



Wei Cai

Professor of Mechanical Engineering and, by courtesy, of Materials Science and Engineering

CONTACT INFORMATION

- **Administrator**

Kelly Chu - Administrative Associate

Email kchu22@stanford.edu

Tel (650) 723-4133

Bio

BIO

Predicting mechanical strength of materials through theory and simulations of defect microstructures across atomic, mesoscopic and continuum scales. Developing new atomistic simulation methods for long time-scale processes, such as crystal growth and self-assembly. Applying machine learning techniques to materials research. Modeling and experiments on the metallurgical processes in metal 3D printing. Understanding microstructure-property relationship in materials for stretchable electronics, such as carbon nanotube networks and semiconducting elastomers.

ACADEMIC APPOINTMENTS

- Professor, Mechanical Engineering
- Professor (By courtesy), Materials Science and Engineering

HONORS AND AWARDS

- Presidential Early Career Award, National Science and Technology Council (2004)
- Career Award, National Science Foundation (2006)
- Young Investigator Award, AFOSR (2006)
- Beer and Johnston Outstanding New Mechanics Educator Award, American Society for Engineering Education (2008)
- T. J. R. Hughes Young Investigator Award, ASME (2013)
- Award of Scientific Achievement in the field of Dislocation Theory and Plasticity, Dislocations 2016 Conference (2016)

BOARDS, ADVISORY COMMITTEES, PROFESSIONAL ORGANIZATIONS

- Editorial Board, Modelling and Simulation in Materials Science and Engineering (2010 - present)

PROFESSIONAL EDUCATION

- PhD, MIT, Nuclear Engineering (2001)

LINKS

- <https://web.stanford.edu/~caiwei>: <https://web.stanford.edu/~caiwei>

- research group site: <https://micronano.stanford.edu/>
- Mechanics and Computation Group: <https://mechanics.stanford.edu/>

Teaching

COURSES

2025-26

- Computational Engineering: ME 123 (Spr)
- Mechanics - Elasticity and Inelasticity: ME 340 (Win)

2024-25

- Computational Engineering: ME 123 (Spr)
- Introduction to Statistical Mechanics: ME 346A (Win)

2023-24

- Material Behaviors and Failure Prediction: ME 152 (Win)
- Mechanics - Elasticity and Inelasticity: ME 340 (Spr)

2022-23

- Computational Engineering: ME 123 (Spr)
- The Science and the Practice of Metal 3D Printing: ME 349 (Win)

STANFORD ADVISEES

Doctoral Dissertation Reader (AC)

Larry Chang, Arijit Majumdar

Doctoral Dissertation Advisor (AC)

Philip DePond, Michael Kim, Eliana Krakovsky, Hanfeng Zhai

Master's Program Advisor

Eric Abdulaziz

Doctoral Dissertation Co-Advisor (AC)

Ben Alessio, Jize Dai

Doctoral (Program)

Daniel Delghandi

Publications

PUBLICATIONS

- **Non-linear jog-dragging effect on the mobility law of edge dislocations in face-centered cubic nickel** *ACTA MATERIALIA*
Jian, W., Wang, Y., Cai, W.
2026; 308
- **Link statistics of dislocation network during strain hardening** *JOURNAL OF THE MECHANICS AND PHYSICS OF SOLIDS*
Akhondzadeh, S., Zhai, H., Jian, W., Sills, R. B., Bertin, N., Cai, W.
2026; 210
- **A printable Nb-based alloy with remarkable high-temperature softening resistance** *ACTA MATERIALIA*
Chen, J., Liu, C., Chen, G., Cai, W., Liao, X., Zou, J., Zhang, L., Qin, M., Qu, X.

2026; 303

- **Tensile behavior of additively manufactured Inconel 718 and stainless steel 316L with compositionally graded joints** *INTERNATIONAL JOURNAL OF PLASTICITY*
Wen, Y., Gao, Y., Narayan, R., Cai, W., Wang, P., Wei, X., Zhang, B., Ramamurty, U., Qu, X.
2025; 189
- **Room-temperature vacancy emission from jog on edge dislocation in FCC nickel under glide force** *SCRIPTA MATERIALIA*
Wang, Y., Jian, W., Cai, W.
2025; 260
- **Characterization of 3D printed micro-blades for cutting tissue-embedding material.** *Extreme Mechanics Letters*
Koppaka, S., Doan, D., Cai, W., Gu, W., Tang, S. K.
2025; 75
- **Lean design of a strong and ductile dual-phase titanium-oxygen alloy.** *Nature materials*
Ding, W., Tao, Q., Liu, C., Chen, G., Yoo, S., Cai, W., Cao, P., Jia, B., Wu, H., Zhang, D., Zhu, H., Zhang, L., Qu, et al
2025
- **Generalizability of Graph Neural Network Force Fields for Predicting Solid-State Properties** *ADVANCED THEORY AND SIMULATIONS*
Mohanty, S., Wang, Y., Cai, W.
2025
- **High absorptivity nanotextured powders for additive manufacturing.** *Science advances*
Tertuliano, O. A., DePond, P. J., Lee, A. C., Hong, J., Doan, D., Capaldi, L., Brongersma, M., Gu, X. W., Matthews, M. J., Cai, W., Lew, A. J.
2024; 10 (36): eadp0003
- **Network Evolution Controlling Strain-Induced Damage and Self-Healing of Elastomers with Dynamic Bonds** *MACROMOLECULES*
Yin, Y., Mohanty, S., Cooper, C. B., Bao, Z., Cai, W.
2024
- **Modeling shortest paths in polymeric networks using spatial branching processes** *JOURNAL OF THE MECHANICS AND PHYSICS OF SOLIDS*
Zhang, Z., Mohanty, S., Blanchet, J., Cai, W.
2024; 187
- **Enhanced mobility of dislocation network nodes and its effect on dislocation multiplication and strain hardening** *ACTA MATERIALIA*
Bertin, N., Cai, W., Aubry, S., Arsenlis, A., Bulatov, V. V.
2024; 271
- **Prediction of yield surface of single crystal copper from discrete dislocation dynamics and geometric learning** *JOURNAL OF THE MECHANICS AND PHYSICS OF SOLIDS*
Jian, W., Xiao, M., Sun, W., Cai, W.
2024; 186
- **Prediction of effective elastic moduli of rocks using Graph Neural Networks** *COMPUTER METHODS IN APPLIED MECHANICS AND ENGINEERING*
Chung, J., Ahmad, R., Sun, W., Cai, W., Mukerji, T.
2024; 421
- **Anomalous temperature dependence of elastic limit in metallic glasses.** *Nature communications*
Wang, Y., Liu, J., Jiang, J. Z., Cai, W.
2024; 15 (1): 171
- **Strong and ductile nanoscale Ti-1Fe dual-phase alloy via deformation twinning** *SCRIPTA MATERIALIA*
Liu, C., Chen, J., Wang, Y., Ding, W., Tao, Q., Chen, G., Cai, W., Qin, M., Qu, X.
2023; 237
- **de Koning et al. Reply.** *Physical review letters*
de Koning, M., Cai, W., Cazorla, C., Boronat, J.
2023; 131 (18): 189602

