thermodynamics of Alloyed Aluminides

2001-2017 **Ni14-Ni25**, *Aubert et Duval, SafranTech, General Electric, TCSAB*, Succession de projets visant à développer une base de données thermodynamiques pour superalliages base Ni

Expérience professionnelle

1998-2025 **Consultante**, *Calcul Thermodynamique, SIRET 41986119000025*, Orcet,
Constitution de bases de données thermodynamiques, calculs avec des bases de données existantes, formation à l'utilisation du logiciel ThermoCalc, à la modélisation thermodynamique pour différents types de matériaux

2021-2023 **Vacataire**, *Sigma Clermont*, Aubière, Initiation au calcul thermodynamique - 20h/an

2018-2019 **Experte senior**, *Eramet Ideas*, Trappes, Thermodynamique et métallurgie - 2 mois

1996-1998 **Post-doc**, *LTPCM, aujourd'hui SIMAP*, Grenoble, en collaboration avec I. Ansara
Constitution de bases de données thermodynamiques pour des alliages base Zr et Ni.

1995-1996 **Post-doc**, *ENSMP*, Evry, en collaboration avec Y. Bienvenu et M. Boussuge
Etude de la réactivité de bétons avec le corium.

1991 **Stage de 6 mois**, *Aubert et Duval*, Les Ancizes, Solidification des superalliages

Diplômes et Études

1995 **Doctorat Science et Génie des Matériaux**, *INP Grenoble*,
Contribution à l'évaluation thermodynamique des alliages polyconstitués à base de nickel, sous la direction de I. Ansara

1991 **Ingénieure Chimiste**, *ENSC Clermont-Ferrand (SIGMA)*, option Matériaux Inorganiques
DEA (Master) Chimie, *Université Blaise Pascal (UCA)*, Clermont-Ferrand

Prix

2016 **Hume-Rothery award**, *Institute of Materials, Minerals and Mining*, Londres, UK

Actions de formation

TRANSVALOR, Sophia Antipolis, 30/01-01/02 2024, Formation à Thermo-Calc pour débutants
CEA, Saclay, 4-5 octobre 2023, Formation à Thermo-Calc pour débutants
CEZUS, Ugine, 5-6 septembre 2023, Formation avancée à Thermo-Calc
CETIM, Sèvres, 30/05-02/06 2023, Formation à DICTRA et TC-PRISMA
SATA 2022, School for Advanced Thermodynamic Assessments, organised by the CIRIMAT laboratory, University of Toulouse in Toulouse, France from June 27 to July 1 2022, Crystallography and ordering, Files integrating experimental data, Finalising and documentation
SIGMA-Clermont - Cours électif S8 - Calphad : Outils numériques de calcul thermodynamique pour les matériaux - Aubière, 2021, 2022 et 2023
Eramet Ideas, Calcul Thermodynamique - Trappes, 24-25 septembre 2019
Safran Aircraft, Formation à lutilisation de Thermo-Calc, Dictra et Prisma - Gennevilliers, 18-19 septembre 2019
IRSN, Orcet, 15 juin 2018, Thermo-Calc, utilisation avancéee
CEA, Cadarache, 11-12 juin 2018, Formation à l'utilisation de la TAF-ID
SATA 2017, School for Advanced Thermodynamic Assessments, organisée par le CEA, Presqu'île de Giens, 3-7 juillet 2017, Crystallography and ordering, Files integrating experimental data, Finalizing and documentation
INDUSTEEL, Le Creusot, 27 et 28 janvier 2016, Formation à Thermo-Calc
SATA 2015, School for Advanced Thermodynamic Assessments, organisée par l'INSTN, Centre Port-Royal, France, 6-10 juillet 2015, Crystallography and ordering, Files integrating experimental data, Finalizing and documentation
CIRIMAT, Toulouse, France, 28 mai 2015, Mise en ordre, Introduction à l'optimisation de paramètres thermodynamiques avec PARROT.
SATA 2014, School for Advanced Thermodynamic Assessments, organisée par l'INSTN, Centre Port-Royal, 23-27 juin 2014, Crystallography and ordering, Finalising and documentation
CEA Valrho, Orcet, 19-20 mai 2014, ThermoCalc version classique
ERAMET, Trappes, 16 mai 2013, Getting into computational thermodynamics
CEA/IRSN, Orcet, 19-21 mars 2013, ThermoCalc version classique
CEA Marcoule, Orcet, 8-9 novembre 2011, ThermoCalc version classique
CEA Cadarache, Orcet, 4-6 juillet 2011, ThermoCalc version classique
INSTN, School Fundamentals of Thermodynamic Modelling of Materials, Saclay, France, 15-19 novembre 2010, Thermodynamic assessemnts
UGITECH, Ugine, 5-6 juillet 2010, ThermoCalc version classique
CEA, Cadarache, June 8-12, 2009, ThermoCalc version classique
SNECMA, Gennevilliers, Mars 2008, ThermoCalc
INPG, LTPCM, Grenoble, 11-13 Mars 2008, Constitution de bases de données thermodynamiques de type Calphad
CEZUS, Ugine, 4 Avril 2007, ThermoCalc Classique version R
AUBERT&DUVAL, Les Ancizes, 26 juin 2006, Formation avancée à ThermoCalc
CEA, Saclay, 25-28 avril 2005, ThermoCalc module 1&2
CEZUS, Ugine, 12-13 mai 2004, Formation thermodynamique

