

CURRICULUM VITAS OF YUNZHI WANG

Department of Materials Science and Engineering
2041 College Road, Columbus, OH43210
The Ohio State University

Phone (614)292-0682; Fax (614)292-1537
e-Mail: wang.363@osu.edu
Web: <https://mse.osu.edu/people/wang.363>

EDUCATION

Ph.D. in Materials Sci. & Eng., 1995, Rutgers, The State University of New Jersey
M.S. in Materials Sci. & Eng., 1992, Rutgers, The State University of New Jersey
M.S. in Metallurgy, 1985, Northeastern University, Shenyang, China
B.S. in Metallurgy, 1982, Northeastern University, Shenyang, China

PROFESSIONAL EXPERIENCE

Oct. 2005 – present Professor, Dept. Mat. Sci. & Eng., The Ohio State University (OSU)
Oct. 2002 – Sept. 2005 Associate Professor, Dept. Mat. Sci. & Eng., OSU
Oct. 1996 – Sept. 2002 Assistant Professor, Dept. Mat. Sci. & Eng., OSU
Apr. 1995 – June 1996 Postdoctoral Associate, Dept. of Ceramics, Rutgers University

SELECTED LIST OF AWARDS AND DISTINCTIONS

- TMS Fellow Award, TMS 2024
- William Hume-Rothery Award, TMS 2024.
- Faculty of Engineering Distinguished Scholar, Monash University, 2023
- Charles Ellison MacQuigg Award for Outstanding Teaching, The Ohio State University, 2022.
- Cyril Stanley Smith Award, TMS, 2020.
- Distinguished Scientist/Engineer Award, MPMD, TMS, 2020.
- MICRSS Award for “*Best Engineering Applications of Phase-Field Modeling*,” 2014.
- Prof. Brahm Prakash Visiting Chair, Indian Institute of Science, 2014.
- Fraunhofer Bessel Research Award, Alexander von Humboldt Foundation, Germany, 2012.
- Harrison Faculty Award for Excellence in Engineering Education, The Ohio State University, 2010.
- 2011, 2006 and 2001 Lumley Research Awards, The Ohio State University, College of Engineering
- Hsun Lee Research Award, Institute of Metal Research, Chinese Academy of Science, March 2006
- KC Wong Research Award, K.C.Wong Education Foundation, Hong Kong, May 2005
- NSF CAREER Award, National Science Foundation, 1997
- Fellow of ASM International, 2016
- ARC International Fellow, Australian Research Council, 2009-2010
- Invited Speaker at Gordon Conference, 2002, 2004 and 2009 Physical Metallurgy Gordon Conferences, New Hampshire.

EXAMPLES OF PROFESSIONAL SERVICES

TMS Technical Committees:

- Chair, TMS/MPMD Phase Transformations Committee (2010-2012)
- Vice Chair, TMS/MPMD Phase Transformations Committee (2008-2010)
- Member, TMS/MPMD Phase Transformations Committee (2002-present)
- Member, TMS/MPMD Computational Materials Science and Engineering Committee (2004-present)
- Member, Integrated Computational Materials Engineering (ICME) Committee, TMS (2010-present)
- Member, Materials Modeling Committee, US Association of Computational Mechanics (2001-present)
- Member, TMS Academic Alliance Committee (2004-2005)
- Member, Joint ASM/TMS Computer Simulation in Materials Science Committee (1999-2003)

*When served as Chair of the Phase Transformation Committee in 2011, initiated the TMS annual meeting symposium on “Phase Transformations and Microstructural Evolution” that has been hold successfully for the past 12 years with over 100 abstracts received for the 2023 symposium.

TMS Technical Journals:

- JOM Phase Transformation Committee Advisor/Editor (2012-2014)
- Metallurgical and Materials Transactions A. Key Reader (2008-present)

Conference Chair/Co-Chair

- International Symposium on Phase-Field Modeling, Chair-Elect, Hongzhou, China, 2024
- International Symposium on Phase-Field Modeling, Co-Chair, Bochum, Germany, 2019
- 8th International Conference on Numerical Methods of Industrial Forming Processes, NUMIFORMi 2004, Co-Chair, Columbus, Ohio, 2004.