- **Strong and ductile niobium-based refractory alloy via deformable zirconia nanoparticles** *INTERNATIONAL JOURNAL OF REFRACTORY METALS & HARD MATERIALS*
Chen, J., Liu, C., Wang, Y., Ding, W., Tao, Q., Chen, G., Cai, W., Qin, M., Qu, X.
2024; 118
- **Stress-dependent activation entropy in thermally activated cross-slip of dislocations.** *Proceedings of the National Academy of Sciences of the United States of America*
Wang, Y., Cai, W.
2023; 120 (34): e2222039120
- **Evaluating the transferability of machine-learned force fields for material property modeling** *COMPUTER PHYSICS COMMUNICATIONS*
Mohanty, S., Yoo, S., Kang, K., Cai, W.
2023; 288
- **Kinetics and mechanism of light-induced phase separation in a mixed-halide perovskite** *MATTER*
Peng, S., Wang, Y., Braun, M., Yin, Y., Meng, A. C., Tan, W., Saini, B., Severson, K., Marshall, A. F., Sytwu, K., Baniecki, J. D., Dionne, J., Cai, et al
2023; 6 (6): 2052-2065
- **One dislocation at a time.** *Nature materials*
Bulatov, V., Cai, W.
2023; 22 (6): 679-680
- **Direct comparison between experiments and dislocation dynamics simulations of high rate deformation of single crystal copper** *ACTA MATERIALIA*
Akhondzadeh, S., Kang, M., Sills, R. B., Ramesh, K. T., Cai, W.
2023; 250
- **Computation of effective elastic moduli of rocks using hierarchical homogenization** *JOURNAL OF THE MECHANICS AND PHYSICS OF SOLIDS*
Ahmad, R., Liu, M., Ortiz, M., Mukerji, T., Cai, W.
2023; 174
- **Hierarchical Homogenization With Deep-Learning-Based Surrogate Model for Rapid Estimation of Effective Permeability From Digital Rocks** *JOURNAL OF GEOPHYSICAL RESEARCH-SOLID EARTH*
Liu, M., Ahmad, R., Cai, W., Mukerji, T.
2023; 128 (2)
- **Absence of Off-Diagonal Long-Range Order in hcp ^4He Dislocation Cores.** *Physical review letters*
de Koning, M., Cai, W., Cazorla, C., Boronat, J.
2023; 130 (1): 016001
- **High energy density flexible and ecofriendly lithium-ion smart battery** *ENERGY STORAGE MATERIALS*
Kuznetsov, O. A., Mohanty, S., Pigos, E., Chen, G., Cai, W., Harutyunyan, A. R.
2023; 54: 266-275
- **Dislocation-position fluctuations in solid He-4 as collective variables in a quantum crystal** *NPJ QUANTUM MATERIALS*
de Koning, M., Cai, W.
2022; 7 (1)
- **Discovery of multimechanisms of screw dislocation interaction in bcc iron from open-ended saddle point searches** *PHYSICAL REVIEW MATERIALS*
Wang, X., Wang, Y., Cai, W., Xu, H.
2022; 6 (12)
- **Computational approaches to model X-ray photon correlation spectroscopy from molecular dynamics** *MODELLING AND SIMULATION IN MATERIALS SCIENCE AND ENGINEERING*
Mohanty, S., Cooper, C. B., Wang, H., Liang, M., Cai, W.
2022; 30 (7)
- **Free energy calculation of crystalline solids using normalizing flows** *MODELLING AND SIMULATION IN MATERIALS SCIENCE AND ENGINEERING*