Présentations sur invitation

TMS Annual Meeting : Hume-Rothery Award Symposium : Thermodynamics, Phase Equilibria and Kinetics for Materials Design and Engineering, San Diego, CA, 24 Févier 2020, Tomorrow fcc ordering model
IMR, Katahira Campus, Tohoku University, Sendai, Japan, 28 février 2018, Constitution of Calphad

multicomponent databases
Aobayama Campus, Tohoku University, Sendai, Japan, 26 février 2018, Thermodynamic modelling of the γ/γ' phases in the Calphad approach
Birmingham University, School of Metallurgy and Materials, Birmingham, UK, 7 novembre 2016, Accuracy of Assessments, a CALPHAD introduction
Imperial College, Engineering Alloys Seminar Series, London, UK, 22 juin 2016, Constitution of Calphad multicomponent databases
Oxford, Computational Thermodynamics and Kinetics Seminar and Workshop, UK, 4-5 avril 2016, Accuracy of Assessments, a CALPHAD introduction
TMS Annual Meeting : Hume-Rothery Award Symposium : Multicomponent Alloy Metallurgy, the Bridge from Materials Science to Materials Engineering, Orlando, FL, 16-19 mars 2015, Constitution of Calphad multicomponent databases
Bochum, Modelling and Simulation of superalloys internatiobal workshop,Germany, 15-17 septembre 2014, Thermodynamic modelling of the γ/γ' phases in the Calphad approach
NIST Calphad Pro data workshop, Gaithersburg, MD, 29-30 avril 2014, Documenting thermodynamic databases
North Western University, Department of Materials Science and Engineering, Evanston, IL, 12 octobre 2013, Calphad at work on ordering
KTH Hero-m, Stockholm, Sweden, 27 aout 2012, Modeling the sigma phase in the ternary system Mo-Ni-Re using DFT
GE GRC, Niskayuna, NY, 31 mai 2012, An investigation of Re containing TCP phases via experiments and first principle calculations to improve their Calphad description
NIST gamma/gamma prime Co-base Superalloys Workshop, Gaithersburg, MD, 2 mai 2011, A deep revision of the Al-Co-Ni-W system calphad description
Saclay, International Information Exchange Meeting on Thermodynamics of Nuclear Fuels, organised by C. Guéneau, Saclay, France 27 novembre - 1 décembre 2007, Introduction to the Calphad approach (CALculation of PHAse Diagram)
TCSAB 10 years symposium, Stockholm, 18 octobre 2007, Modelling chemical ordering with Thermo-Calc
THALU, Final meeting of COST 535, Interlaken, Switzerland, 21-24 octobre 2007, fcc, bcc, hcp based binary phase diagram in the Al-Fe-Ni-Ti COST 535 system and their extrapolation into ternary : a Calphad-First-Principles study
ICMPE, Journée Modélisation et simulation, organised by J.M. Joubert, Thiais, France, 28 février 2006, Introduction à l'approche CALPHAD (CALculation of PHAse Diagram)
TofA, Wien, Austria, 12-18 septembre 2004, Modeling of the bcc ordering using the sublattice formalism
Himo Ansara memoriam symposium, Grenoble, France, 9 juin 2004, A case study of the modelling order-disorder transformations : Al-Fe-Ni
Calphad XXVIII, Grenoble, France, 2-7 mai 1999, Modelling intermetallics Phases II Laves mu and sigma phases, combining the Cluster Expansion and the Compound Energy Formalism
Calphad XXVI, Palm Coast, FL, 17-23 mai 1997, Ordering models in the Calphad approach