Symposium Organizer/Co-organizer

- Organized or co-organized more than a dozen symposium at national and international conferences (see Section 11 of the Nomination Form for details)

Guest Editor: Philosophical Magazine A, a special issue (2008-2009)

Member of Editorial Board

- Materials Research Letter (2017-present)
- Entropy, Reviewer Board (2020-present).
- Materials Informatics (2020-present)
- npj Computational Materials (2017-present)
- Modeling and Simulation in Materials Science and Engineering (MSMSE) (2010-2020)
- Computers, Materials, & Continua (CMC) (2008-present)

Working with Industry

Worked extensively with industry, national labs and software companies for the development and adoption of ICME tools, including Ford, GM, GE Aviation, GE Power, GE Global Research Centers, Pratt & Whitney, Rolls-Royce, Honeywell, Wyman-Gordon, Ladish, Timet, Air Force Research Lab, Idaho National Lab, National Energy Technology Lab, NIST, Knoll Atomic Power Lab, Scientific Forming, BlueQuartz Software LLC, CompuTherm LLC, ThermoCalc Software, and OpenPhase Solutions GmbH.

RESEARCH INTERESTS AND EXPERTISE

- Microstructural evolution during phase transformations and plastic deformation in multiphase and/or polycrystalline alloys; phase transformation and nanodomain engineering in ferroics and ferroic glasses; shear-banding in metallic glasses; grain growth and domain coarsening; segregation, segregation transition and localized phase transformation at extended defects; variant selection and texture evolution.
- Computational materials science and engineering: mesoscale modeling; computational materials design; phase-field method, diffusive molecular dynamics (DMD) method, heterogeneously randomized STZ dynamics method, integrated phase-field and FFT-based crystal plasticity FEM modeling.
- Alloy systems: high-temperature superalloys, light structural materials (Ti-, Al- and Mg-alloys), high entropy alloys (HEAs), bulk metallic glasses, superelastic and shape memory alloys (SMAs), ferroelectric and ferromagnetic materials, GUM metals, Invar and Elinvar alloys.

PUBLICATIONS AND PRESENTATIONS

- Over 300 refereed journal articles (including over 130 in Acta Materialia, one Overview), with over 17,000 citations and an h-index of 75, over 55 papers having over 100 citations in Google Scholar, and over 15,000 citations and an h-index of 67 in SCI ([Web of Science ResearcherID B-2557-2010](#)).

- 7 chapters in materials handbooks published by ASM, John Wiley & Sons and Springer, an Overview in Acta Materialia and several reviews in Progress in Materials Science and MRS Bulletin.
- Since 2001, Prof. Wang has delivered ~260 Invited, Keynote or Plenary presentations (including 3 Gordon Conferences) and ~230 contributed talks at professional conferences, colloquia and workshops hold nationally and internationally.

SPECIFIC NOTABLE ACCOMPLISHMENTS AND IMPACT OF WORK

Prof. Wang and his group at OSU are highly respected internationally for their work in developing computational techniques to model complex multi-phase and polycrystalline materials. As a principal developer and practitioner, Prof. Wang is at the forefront of advancing the phase-field method for use in engineering applications [1] (for Refs cited, please see **LIST OF REPRESENTATIVE PUBLICATION**). His research has led to the widespread adoption of this method for predicting microstructural evolution during phase transformations and deformation in a variety of alloy systems, including Ni- and Co-base superalloys, Ti-, Al-, and Mg-alloys, shape memory alloys (SMAs), high-entropy alloys, and ferroelectric and ferromagnetic alloys. Apart from his work on the phase-field method, Prof. Wang is also a principal developer and practitioner of two other novel techniques: (a) diffusive molecular dynamics (DMD) for predicting coupled displacive/diffusional processes at the atomic resolution but diffusion time scale [2] and (b) heterogeneously randomized Shear Transformation Zone (STZ) dynamics for predicting deformation behavior in bulk metallic glasses [3]. Most recently, Prof. Wang's group has also developed a new theoretical framework known as the phase transition graph (PTG) analysis for analyzing structural transformations and deformation twinning (for review see [4]). PTG can be used in conjunction with phase diagrams to guide the design of new alloys whose properties are dictated by structural phase transformations and mechanical twinning.