- Ahmad, R., Cai, W.
2022; 30 (6)
- **Nanoparticle-enhanced absorptivity of copper during laser powder bed fusion** *ADDITIVE MANUFACTURING*
Tertuliano, O. A., DePond, P. J., Doan, D., Matthews, M. J., Gu, X., Cai, W., Lew, A. J.
2022; 51
 - **Correlative image learning of chemo-mechanics in phase-transforming solids.** *Nature materials*
Deng, H. D., Zhao, H., Jin, N., Hughes, L., Savitzky, B. H., Ophus, C., Fraggedakis, D., Borbely, A., Yu, Y., Lomeli, E. G., Yan, R., Liu, J., Shapiro, et al
2022
 - **Phagocytic 'teeth' and myosin-II 'jaw' power target constriction during phagocytosis.** *eLife*
Vorselen, D., Barger, S. R., Wang, Y., Cai, W., Theriot, J. A., Gauthier, N. C., Krendel, M.
2021; 10
 - **Phagocytic 'teeth' and myosin-II 'jaw' power target constriction during phagocytosis** *ELIFE*
Vorselen, D., Barger, S. R., Wang, Y., Cai, W., Theriot, J. A., Gauthier, N. C., Krendel, M.
2021; 10
 - **Bending and precipitate formation mechanisms in epitaxial Ge-core/GeSn-shell nanowires.** *Nanoscale*
Meng, A. C., Wang, Y., Braun, M. R., Lentz, J. Z., Peng, S., Cheng, H., Marshall, A. F., Cai, W., McIntyre, P. C.
2021
 - **Electro-chemo-mechanical charge carrier equilibrium at interfaces.** *Physical chemistry chemical physics : PCCP*
Chen, C., Yin, Y., Kang, S. D., Cai, W., Chueh, W. C.
2021
 - **Pipe-diffusion-enriched dislocations and interfaces in SnSe/PbSe heterostructures** *PHYSICAL REVIEW MATERIALS*
Hughes, E. T., Haidet, B. B., Bonef, B., Cai, W., Mukherjee, K.
2021; 5 (7)
 - **A critical look at the prediction of the temperature field around a laser-induced melt pool on metallic substrates.** *Scientific reports*
Shu, Y., Galles, D., Tertuliano, O. A., McWilliams, B. A., Yang, N., Cai, W., Lew, A. J.
2021; 11 (1): 12224
 - **Oxidation behavior of low-cost CP-Ti powders for additive manufacturing via fluidization** *CORROSION SCIENCE*
Ding, W., Wang, Z., Chen, G., Cai, W., Zhang, C., Tao, Q., Qu, X., Qin, M.
2021; 178
 - **A novel experimental method for in situ strain measurement during selective laser melting** *VIRTUAL AND PHYSICAL PROTOTYPING*
Wen, Y., Zhang, B., Liu, S., Cai, W., Wang, P., Lee, C., Ma, J., Qu, X.
2020; 15: 583–95
 - **Dislocation density-based plasticity model from massive discrete dislocation dynamics database** *JOURNAL OF THE MECHANICS AND PHYSICS OF SOLIDS*
Akhondzadeh, S., Sills, R. B., Bertin, N., Cai, W.
2020; 145
 - **Stress effects on the energy barrier and mechanisms of cross-slip in FCC nickel** *JOURNAL OF THE MECHANICS AND PHYSICS OF SOLIDS*
Kuykendall, W. P., Wang, Y., Cai, W.
2020; 144
 - **Growth mode control for direct-gap core/shell Ge/GeSn nanowire light emission** *MATERIALS TODAY*
Meng, A. C., Braun, M. R., Wang, Y., Peng, S., Tan, W., Lentz, J., Xue, M., Pakzad, A., Marshall, A. F., Harris, J. S., Cai, W., McIntyre, P. C.
2020; 40: 101–13
 - **Topological origin of strain induced damage of multi-network elastomers by bond breaking** *EXTREME MECHANICS LETTERS*
Yin, Y., Bertin, N., Wang, Y., Bao, Z., Cai, W.
2020; 40

- **Intrinsic size dependent plasticity in BCC micro-pillars under uniaxial tension and pure torsion** *EXTREME MECHANICS LETTERS*
Ryu, I., Gravell, J. D., Cai, W., Nix, W. D., Gao, H.
2020; 40
- **Selective laser melting of CP-Ti to overcome the low cost and high performance trade-off** *ADDITIVE MANUFACTURING*
Tao, Q., Wang, Z., Chen, G., Cai, W., Cao, P., Zhang, C., Ding, W., Lu, X., Luo, T., Qu, X., Qin, M.
2020; 34
- **Roadmap on multiscale materials modeling** *MODELLING AND SIMULATION IN MATERIALS SCIENCE AND ENGINEERING*
van der Giessen, E., Schultz, P. A., Bertin, N., Bulatov, V. V., Cai, W., Csanyi, G., Foiles, S. M., Geers, M. D., Gonzalez, C., Hutter, M., Kim, W., Kochmann, D. M., LLorca, et al
2020; 28 (4)
- **Microparticle traction force microscopy reveals subcellular force exertion patterns in immune cell-target interactions.** *Nature communications*
Vorselen, D. n., Wang, Y. n., de Jesus, M. M., Shah, P. K., Footer, M. J., Huse, M. n., Cai, W. n., Theriot, J. A.
2020; 11 (1): 20
- **Multivalent Assembly of Flexible Polymer Chains into Supramolecular Nanofibers.** *Journal of the American Chemical Society*
Cooper, C. B., Kang, J. n., Yin, Y. n., Yu, Z. n., Wu, H. C., Nikzad, S. n., Ochiai, Y. n., Yan, H. n., Cai, W. n., Bao, Z. n.
2020
- **Frontiers in the Simulation of Dislocations** *ANNUAL REVIEW OF MATERIALS RESEARCH, VOL 50, 2020*
Bertin, N., Sills, R. B., Cai, W.
edited by Clarke, D. R.
2020; 50: 437–64
- **Phase-field investigation of the stages in radial growth of core-shell Ge/Ge_{1-x}Sn_x nanowires.** *Nanoscale*
Wang, Y., Meng, A. C., McIntyre, P. C., Cai, W.
2019
- **Stretchable self-healable semiconducting polymer film for active-matrix strain-sensing array.** *Science advances*
Oh, J. Y., Son, D., Katsumata, T., Lee, Y., Kim, Y., Lopez, J., Wu, H., Kang, J., Park, J., Gu, X., Mun, J., Wang, N. G., Yin, et al
2019; 5 (11): eaav3097
- **GPU-accelerated dislocation dynamics using subcycling time-integration** *MODELLING AND SIMULATION IN MATERIALS SCIENCE AND ENGINEERING*
Bertin, N., Aubry, S., Arsenlis, A., Cai, W.
2019; 27 (7)
- **Spherical harmonics method for computing the image stress due to a spherical void** *JOURNAL OF THE MECHANICS AND PHYSICS OF SOLIDS*
Wang, Y., Zhang, X., Cai, W.
2019; 126: 151–67
- **Strengthening Mechanism of a Single Precipitate in a Metallic Nanocube** *NANO LETTERS*
Kiani, M. T., Wang, Y., Bertin, N., Cai, W., Gu, X.
2019; 19 (1): 255–60
- **Coupling of coherent misfit strain and composition distributions in core-shell Ge/Ge_{1-x}Sn_x nanowire light emitters** *Materials Today Nano*
Meng, A. C.
2019; 5: 100026
- **High-Throughput Growth of Microscale Gold Bicrystals for Single-Grain-Boundary Studies.** *Advanced materials (Deerfield Beach, Fla.)*
Gan, L. T., Yang, R. n., Traylor, R. n., Cai, W. n., Nix, W. D., Fan, J. A.
2019: e1902189
- **Properties of the Eshelby tensor and existence of the equivalent ellipsoidal inclusion solution** *JOURNAL OF THE MECHANICS AND PHYSICS OF SOLIDS*
Barnett, D. M., Cai, W.