Publications

1. B. Sundman, N. Dupin, M. H. F. Sluiter, S. G. Fries, C. Guéneau, B. Hallstedt, U. R. Kattner, M. Selleby, The Legacy of " The Regular Model for Stoichimetric Phases and Ionic Melts" Journal of Phase Equilibria and Diffusion (2024), doi.org/10.1007/s11669-024-01163-2
2. J. C. Pereira dos Santos, S. Griesemer, N. Dupin, U. R. Kattner, Chuan Liu, D. Ivanova, T. Hammerschmidt, S. G. Fries, C. Wolverton, C. E. Campbell, Applying the Effective Bond Energy Formalism (EBEF) to Describe the Sigma (σ) Phase in the Co-Cr-Ni-Re System, Journal of Phase Equilibria and Diffusion (2023) doi.org/10.1007/s11669-023-01079-3
3. B. Sundman, N. Dupin, B. Hallstedt, Algorithms useful for calculating multi-component equilibria, phase diagrams and other kinds of diagrams, Calphad (2021)

doi.org/10.1016/j.calphad.2021.102330

4. A. Smith, M. Rutten, L. Hermann, E. Epifano, R.J.M. Konings, E. Colineau, J.-C. Griveau, C. Guéneau, N. Dupin, Experimental studies and thermodynamic assessment of the Ba-Mo-O system by the CALPHAD method, Journal of the European Ceramic Society (2021) doi.org/10.1016/j.jeurceramsoc.2021.01.010
5. C. Guéneau, N. Dupin, L. Kjellqvist, E. Geiger, M. Kurata, S. Gossé, E. Corcoran, A. Quaini, R. Hania, A.L. Smith, M.H.A. Piro, T. Besmann, P.E.A Turchi, J.C. Dumas, M.J. Welland, T. Ogata, B.O. Lee, J.R. Kennedey, C. Adkins, M. Bankhead, D. Costa, TAF-ID : An international thermodynamic database for nuclear fuels applications, Calphad 72 (2020) 102212. doi.org/10.1016/j.calphad.2020.102212
6. N. Dupin, U.R. Kattner, B. Sundman, M. Palumbo, S.G. Fries, Implementation of an Effective Bond Energy Formalism in the Multicomponent Calphad Approach, J. Res. Natl. Inst. Stand. Technol. 123 (2018) 123020. doi :10.6028/jres.123.020.
7. A. Quaini, C. Guéneau, S. Gossé, N. Dupin, B. Sundman, E. Brackx, R. Domenger, M. Kurata, F. Hodaj, Contribution to the themodynamic description of the corium - the U-Zr-O System, J. Nucl. Mat., 501C, 104-131 (2018).
8. E. C. Corcoran, J.-L. Flèche, N. Dupin, B. Sundman, and C. Guéneau, Thermodynamic Investigations of the Uranium-Molybdenum-Oxygen System by a Coupling of Density Functional Theory and CALPHAD Methodologies, Calphad, 63 196-211 (2018).
9. S. Gossé, N. Dupin, C. Guéneau, J.-C. Crivello and J.-M. Joubert, Thermodynamic assessment of the Pd-Rh-Ru system using calphad and first principles methods, J. Nucl. Mat., 474, 163-173 (2016).