In his core research, Prof. Wang develops and advances these methods to address new scientific and technical challenges, and through his widespread collaborations, he integrates these theoretical analyses and simulation methods with (a) CALPHAD, *ab initio* calculation, MD simulation, FFT-based crystal plasticity model and continuum FEM and (b) advanced experimental characterization, to advance fundamental understanding of phase transformation and deformation mechanisms in both crystalline and amorphous alloys, as well as to develop computational design tools for practical ICME applications. The following are the major contributions of Prof. Wang's scholarly work to the discipline of physical metallurgy.

- ***Major Contributions to the Development of New Alloy Design Principles***

Prof. Wang's group has demonstrated several novel alloy design approaches to achieve (a) linear-superelasticity with large elastic strain limit, nearly zero hysteresis and ultralow modulus [5-10], (b) high strength and prolonged TRIP effect for high work-hardenability and large uniform elongation of a new class of Ti-alloys enable by additive manufacturing [11], and (c) much enhanced creep performance of a new class of Ni-base superalloys strengthened by mechanically driven localized phase transformations at stacking faults and twin boundaries [12]. These new alloy design principles are based on a novel concept of microscale compositionally and/or structurally modulated (microCM or microSM) materials, which is in a direction radically different from traditional homogeneous alloys. Guided by mechanism-based computer simulations and validated by experiments, these microCMs and microSMs are proven effective in controlling strain release during superelastic and plastic deformation. These studies clearly demonstrate how the MGI/ICME philosophy can accelerate the design and development of novel alloys with exceptional properties.

- ***Major Contributions to Materials Theory***

- *Phase Transition Graph (PTG) – a New Alloy Design Tool*

Most alloy phases change their structure in response to external fields such as temperature, stress, electrical, etc. Such structural phase transitions underpin the microstructure and properties of many

smart materials. Because of symmetry-breaking associated with structural changes, there are multiple phase transition pathways (PTPs) to transform from one crystal structure to another, leading to multiple structural states. The interconnection of these structural states through either PTPs or non-PTPs (such as deformation twinning) yields a complicated network. Using group and graph theories, Prof. Wang's group has established a rigorous mathematical description of this network and introduced *a new alloy design tool*, i.e., the phase transition graph (PTG) (for a recent review, see [4]). The PTG analysis goes beyond crystal physics and Landau theory of phase transitions and twinning and captures the characteristics of traversal from multiple structural states of one phase to those of the other during transformation cycling. Using PTG topology as a new design criterion, ferroic alloys potentially having giant piezoelectricity and giant electro- and magneto-strictions have been identified [13], and strategies to improve functional fatigue resistance of SMAs [14] have been proposed. The PTG analysis has also revealed an intrinsic coupling between structural phase transformation and deformation twinning [15,16], which has the promise to design alloys having controlled strain release by coupling the transformation-induced plasticity (TRIP) and twinning-induced plasticity (TWIP) effects. Thus, PTG could be used in combination with alloy phase diagrams to guide the design of new alloys whose properties are dictated by structural phase transformations and mechanical twinning.