2018; 121: 71–80

- **Energy of periodic discrete dislocation networks** *JOURNAL OF THE MECHANICS AND PHYSICS OF SOLIDS*
Bertin, N., Cai, W.
2018; 121: 133–46
- **Predicting stability of nanofin arrays against collapse by phase field modeling** *JOURNAL OF VACUUM SCIENCE & TECHNOLOGY B*
Wang, Y., Woytowicz, P., Mui, D., Cai, W.
2018; 36 (5)
- **Dislocation Networks and the Microstructural Origin of Strain Hardening.** *Physical review letters*
Sills, R. B., Bertin, N., Aghaei, A., Cai, W.
2018; 121 (8): 085501
- **A spectral approach for discrete dislocation dynamics simulations of nanoindentation** *MODELLING AND SIMULATION IN MATERIALS SCIENCE AND ENGINEERING*
Bertin, N., Glavas, V., Datta, D., Cai, W.
2018; 26 (5)
- **Computation of virtual X-ray diffraction patterns from discrete dislocation structures** *COMPUTATIONAL MATERIALS SCIENCE*
Bertin, N., Cai, W.
2018; 146: 268–77
- **Discrete shear band plasticity through dislocation activities in body-centered cubic tungsten nanowires** *SCIENTIFIC REPORTS*
Wang, J., Wang, Y., Cai, W., Li, J., Zhang, Z., Mao, S. X.
2018; 8: 4574
- **Microstructural origin of resistance-strain hysteresis in carbon nanotube thin film conductors** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
Jin, L., Chortos, A., Lian, F., Pop, E., Linder, C., Bao, Z., Cai, W.
2018; 115 (9): 1986–91
- **Reliability of Single Crystal Silver Nanowire-Based Systems: Stress Assisted Instabilities.** *ACS nano*
Ramachandramoorthy, R., Wang, Y., Aghaei, A., Richter, G., Cai, W., Espinosa, H. D.
2017; 11 (5): 4768-4776
- **Phase Field Model for Morphological Transition in Nanowire Vapor-Liquid-Solid Growth** *CRYSTAL GROWTH & DESIGN*
Wang, Y., McIntyre, P. C., Cai, W.
2017; 17 (4): 2211-2217
- **Highly stretchable polymer semiconductor films through the nanoconfinement effect** *SCIENCE*
Xu, J., Wang, S., Wang, G. N., Zhu, C., Luo, S., Jin, L., Gu, X., Chen, S., Feig, V. R., To, J. W., Rondeau-Gagne, S., Park, J., Schroeder, et al
2017; 355 (6320): 59-?
- **Stability of Eshelby dislocations in FCC crystalline nanowires** *INTERNATIONAL JOURNAL OF PLASTICITY*
Ryu, S., Cai, W.
2016; 86: 26-36
- **Spatiotemporal periodicity of dislocation dynamics in a two-dimensional microfluidic crystal flowing in a tapered channel.** *Proceedings of the National Academy of Sciences of the United States of America*
Gai, Y., Leong, C. M., Cai, W., Tang, S. K.
2016; 113 (43): 12082-12087
- **Dislocation Structure and Mobility in hcp ⁴He.** *Physical review letters*
Landinez Borda, E. J., Cai, W., de Koning, M.
2016; 117 (4): 045301-?
- **Dislocation Structure and Mobility in hcp He-4** *PHYSICAL REVIEW LETTERS*
Borda, E. J., Cai, W., de Koning, M.
2016; 117 (4)