10. F. Royer, N. Dupin, Y. Bienvenu, Degré de métastabilité obtenu en fabrication additive (SLM) de superalliages à base de nickel, Récents progrès en Génie des Procédés, Numéro 107, 2015, ISSN : 1775-335X ; ISBN : 978-2-910239-81-7, Ed. SFGP, Paris, France
11. T.N.P. Thi, J.-C. Dumas, V. Bouineau, N. Dupin, C. Guéneau, S. Gossé, P. Benigni, P. Maugis, J. Rogez, Thermodynamic assessment of the Cs-Te binary system, Calphad, 48, 1-12 (2015).
12. A. Breidi, M. Andasmas, J.-C. Crivello, N. Dupin and J.-M. Joubert, Experimental and computed phase diagrams of FeRe system, Journal of Physics : Condensed Matter, 26, 485402, 2014.
13. F. Körmann, A.A.H. Breidi, S.L. Dudarev, N. Dupin, G. Ghosh, T. Hickel, P. Korzhavyi, J.A. Muñoz, I. Ohnuma, Lambda transitions in materials science : Recent advances in Calphad and first-principles modelling, Phys. Status Solidi B, 251 (1), 53-80 (2014).
14. F. Stein, C. He, N. Dupin, Melting behaviour and homogeneity range of B2 CoAl and updated thermodynamic description of the Al-Co system, Intermetallics, 39, 58-68 (2013).
15. R. Mathieu, N. Dupin, J.C Crivello, K. Yaqoob, A. Breidi, J.M. Fiorani, N. David, J.M. Joubert, CALPHAD description of the Mo-Re system focused on the sigma phase modeling, CALPHAD, 43, 18-31 (2013).
16. D. Manara, R. Böhler, K. Boboridis, L. Capriotti, A. Quaini, L. Luzzi, F. De Bruycker, C. Guéneau, N. Dupin, R. Konings, The Melting Behaviour of Oxide Nuclear Fuels : Effects of the Oxygen Potential Studied by Laser Heating, Procedia Chemistry, 7, 505-512 (2012).
17. A. Berche, N. Dupin, C. Guéneau, C. Rado, B. Sundman, JC. Dumas, Calphad thermodynamic description of some binary systems involving U, Journal of Nuclear Materials, 411, 131-143 (2011).
18. C. Guéneau, N. Dupin, B. Sundman, C. Martial, J.-C. Dumas, S. Gossé, S. Chatain, F. De Bruycker, D. Manara, R.J.M. Konings, Thermodynamic modelling of advanced oxide and carbide nuclear fuels : description of the U-Pu-O-C systems, J. Nucl. Mat. 419 (1-3), 145-167 (2011).
19. P. Gotcu-Freis, J.-Y. Colle, C. Guéneau, N. Dupin, B. Sundman, R.J.M. Konings, A thermodynamic study of the Pu-Am-O system, J. Nucl. Mat., 414 (3) 408-421 (2011).
20. B. Sundman, C. Guéneau, N. Dupin, Modelling multiple defects in ionic phases like UO2$\pm$x using the compound energy formalism, Acta Materialia, 59 (15) 6039-6047 (2011).