➤ *Advancing Theory of Heterogeneous Nucleation*

Nucleation is one of the most fundamental problems in materials science, but also the most challenging problem for both experimental and computational studies. By applying transition pathway search algorithms such as the nudged elastic band (NEB) method to the *ab initio* and CLAPHAD informed phase-field free energy landscape [17], Prof. Wang's group is able to consider any arbitrary critical nucleus shapes that are fully determined by the saddle point along the minimum energy path (MEP) on the free energy surface without any a priori constraints. Even though more than 60 years have passed since the first theory on heterogeneous nucleation (HN) at grain boundaries (GBs) was established in the 1950s, the existing models cannot account for the concurrent shape changes of both the nucleus and the GB plane that hosts the nucleus. Prof. Wang's fully variational approach [18,19] has demonstrated that both the nucleus and the GB plane are highly deformable in response to their interactions. As a consequence, *the activation energy barrier for HN can be reduced by orders of magnitude relative to predictions by previous models, which is now more in line with the experiment.*

➤ *Understanding the Effect of Anisotropy in Grain Boundary Energy and Mobility on Grain Growth*

Prof. Wang's group first introduced anisotropy in both energy and mobility of grain boundaries into a phase-field model of grain growth and demonstrated, for the first time, drastically different effects of energy anisotropy from that of mobility anisotropy on grain growth kinetics and texture evolution [20-22].

• ***Major Contributions to Understanding Transformation and Deformation Mechanisms***

➤ *Uncovering Transformation and Deformation Mechanisms in Complex Engineering Alloys*

Solid-state phase transformations play a critical role in the design of multi-phase alloys. Prof. Wang and his collaborators have made significant contributions in this field by incorporating microelasticity into the phase-field method using Green's function approach and fast Fourier transforms (FFT), which made it applicable to solid-state phase transformations where long-range elastic interactions play a dominant role in governing the multi-phase microstructures. They are the first to predict many unique phenomena dominated by the long-range elastic interactions, including particle translational motion, splitting, inverts coarsening, spatial alignment of precipitates, autocatalytic and collective nucleation, and formation of tweed and twin patterns during phase transformations with symmetry breaking [23-27].

By incorporating *ab initio* defect energetics and CALPHAD thermodynamic and mobility databases, Prof. Wang's group has developed quantitative phase-field models at multiple length scales (nm to μm) to predict the collective behaviour of mutually interacting phases and defects of arbitrary configurations

in both elastically anisotropic and inhomogeneous multi-phase alloys. A hallmark of Prof. Wang's work has been its usefulness in helping to understand experimental observations and then to inspire and guide new experiments to achieve enhanced or novel properties. Examples include (a) uncovering the transformation and deformation mechanisms of intermetallic phases and development of deformation mechanism maps for superalloys [28-36], (b) uncovering the non-conventional transformation pathways leading to novel microstructures in Ti-alloys [6,8, 37-47], (c) quantifying contributions from modulus mismatch and dislocation plasticity to γ' rafting in superalloys [48-50], uncovering the mechanisms of strain glass transitions [51] in ferroelastic alloys and mechanisms of phase transitions at ferroelectric morphotropic phase boundaries and domain structure development [52].