- **Advanced time integration algorithms for dislocation dynamics simulations of work hardening** *MODELLING AND SIMULATION IN MATERIALS SCIENCE AND ENGINEERING*
Sills, R. B., Aghaei, A., Cai, W.
2016; 24 (4)
- **Solute drag on perfect and extended dislocations** *PHILOSOPHICAL MAGAZINE*
Sills, R. B., Cai, W.
2016; 96 (10): 895-921
- **Spontaneous, Defect-Free Kinking via Capillary Instability during Vapor-Liquid-Solid Nanowire Growth.** *Nano letters*
Li, Y., Wang, Y., Ryu, S., Marshall, A. F., Cai, W., McIntyre, P. C.
2016; 16 (3): 1713-1718
- **Direct observation of mineral-organic composite formation reveals occlusion mechanism.** *Nature communications*
Rae Cho, K., Kim, Y., Yang, P., Cai, W., Pan, H., Kulak, A. N., Lau, J. L., Kulshreshtha, P., Armes, S. P., Meldrum, F. C., De Yoreo, J. J.
2016; 7: 10187-?
- **Anisotropic Size-Dependent Plasticity in Face-Centered Cubic Micropillars Under Torsion** *JOM*
Ryu, I., Cai, W., Nix, W. D., Gao, H.
2016; 68 (1): 253-260
- **Shape-Controlled, Self-Wrapped Carbon Nanotube 3D Electronics** *ADVANCED SCIENCE*
Wang, H., Wang, Y., Tee, B. C., Kim, K., Lopez, J., Cai, W., Bao, Z.
2015; 2 (9)
- **Shape-Controlled, Self-Wrapped Carbon Nanotube 3D Electronics.** *Advanced science (Weinheim, Baden-Wurtemberg, Germany)*
Wang, H., Wang, Y., Tee, B. C., Kim, K., Lopez, J., Cai, W., Bao, Z.
2015; 2 (9): 1500103
- **Stochastic behaviors in plastic deformation of face-centered cubic micropillars governed by surface nucleation and truncated source operation** *ACTA MATERIALIA*
Ryu, I., Cai, W., Nix, W. D., Gao, H.
2015; 95: 176-183
- **A Bamboo-Inspired Nanostructure Design for Flexible, Foldable, and Twistable Energy Storage Devices** *NANO LETTERS*
Sun, Y., Sills, R. B., Hu, X., Seh, Z. W., Xiao, X., Xui, H., Luo, W., Jin, H., Xin, Y., Li, T., Zhang, Z., Zhou, J., Cai, et al
2015; 15 (6): 3899-3906
- **Intrinsic bauschinger effect and recoverable plasticity in pentatwinned silver nanowires tested in tension.** *Nano letters*
Bernal, R. A., Aghaei, A., Lee, S., Ryu, S., Sohn, K., Huang, J., Cai, W., Espinosa, H.
2015; 15 (1): 139-146
- **A three-dimensional phase field model for nanowire growth by the vapor-liquid-solid mechanism** *MODELLING AND SIMULATION IN MATERIALS SCIENCE AND ENGINEERING*
Wang, Y., Ryu, S., McIntyre, P. C., Cai, W.
2014; 22 (5)
- **Modeling a distribution of point defects as misfitting inclusions in stressed solids** *JOURNAL OF THE MECHANICS AND PHYSICS OF SOLIDS*
Cai, W., Sills, R. B., Barnett, D. M., Nix, W. D.
2014; 66: 154-171
- **Ideal Shear Strength of a Quantum Crystal** *PHYSICAL REVIEW LETTERS*
Landinez Borda, E. J., Cai, W., de Koning, M.
2014; 112 (15)
- **Efficient time integration in dislocation dynamics** *MODELLING AND SIMULATION IN MATERIALS SCIENCE AND ENGINEERING*
Sills, R. B., Cai, W.
2014; 22 (2)

- **Efficient Time Integrators for Dislocation Dynamics Simulations** *Modelling and Simulation in Materials Science and Engineering*
Sills, R., Cai, W.
2014; 24: 025003
- **Stress dependence of cross slip energy barrier for face-centered cubic nickel** *JOURNAL OF THE MECHANICS AND PHYSICS OF SOLIDS*
Kang, K., Yin, J., Cai, W.
2014; 62: 181-193
- **Stress Dependence of Cross Slip Energy Barrier for Face-Centered Cubic Metals** *Journal of the Mechanics and Physics of Solids*
Kang, K., Yin, J., Cai, W.
2014; 62: 181
- **Zippering, entanglement, and the elastic modulus of aligned single-walled carbon nanotube films** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
Won, Y., Gao, Y., Panzer, M. A., Xiang, R., Maruyama, S., Kenny, T. W., Cai, W., Goodson, K. E.
2013; 110 (51): 20426-20430
- **Conditional convergence in two-dimensional dislocation dynamics** *MODELLING AND SIMULATION IN MATERIALS SCIENCE AND ENGINEERING*
Kuykendall, W. P., Cai, W.
2013; 21 (5)
- **Atomistic simulations of grain boundary segregation in nanocrystalline yttria-stabilized zirconia and gadolinia-doped ceria solid oxide electrolytes** *ACTA MATERIALIA*
Lee, H. B., Prinz, F. B., Cai, W.
2013; 61 (10): 3872-3887
- **Plasticity of bcc micropillars controlled by competition between dislocation multiplication and depletion** *ACTA MATERIALIA*
Ryu, I., Nix, W. D., Cai, W.
2013; 61 (9): 3233-3241
- **Zippering, Entanglement, and the Modulus of Aligned Single-Walled Carbon Nanotube Films**
Won, Y., Gao, Y., Panzer, Matthew, A., Xiang, R., Maruyama, S., Kenny, Thomas, W., Cai, W.
2013
- **Modeling Dislocation Mechanisms of the Acoustic Nonlinearity in Metallic Crystals** *9th International Workshop on Structural Health Monitoring (IWSHM)*
CASH, W. D., Cai, W.
DESTECH PUBLICATIONS, INC.2013: 1065–1072
- **Modelling plasticity of BCC micro-pillars using dislocation dynamics** *Acta Materialia*
Ryu, I., Nix, William, D., Cai, W.
2013; 61: 3233
- **On the existence of Eshelby's equivalent ellipsoidal inclusion solution** *MATHEMATICS AND MECHANICS OF SOLIDS*
Kuykendall, W. P., Cash, W. D., Barnett, D. M., Cai, W.
2012; 17 (8): 840-847
- **Nucleation-Controlled Distributed Plasticity in Penta-twinned Silver Nanowires** *SMALL*
Filleter, T., Ryu, S., Kang, K., Yin, J., Bernal, R. A., Sohn, K., Li, S., Huang, J., Cai, W., Espinosa, H. D.
2012; 8 (19): 2986-2993
- **Singular orientations and faceted motion of dislocations in body-centered cubic crystals** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
Kang, K., Bulatov, V. V., Cai, W.
2012; 109 (38): 15174-15178
- **Ab initio kinetic Monte Carlo model of ionic conduction in bulk yttria-stabilized zirconia** *MODELLING AND SIMULATION IN MATERIALS SCIENCE AND ENGINEERING*
Lee, E., Prinz, F. B., Cai, W.