21. F. De Bruycker, K. Boboridis, R.J.M. Konings, M. Rini, R. Eloirdi, C. Guéneau, N. Dupin, D. Manara, On the melting behaviour of uranium/plutonium mixed dioxides with high-Pu content : a laser heating study, J. Nucl. Mat., 419 (1-3), 186-193 (2011).
22. C. Toffolon-Masclet, J.-C. Brachet, C. Servant, J.-M. Joubert, P. Barberis, N. Dupin, P. Zeller, Contribution of Thermodynamic Calculations to Metallurgical Studies of Multi-Component Zirconium Based Alloys Eds. B. Kammenzind and M. Limback, Zirconium in the Nuclear Industry : 15th International symmposium, Book Series : American Society for Testing and Materials Special Technical Publications, Vol. 1505, p. 754-775 (2009).
23. J De Keyzer, G Cacciamani, N Dupin, P Wollants, Thermodynamic modeling and optimization of the Fe-Ni-Ti system, Calphad 33 (1), 109-123 (2009)
24. B. Sundman, I. Ohnuma, N. Dupin, U.R. Kattner, S.G. Fries, An assessment of the entire Al-Fe system including D03 ordering, Acta Materialia. 57 (2009) 2896.
25. N. Warnken, B. Böttger, S. G. Fries, N. Dupin, B. Sundman, Microstructure of a five-component Ni-base superalloy : experiments and simulation, The SGTE Casebook (Second Edition) 2008, 405-414.
26. B. Hallstedt, N. Dupin, M. Hillert, L. Hoglund, H. L. Lukas, J. C. Schuster, N. Solak, Thermodynamic models for crystalline phases. Composition dependent models for volume, bulk modulus and thermal expansion, Calphad, 31, 28-37 (2007)
27. N. Dupin, S.G. Fries, J.-M. Joubert, B. Sundman, M. Sluiter, Y. Kawazoe, A. Pasturel, Using first-principles results to calculate finite temperature thermodynamic properties of the Nb-Ni mu-phase in the Bragg-Williams approximation, Phil. Mag. 86, 1631-1641 (2006).
28. P. Barberis , N. Dupin , C. Lemaignan, A. Pasturel, J.M. Grange, ASTM No1467, 129 (2006)
29. J.-M. Joubert, N. Dupin, Mixed site occupancies in the mu phase, Intermetallics, 12, 1373-1380 (2004).
30. J.M. Joubert, B. Sundman, and N. Dupin, Assessment of. the Niobium-Nickel System, Calphad, 2004, 28(3), p 299-306
31. G. Reumont, P. Perrot, N. Dupin, Y. Dutheillet,Thermochemical prediction of high temperature corrosion of a Fe-20wt%Cr-10wt%Ni alloy : waste incinerator application, J. of Materials Science Letters, 22 (13), 975-977 (2003).
32. N. Dupin, B. Sundman, A thermodynamic database for Ni-base superalloys, Scand. J. Metall., 30, 184-192 (2001).
33. B.P. Burton, N. Dupin, S.G. Fries, G. Grimvall, A. Fernandez Guillermet, P. Miodownik, W. Alan Oates, V. Vinograd, Using Ab Initio Calculations in the Calphad Environment, Z. Metallkde, 92 (6), 514-525 (2001).
34. N. Dupin, I. Ansara, B. Sundman, Thermodynamic Re-Assessment of the Ternary System Al-Cr-Ni, Calphad, 25 (2), 279-298 (2001).
35. P. Liang, N. Dupin, S.G. Fries, H.J. Seifert, I. Ansara, H.L. Lukas, F. Aldinger, Thermodynamic assessment of the Zr-O binary system Z. fur Metallkunde, 92 (7), 747-756, (2001).
36. A. Kusoffsky, N. Dupin, B. Sundman, On the Compound Energy Formalism Applied to fcc Ordering, Calphad, 25 (4), 549-565 (2001).
37. G. Cacciamani, R. Ferro, I. Ansara, N. Dupin, Thermodynamic modelling of the Co-Ti system, Intermetallics, 8, 213-222 (2000).
38. N. Dupin, I. Ansara, On the Sublattice Formalism Applied to the B2 phase, Z. Metallkde, 90 (1), 76-85 (1999).
39. N. Dupin, I. Ansara, C. Servant, C. Toffolon, C. Lemaignan, J.C. Brachet, A thermodynamic database for zirconium alloys, J. Nucl. Mater., 275, 287-295 (1999).
40. I. Ansara, N. Dupin, J.M. Joubert, M. Latroche, A. Percheron-Guégan, Thermodynamic Study of the Cr-Ni-Zr system, J. Phase Equil., 19 (1), 6-10 (1998).

41. N. Dupin, I. Ansara, Evaluation Thermodynamique du système Al-Co, Rev. Métallurgique - CIT/Sci. Génie Matériaux, 9, 1121-1129 (1998).
42. I. Ansara, N. Dupin, H.L. Lukas, B. Sundman, Thermodynamic assessment of the Al-Ni system, J. Alloys and Comp., 247 (1-2), 20-30 (1997).
43. I. Ansara, N. Dupin, B. Sundman, Reply to the paper : When is a compound energy not a compound energy ? A critique of the 2-Sublattice Order/disorder model, Calphad, 21 (4), 535-542 (1997).
44. N. Dupin, I. Ansara, Thermodynamic assessment of the Cr-Ni-Ta system, Z. Metallkde, 87 (7), 555-561 (1996).
45. C. Guéneau, C. Servant, I. Ansara, N. Dupin, Thermodynamic assessment of the Si-Zr system, Calphad, 18 (3), 319-327 (1994).
46. N. Dupin, I. Ansara, Thermodynamic assessment of the Cr-Ta system, J. Phase Equil., 14 (4), 451-456 (1993).