- *Discovering New Mechanism Underlying the Anomalies of Invar and Elinvar Alloys*
By phase-field simulations, Prof. Wang's group and collaborators have discovered a new mechanism that accounts for Invar and Elinvar anomalies in both magnetic and non-magnetic alloys [53]. Motivated by this work, new experiments have been carried out on the century-old Invar and Elinvar alloys, i.e., Fe-Ni alloys. These studies have shown that these classical magnetic alloys and the non-magnetic GUM metals [6-8,54] could share the same physical origin for the Invar and Elinvar anomalies, i.e., the strain glass transition [51].
- ***Major Contributions to Computational Materials Science and Engineering***
- *Bridging Phase-Field Method with Ab Initio Calculations*
Prof. Wang's group is the first to incorporate the generalized stacking fault (GSF) energy from *ab initio* calculations into the phase-field method of dislocations and the first to apply transition pathway search algorithms such as NEB method to *ab initio* informed phase field Hamiltonians. This work has led to the development of the microscopic phase-field (MPF) model of nano-mechanics [55,56] and has opened a new avenue for quantitative characterization of elementary defects and defect processes. Examples are critical nucleus configuration and formation energy during solid state phase transformations [17-19] and their incorporation into the phase-field method [27,57], core energy, structure and Peierls stress of dislocations and grain boundaries [55,56], and critical stress, activation energy and activation volume of dislocation shearing of an individual or a group of precipitates [29-36]. These are critical parameters needed for quantitative descriptions of materials behavior, but extremely difficult to obtain by experiment alone (see [1] for reviews).
- *Bridging Phase Field Method with FFT-Based Crystal Plasticity Method*
In collaboration with colleague (Prof. Niezgoda), Prof. Wang's group developed an integrated full-field modeling approach [58-60] that couples the mechanical response, simulated by an image-based FFT crystal plasticity model, with the underlying microstructure evolution, simulated by the phase-field method. This approach allows one to study efficiently co-evolution of dislocation density and grain/precipitate microstructures during thermal mechanical processing, with a promising potential of leading to the development of fast-acting ICME tools for practical industrial applications.
- *Development of DMD Method and Heterogeneously Randomized STZ Model*
In collaboration with colleague (Prof. Ju Li, now at MIT), Prof. Wang's group has developed (a) a new computational method, Diffusive Molecular Dynamics (DMD) [2], which provides a capability for overcoming time-scale limitations that have prevented conventional MD from capturing coupled displacive/diffusional atomic processes [61], and (b) a heterogeneously randomized shear transformation zone (STZ) model with a kinetic Monte Carlo algorithm [62] for the prediction of deformation and shear band formation in BMGs. The former has revealed, for the first time, atomistic descriptions of climb of a dissociated dislocation and void growth by simultaneous accumulation of vacancies and dislocation emission [61], while the latter has demonstrated the effects of structural heterogeneities in BMGs on strain localization and shear banding [62-64].

MAJOR IMPACT ON ALLOY DESIGN AND DEVELOPMENT COMMUNITY

Prof. Wang's group at OSU has a long track record of working with major alloy development companies, software companies, national labs and universities to develop computational alloy design tools, and to share software applications, source codes and synthetic digital microstructure datasets with the community.

- **Major Contributions to ICME**

Prof. Wang's group has played key roles in numerous large team research efforts on ICME, including the ONR D3-D program, multiple AFRL MAI programs and STW-21 programs, AFOSR MEANS and MEANS-2 programs, and NSF FRG programs and DMREF programs, which systematically coupled multiscale computational simulations with experimental characterization and testing for ICME tool development. His computational tools are not only being used by students in classrooms for learning, but also being practiced by materials engineers in major US aerospace engine companies who have participated in these programs, including GE Aviation, Pratt & Whitney, Rolls-Royce, Honeywell, Wyman-Gordon, Ladish, and Timet. His group has also worked and been working closely with GM, Ford Motor Company, GE Power, GE Global Research Centers, CompuTherm, Thermo_Calc Software, Scientific Forming SFTC, BlueQuartz Software, Air Force Research Lab, Idaho National Lab, National Energy Technology Lab, NIST, and Knoll Atomic Power Lab to develop computer simulation codes for ICME applications.

Many of Prof. Wang's students and postdocs are now working at major US corporations (such as GE, Pratt & Whitney, ExxonMobil, and Carpenter), national labs (such as NETL, INL, and LLNL) and software companies (such as Thermo_Calc, CompuTherm and Scientific Forming) and continue to contribute to ICME.

- **Commercial Software Application Developed**

Developed the 1st version of PanPhaseField with CompuTerm (<https://compuTherm.com/panphasefield>).

- **Shared computer codes, synthetic microstructure datasets, and deformation mechanism map**

- OpenFP, an open-source phase field code, jointly developed with Dr. Simmons at AFRL has been distributed to 8 US industrial companies, 4 government agencies research labs, and 14 universities.
- The diffusive molecular dynamics (DMD) codes and documentation, jointly developed with colleague Ju Li (now at MIT) have been distributed to over a dozen research groups over the world. This distribution includes the main codes (as a standard LAMMPS user-package), potential preparation tools and many other pre-processing and post-processing tools that are essential to perform DMD simulations. (<http://alum.mit.edu/www/liju99/DMD>)

Synthetic microstructure data and dislocation activity diagrams (DADs) generated by phase-field simulations have been distributed to over a dozen research groups worldwide.