2012; 20 (6)

- **Computing dislocation stress fields in anisotropic elastic media using fast multipole expansions** *MODELLING AND SIMULATION IN MATERIALS SCIENCE AND ENGINEERING*
Yin, J., Barnett, D. M., Fitzgerald, S. P., Cai, W.
2012; 20 (4)
- **Dislocation dynamics simulation of Frank-Read sources in anisotropic alpha-Fe** *MODELLING AND SIMULATION IN MATERIALS SCIENCE AND ENGINEERING*
Fitzgerald, S. P., Aubry, S., Dudarev, S. L., Cai, W.
2012; 20 (4)
- **Contribution of dislocation dipole structures to the acoustic nonlinearity** *JOURNAL OF APPLIED PHYSICS*
CASH, W. D., Cai, W.
2012; 111 (7)
- **Stress-driven migration of simple low-angle mixed grain boundaries** *ACTA MATERIALIA*
Lim, A. T., Haataja, M., Cai, W., Srolovitz, D. J.
2012; 60 (3): 1395-1407
- **Plasticity of metal nanowires** *JOURNAL OF MATERIALS CHEMISTRY*
Weinberger, C. R., Cai, W.
2012; 22 (8): 3277-3292
- **Molecular Dynamics** *Comprehensive Nuclear Materials*
Cai, W., Li, J., Yip, S.
edited by Konings, R. J., M.
Elsevier.2012: 249–265
- **Molecular Dynamics** *Comprehensive Nuclear Materials*
Cai, W., Li, J., Yip, S.
edited by Konings, R.
Elsevier.2012: 249–265
- **Equilibrium shape of dislocation shear loops in anisotropic alpha-Fe** *MODELLING AND SIMULATION IN MATERIALS SCIENCE AND ENGINEERING*
Aubry, S., Fitzgerald, S. P., Dudarev, S. L., Cai, W.
2011; 19 (6)
- **Predicting the dislocation nucleation rate as a function of temperature and stress** *JOURNAL OF MATERIALS RESEARCH*
Ryu, S., Kang, K., Cai, W.
2011; 26 (18): 2335-2354
- **Molecular dynamics simulations of gold-catalyzed growth of silicon bulk crystals and nanowires** *JOURNAL OF MATERIALS RESEARCH*
Ryu, S., Cai, W.
2011; 26 (17): 2199-2206
- **Energy barrier for homogeneous dislocation nucleation: Comparing atomistic and continuum models** *SCRIPTA MATERIALIA*
Aubry, S., Kang, K., Ryu, S., Cai, W.
2011; 64 (11): 1043-1046
- **Entropic effect on the rate of dislocation nucleation** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
Ryu, S., Kang, K., Cai, W.
2011; 108 (13): 5174-5178
- **Dislocation junctions and jogs in a free-standing FCC thin film** *MODELLING AND SIMULATION IN MATERIALS SCIENCE AND ENGINEERING*
Lee, S., Aubry, S., Nix, W. D., Cai, W.
2011; 19 (2)

- **The stability of Lomer-Cottrell jogs in nanopillars** *SCRIPTA MATERIALIA*
Weinberger, C. R., Cai, W.
2011; 64 (6): 529-532
- **Enhancing ionic conductivity of bulk single-crystal yttria-stabilized zirconia by tailoring dopant distribution** *PHYSICAL REVIEW B*
Lee, E., Prinz, F. B., Cai, W.
2011; 83 (5)
- **Dislocation contribution to acoustic nonlinearity: The effect of orientation-dependent line energy** *JOURNAL OF APPLIED PHYSICS*
Cash, W. D., Cai, W.
2011; 109 (1)
- **Entropic Effect on the Rate of Dislocation Nucleation**
Ryu, S., Kang, K., Cai, W.
2011
- **Nanoscale patterning controls inorganic-membrane interface structure** *NANOSCALE*
Almquist, B. D., Verma, P., Cai, W., Melosh, N. A.
2011; 3 (2): 391-400
- **Role of Surface Roughness in Hysteresis during Adhesive Elastic Contact.** *Philosophical magazine letters*
Kesari, H., Doll, J. C., Pruitt, B. L., Cai, W., Lew, A. J.
2010; 90 (12): 891-902
- **Analysis of the elastic strain energy driving force for grain boundary migration using phase field simulation** *SCRIPTA MATERIALIA*
Tonks, M., Millett, P., Cai, W., Wolf, D.
2010; 63 (11): 1049-1052
- **Size and temperature effects on the fracture mechanisms of silicon nanowires: Molecular dynamics simulations** *INTERNATIONAL JOURNAL OF PLASTICITY*
Kang, K., Cai, W.
2010; 26 (9): 1387-1401
- **Numerical tests of nucleation theories for the Ising models** *PHYSICAL REVIEW E*
Ryu, S., Cai, W.
2010; 82 (1)
- **Plasticity of metal wires in torsion: Molecular dynamics and dislocation dynamics simulations** *JOURNAL OF THE MECHANICS AND PHYSICS OF SOLIDS*
Weinberger, C. R., Cai, W.
2010; 58 (7): 1011-1025
- **Efficient computation of forces on dislocation segments in anisotropic elasticity** *MODELLING AND SIMULATION IN MATERIALS SCIENCE AND ENGINEERING*
Yin, J., Barnett, D. M., Cai, W.
2010; 18 (4)
- **Atomistic simulations of surface segregation of defects in solid oxide electrolytes** *ACTA MATERIALIA*
Lee, H. B., Prinz, F. B., Cai, W.
2010; 58 (6): 2197-2206
- **Validity of classical nucleation theory for Ising models** *PHYSICAL REVIEW E*
Ryu, S., Cai, W.
2010; 81 (3)
- **A gold-silicon potential fitted to the binary phase diagram** *JOURNAL OF PHYSICS-CONDENSED MATTER*
Ryu, S., Cai, W.
2010; 22 (5)
- **Kinetic Monte Carlo simulations of oxygen vacancy diffusion in a solid electrolyte: Computing the electrical impedance using the fluctuation-dissipation theorem** *ELECTROCHEMISTRY COMMUNICATIONS*