LIST OF REPRESENTATIVE PUBLICATION

1. Y. Wang and J. Li, "Acta Materialia Overview 150: Phase Field Modeling of Defects and Deformation," *Acta Mater.* **58** (2010) 1212-1235.
2. J. Li, S. Sarkar, W.T. Cox, T.J. Lenosky, E.B. Bitzek and Y. Wang, "Diffusive Molecular Dynamics and Its Application to Nanoindentation and Sintering" *PRB* **84**, 054103 (2011).
3. P.Y. Zhao, J. Li and Y. Wang, "Heterogeneously Randomized STZ Model of Metallic Glasses: Softening and Extreme Value Statistics during Deformation," *Int. J. Plasticity* **40** (2013) 1-22.
4. Y. Gao, T. Yu and Y. Wang, "Phase Transformation Graph and Transformation Pathway Engineering for Shape Memory Alloys." *Shap. Mem. Superelasticity* **6** (2020) 115-130.
5. J.M. Zhu, Y.P. Gao, D. Wang, T.Y. Zhang and Y. Wang, "Taming Martensitic Transformation via Concentration Modulation at Nanoscale," *Acta Mater.* **130** (2017) 196-207.
6. J.M. Zhu, Y. Gao, D. Wang, J. Li, T.Y. Zhang, Y. Wang, "Making metals linear super-elastic with ultralow modulus and nearly zero hysteresis," *Mater. Horiz.* **6** (2019) 515-523.

7. J.M. Zhu, D. Wang, Y. Gao, T.Y. Zhang, Y. Wang, "Linear-Superelastic Metals by Controlled Strain Release via Nanoscale Concentration-Gradient Engineering," *Materials Today* 33 (2020) 17-23.
8. Y.T. Su, C.X. Liang, X. Sun, H.L. Zhang, Q.L. Liang, Y.F. Zheng, Y.L. Hao, R. Yang, D. Wang, D. Banerjee, Y. Wang, "Composition-dependent shuffle-shear coupling and shuffle-regulated strain glass transition in compositionally modulated Ti-Nb alloys," *Acta Mater.* 246 (2023) 118697.
9. Q.L. Liang, S.S. Zhao, D. Wang, J. Zhang, S.L. Li, Y.D. Wang, Y.F. Zheng, X.B. Ren, M.J. Mills and Y. Wang, "Strain States and Unique Properties in Cold-Rolled TiNi Shape Memory Alloys," *Acta Mater.* 231 (2022) 117890.
10. Q.L. Liang, D. Wang, J. Zhang, Y.C. Ji, X.D. Ding, Yu. Wang, X.B. Ren, Y. Wang, "Novel B19' Strain Glass with Large Recoverable Strain," *Phys. Rev. Materials* 1, 033608 (2017).
11. T.L. Zhang, Z.H. Huang, T. Yang, H.J. Kong, J.H. Luan, A.D. Wang, D. Wang, Y. Wang, C.T. Liu, "In Situ Design of Advanced Ti-Alloy with Concentration Modulations by Additive Manufacturing," *Science* 374 (2021) 478-482.
12. L.S. Feng, S.B. Kannan, A. Egan, T. Smith, M.J. Mills, M. Ghazisaeidi, Y. Wang, "Localized Phase Transformation at Stacking Faults and Mechanism-Based Alloy Design," *Acta Mater.* 240 (2022) 118287.
13. Y.P. Gao, S.A. Dregia and Y. Wang, "A Universal Symmetry Criterion for the Design of High Performance Ferroic Materials," *Acta Mater.* 127 (2017) 438-449.
14. Y.P. Gao, L. Casalena, M. Bowers, R. Noebe, M.J. Mills and Y. Wang, "An Origin of Functional Fatigue of Shape Memory Alloys," *Acta Mater.* 126 (2017) 389-400.
15. Y.P. Gao, Y.F. Zheng, H.L. Fraser, Y. Wang, "Intrinsic coupling between twinning plasticity and transformation plasticity in metastable β Ti-alloys: a symmetry and pathway analysis," *Acta Mater.* 196 (2020) 488-504.
16. Y.P. Gao, Y.F. Zhang and Y. Wang, "Determination of Twinning Path from Broken Symmetry: a Revisit to Deformation Twinning in BCC Metals," *Acta Mater.* 196 (2020) 280-294.
17. C. Shen, J. Li and Y. Wang, "Finding Critical Nucleus in Solid State Phase Transformations," *Met. Mat. Trans. A*. 39A (2008) 976-983 (Editor's choice).
18. R.P. Shi, C. Shen, S.A. Dregia and Y. Wang, "Form of Critical Nuclei at homo-phase Boundaries," *Scripta Mater.* 146 (2018) 276-280.
19. R.P. Shi, T.W. Heo, B.C. Wood, Y. Wang, "Critical nuclei at hetero-phase interfaces," *Acta Mater.* 200 (2020) 510-525.
20. A. Kazaryan, Y. Wang and B. R. Patton, "Generalized Phase Field Approach for Computer Simulation of Sintering: Incorporation of Rigid-Body Motion," *Scripta Mater.* 41 (1999) 487-492.
21. A. Kazaryan, Y. Wang, S. A. Dregia and B. R. Patton, "Grain Growth in Systems with Anisotropic Boundary Mobility: Analytical Model and Computer Simulation," *Phy. Rev. B*. 63 (2001) 1841021.
22. A. Kazaryan, Y. Wang, S. A. Dregia and B. R. Patton, "Grain Growth in Anisotropic Systems: Comparison of Effect of Energy and Mobility," *Acta Mater.* 50 (2002) 2491-2502.
23. Y. Wang, L. Q. Chen and A. G. Khachaturyan, "Kinetics of Strain-Induced Morphological Transformation in Cubic Alloys with a Miscibility Gap", *Acta Metall. et Mater.*, 41 (1993) 279.
24. C. Shen and Y. Wang, *Coherent Precipitation – Phase Field Method*, pp2117-2142 in *Handbook of Materials Modeling*, Part B: Models, ed. by S. Yip, Springer, New York (2005).
25. Y. Wang and A. G. Khachaturyan, "Three-Dimensional Field Model and Computer Modeling of Martensitic Transformation", *Acta Metall. et Mater.* , 45 (1997) 759-773.
26. C. Shen, J. P. Simmons and Y. Wang, "Effect of Elastic Interaction on Nucleation – I. Calculation of Strain Energy of Nucleus Formation in Elastically Anisotropic Crystal of Arbitrary Microstructure," *Acta Mater.* 54 (2006) 5617-5630.
27. C. Shen, J. P. Simmons and Y. Wang, "Effect of Elastic Interaction on Nucleation – II. Simulation Study using Phase Field Method," *Acta Mater.* 55 (2007) 1457-1466.
28. Y. Wang, D. Banerjee, C. C. Su and A. G. Khachaturyan, "Field Kinetic Model and Computer Simulation of Precipitation of L1₂ ordered Intermetallic from FCC Solid Solution", *Acta Mater.* 46, 2983-3001 (1998).