-
- Lee, E., Prinz, F. B., Cai, W.
2010; 12 (2): 223-226
- **Orientation-Dependent Plasticity in Metal Nanowires under Torsion: Twist Boundary Formation and Eshelby Twist** *NANO LETTERS*
Weinberger, C. R., Cai, W.
2010; 10 (1): 139-142
 - **The Validity of Classical Nucleation Theory for Ising Models** *Physical Review E (Rapid Communications)*
Ryu, S., Cai, W.
2010; 81: 030601
 - **Role of surface roughness in hysteresis during adhesive elastic contact** *PHILOSOPHICAL MAGAZINE LETTERS*
Kesari, H., Doll, J. C., Pruitt, B. L., Cai, W., Lew, A. J.
2010; 90 (12): 891-902
 - **Improved modified embedded-atom method potentials for gold and silicon** *MODELLING AND SIMULATION IN MATERIALS SCIENCE AND ENGINEERING*
Ryu, S., Weinberger, C. R., Baskes, M. I., Cai, W.
2009; 17 (7)
 - **Modelling dislocations in a free-standing thin film** *MODELLING AND SIMULATION IN MATERIALS SCIENCE AND ENGINEERING*
Weinberger, C. R., Aubry, S., Lee, S., Nix, W. D., Cai, W.
2009; 17 (7)
 - **Mechanics of Crystalline Nanowires** *MRS BULLETIN*
Park, H. S., Cai, W., Espinosa, H. D., Huang, H.
2009; 34 (3): 178-183
 - **Energy of a Prismatic Dislocation Loop in an Elastic Cylinder** *MATHEMATICS AND MECHANICS OF SOLIDS*
Cai, W., Weinberger, C. R.
2009; 14 (1-2): 192-206
 - **Dislocation dynamics simulations in a cylinder** *International Conference on the Fundamentals of Plastic Deformation (DISLOCATIONS)*
Weinberger, C. R., Aubry, S., Lee, S., Cai, W.
IOP PUBLISHING LTD.2009
 - **Comparison of thermal properties predicted by interatomic potential models** *MODELLING AND SIMULATION IN MATERIALS SCIENCE AND ENGINEERING*
Ryu, S., Cai, W.
2008; 16 (8)
 - **Torsion and bending periodic boundary conditions for modeling the intrinsic strength of nanowires** *JOURNAL OF THE MECHANICS AND PHYSICS OF SOLIDS*
Cai, W., Fong, W., Eisen, E., Weinberger, C. R.
2008; 56 (11): 3242-3258
 - **Comparing the strength of f.c.c. and b.c.c. sub-micrometer pillars: Compression experiments and dislocation dynamics simulations** *Symposium on Mechanical Behavior of Nanostructured Materials held TMS 2007 Annual Meeting*
Greer, J. R., Weinberger, C. R., Cai, W.
ELSEVIER SCIENCE SA.2008: 21-25
 - **Surface-controlled dislocation multiplication in metal micropillars** *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*
Weinberger, C. R., Cai, W.
2008; 105 (38): 14304-14307
 - **Quantum entanglement of formation between qudits** *PHYSICAL REVIEW A*
Ryu, S., Cai, W., Caro, A.
2008; 77 (5)
 - **Electronic structure calculations in a uniform magnetic field using periodic supercells** *JOURNAL OF COMPUTATIONAL PHYSICS*
-

- Lee, E., Cai, W., Galli, G. A.
2007; 226 (2): 1310-1331
- **Computing image stress in an elastic cylinder** *JOURNAL OF THE MECHANICS AND PHYSICS OF SOLIDS*
Weinberger, C. R., Cai, W.
2007; 55 (10): 2027-2054
 - **Enabling strain hardening simulations with dislocation dynamics** *MODELLING AND SIMULATION IN MATERIALS SCIENCE AND ENGINEERING*
Arsenlis, A., Cai, W., Tang, M., Rhee, M., Opperstrup, T., Hommes, G., Pierce, T. G., Bulatov, V. V.
2007; 15 (6): 553-595
 - **Brittle and ductile fracture of semiconductor nanowires - molecular dynamics simulations** *PHILOSOPHICAL MAGAZINE*
Kang, K., Cai, W.
2007; 87 (14-15): 2169-2189
 - **A hybrid method for computing forces on curved dislocations intersecting free surfaces in three-dimensional dislocation dynamics** *MODELLING AND SIMULATION IN MATERIALS SCIENCE AND ENGINEERING*
Tang, M., Cai, W., Xu, G., Bulatov, V. V.
2006; 14 (7): 1139-1151
 - **Geometric aspects of the ideal shear resistance in simple crystal lattices** *PHILOSOPHICAL MAGAZINE*
Bulatov, V. V., Cai, W., Baran, R., Kang, K.
2006; 86 (25-26): 3847-3859
 - **Dislocation multi-junctions and strain hardening** *NATURE*
Bulatov, V. V., Hsiung, L. L., Tang, M., Arsenlis, A., Bartelt, M. C., Cai, W., Florando, J. N., Hiratani, M., Rhee, M., Hommes, G., Pierce, T. G., de la Rubia, T. D.
2006; 440 (7088): 1174-1178
 - **A non-singular continuum theory of dislocations** *JOURNAL OF THE MECHANICS AND PHYSICS OF SOLIDS*
Cai, W., Arsenlis, A., Weinberger, C. R., Bulatov, V. V.
2006; 54 (3): 561-587
 - **Computer Simulations of Dislocations**
Bulatov, V. V., Cai, W.
Oxford University Press.2006
 - **Stochastic simulation of dislocation glide in tantalum and Ta-based alloys** *JOURNAL OF THE MECHANICS AND PHYSICS OF SOLIDS*
Deo, C. S., Srolovitz, D. J., Cai, W., Bulatov, V. V.
2005; 53 (6): 1223-1247
 - **Adaptive importance sampling Monte Carlo simulation of rare transition events** *JOURNAL OF CHEMICAL PHYSICS*
de Koning, M., Cai, W., Sadigh, B., Opperstrup, T., Kalos, M. H., Bulatov, V. V.
2005; 122 (7)
 - **Kinetic Monte Carlo method for dislocation migration in the presence of solute** *PHYSICAL REVIEW B*
Deo, C. S., Srolovitz, D. J., Cai, W., Bulatov, V. V.
2005; 71 (1)
 - **Modelling Dislocations using a Periodic Supercell** *Handbook of Materials Modelling*
Cai, W.
edited by Yip, S.
Springer.2005
 - **Modeling Dislocations using a Periodic Supercell** *Handbook of Materials Modelling*
Cai, W.
edited by Yip, S.
Springer.2005