29. L. Kovarik, R.R. Unocic, J. Li, P. Sarosi, C. Shen, Y. Wang and M.J. Mills, "Microtwinning and Other Shearing Mechanisms at Intermediate Temperatures in Ni-Base Superalloys," *Prog. Mat. Sci.* **54** (2009) 839-873.
30. R.R. Unocic, N. Zhou, L. Kovarik, C. Shen, Y. Wang, and M.J. Mills, "Dislocation decorrelation and relationship to deformation microtwins during creep of a γ' precipitate strengthened Ni-base superalloy," *Acta Mater.* **59** (2011) 7325-7339.
31. D.C. Lv, D. McAllister, M.J. Mills and Y. Wang, "Deformation Mechanisms of D0₂₂ Ordered Intermetallic Phase in Superalloys," *Acta Mater.* **118** (2016) 350-361.
32. L.S. Feng, D. Lv, R.K. Rhein, J.G. Goiri, M.S. Titus, A. Van der Ven, T.M. Pollock, Y. Wang, "Shearing of γ' particles in Co-base and Co-Ni-base superalloys," *Acta Mater.* **161** (2018) 99-109.
33. N. Zhou, C. Shen, M.J. Mills, J. Li and Y. Wang, "Modeling Displacive-Diffusional Coupled Dislocation Shearing of γ' Precipitates in Ni-Base Superalloys," *Acta Mater.* **59** (2011) 3484-3497.
34. V.A. Vorontsov, C. Shen, Y. Wang, D. Dye and C.M.F. Rae, "Shearing of γ' Precipitates by a $\langle 112 \rangle$ Dislocation Ribbons in Ni-Base Superalloys: A Phase Field Approach," *Acta Mater.* **58** (2010) 4110.
35. L.S. Feng, M.J. Mills and Y. Wang, "Generalized Stacking Fault Energy Surface Mismatch and Dislocation Transformation" *npj Computational Materials* (2021) 7:201
36. L.S. Feng, R.P. Shi, C.H. Zenk, M.J. Mills, Y. Wang, "Phase field modeling of shearing processes of a dual-lobed $\gamma''|\gamma'|\gamma''$ coprecipitate," *Acta Mater.* **246** (2023) 118693.
37. R.P. Shi, D. Wang and Y. Wang, "Modeling and Simulation of Microstructure Evolution during Heat Treatment of Titanium-Alloys," pp573-603 in *ASM Handbook* Volume **4E**: Heat Treating of Nonferrous Alloys, ed. George E. Totten, ASM (2016).
38. D. Wang, R. Shi, Y. Zheng, R. Banerjee, H.L. Fraser, Y. Wang, "Integrated Computational Materials Engineering (ICME) Approach to Design of Novel Microstructures for Ti-Alloys," *JOM.* **66** (2014) 1287-1298.
39. A. Boyne, D. Wang, R.P. Shi, Y. Zheng, A. Behera, S. Nag, J.S. Tiley, H.L. Fraser, R. Banerjee, Y. Wang, "Pseudospinodal mechanism for fine α/β microstructures in β -Ti alloys," *Acta Mater.* **64** (2014) 188-197.
40. R.P. Shi, Y.F. Zheng, R. Banerjee, H.L. Fraser, Y. Wang, " ω -assisted α nucleation in a metastable β titanium alloy," *Scripta Mater.* **171** (2019) 62-66.
41. D. Qiu, R.P. Shi, P. Zhao, D. Zhang, W. Lv and Y. Wang, "Effect of low angle grain boundaries on morphology and variant selection of grain boundary allotriomorphs and Widmanstätten side-plates," *Acta Mater.* **112** (2016) 347-360.
42. R.P. Shi, N. Zhou, S. Niezgoda and Y. Wang, "Microstructure and Transformation Texture Evolution during α Precipitation in Polycrystalline α/β Titanium Alloys – A Simulation Study," *Acta Mater.* **94** (2015) 224-243.
43. D. Qiu, R.P. Shi, D. Zhang, W. Lu and Y. Wang, "Variant selection by dislocations during α precipitation in α/β titanium alloys," *Acta Mater.* **88** (2015) 218-231.
44. R.P. Shi and Y. Wang, "Variant selection during α precipitation in Ti-6Al-4V under the influence of local stress – A simulation study," *Acta Mater.* **61** (2013) 6006-6024.
45. R.P. Shi, N. Ma and Y. Wang, "Predicting Equilibrium Shape of Precipitates as Function of Coherency State", *Acta Mater.* **60** (2012) 4172-4184.
46. T.L. Zhang, D. Wang, Y. Wang, "Novel transformation pathway and heterogeneous microstructure in Ti-Alloys," *Acta Mater.* **196** (2020) 409-417.
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