- **Mobility laws in dislocation dynamics simulations** *13th International Conference on the Strength of Materials (ICSMA 13)*
Cai, W., Bulatov, V. V.
ELSEVIER SCIENCE SA.2004: 277–281
- **Core energy and Peierls stress of a screw dislocation in bcc molybdenum: A periodic-cell tight-binding study** *PHYSICAL REVIEW B*
Li, J., Wang, C. Z., CHANG, J. P., Cai, W., Bulatov, V. V., Ho, K. M., Yip, S.
2004; 70 (10)
- **Ab initio calculations in a uniform magnetic field using periodic supercells** *PHYSICAL REVIEW LETTERS*
Cai, W., Galli, G.
2004; 92 (18)
- **Dynamic transitions from smooth to rough to twinning in dislocation motion** *NATURE MATERIALS*
Marian, J., Cai, W., Bulatov, V. V.
2004; 3 (3): 158-163
- **Massively-parallel dislocation dynamics simulations** *IUTAM Symposium on Mesoscopic Dynamics of Fracture Process and Materials Strength*
Cai, W., Bulatov, V. V., Pierce, T. G., Hiratani, M., Rhee, M., Bartelt, M., Tang, M.
SPRINGER.2004: 1–11
- **Dislocation Core Effects on Mobility** *Dislocations in Solids*
Cai, W., Bulatov, V. V., Chang, J., Li, J., Yip, S.
edited by Nabarro, F. R., N., Hirth, J., P.
North-Holland Pub.2004: 1
- **Dislocation Core Effects on Mobility** *Dislocations in Solids*
Cai, W., Bulatov, V. V., Chang, J., Li, J., Yip, S.
North-Holland Pub.2004: 1–80
- **Scalable Line Dynamics in ParaDiS, Conference on High Performance Networking and Computing**
Bulatov, V., Cai, W., Fier, J., Hiratani, M., Pierce, T., Tang, M.
2004
- **Dislocation image stresses at free surfaces by the finite element method** *Symposium on Thin Films - Stresses and Mechanical Properties X held at the 2003 MRS Fall Meeting*
Tang, M. J., Xu, G. S., Cai, W., Bulatov, V.
MATERIALS RESEARCH SOCIETY.2004: 29–33
- **Modeling of dislocation-grain boundary interactions in FCC metals** *Workshop on Modeling and Experimental Validation*
de Koning, M., Kurtz, R. J., Bulatov, V. V., Henager, C. H., Hoagland, R. G., Cai, W., Nomura, M.
ELSEVIER SCIENCE BV.2003: 281–89
- **Anomalous dislocation multiplication in FCC metals** *PHYSICAL REVIEW LETTERS*
de Koning, M., Cai, W., Bulatov, V. V.
2003; 91 (2)
- **Periodic image effects in dislocation modelling** *PHILOSOPHICAL MAGAZINE*
Cai, W., Bulatov, V. V., CHANG, J. P., Li, J., Yip, S.
2003; 83 (5): 539-567
- **Atomistic measures of materials strength and deformation** *Conference of the NATO-Advanced-Study-Institute on Computational Materials Science*
Li, J., Cai, W., CHANG, J. P., Yip, S.
I O S PRESS.2003: 359–387
- **Importance sampling of rare transition events in Markov processes** *PHYSICAL REVIEW E*
Cai, W., Kalos, M. H., de Koning, M., Bulatov, V. V.
2002; 66 (4)
- **Nodal effects in dislocation mobility** *PHYSICAL REVIEW LETTERS*

- Bulatov, V. V., Cai, W.
2002; 89 (11)
- **Molecular dynamics simulations of motion of edge and screw dislocations in a metal** *Meeting of the International Union of Materials Research Societies (IUMRS)*
Chang, J. P., Cai, W., Bulatov, V. V., Yip, S.
ELSEVIER SCIENCE BV.2002: 111–15
 - **Kinetic Monte Carlo approach to modeling dislocation mobility** *Meeting of the International Union of Materials Research Societies (IUMRS)*
Cai, W., Bulatov, V. V., Justo, J. F., Argon, A. S., Yip, S.
ELSEVIER SCIENCE BV.2002: 124–30
 - **Dislocation motion in BCC metals by molecular dynamics** *International Conference on the Fundamentals of Plastic Deformation*
CHANG, J. P., Cai, W., Bulatov, V. V., Yip, S.
ELSEVIER SCIENCE SA.2001: 160–163
 - **Kinetic Monte Carlo modeling of dislocation motion in BCC metals** *International Conference on the Fundamentals of Plastic Deformation*
Cai, W., Bulatov, V. V., Yip, S., Argon, A. S.
ELSEVIER SCIENCE SA.2001: 270–273
 - **Point defect interaction with dislocations in silicon** *International Conference on the Fundamentals of Plastic Deformation*
Justo, J. F., de Koning, M., Cai, W., Bulatov, V. V.
ELSEVIER SCIENCE SA.2001: 129–132
 - **Anisotropic elastic interactions of a periodic dislocation array** *PHYSICAL REVIEW LETTERS*
Cai, W., Bulatov, V. V., CHANG, J. P., Li, J., Yip, S.
2001; 86 (25): 5727-5730
 - **Parameter-free modelling of dislocation motion: the case of silicon** *PHILOSOPHICAL MAGAZINE A-PHYSICS OF CONDENSED MATTER STRUCTURE DEFECTS AND MECHANICAL PROPERTIES*
Bulatov, V. V., Justo, J. F., Cai, W., Yip, S., Argon, A. S., Lenosky, T., de Koning, M., de la Rubia, T. D.
2001; 81 (5): 1257-1281
 - **Commentary on Atomistic Simulations of Materials Strength and Deformation: Prospects for Mechanistic Insights**, *Materials Science for the 21st Century*
Li, J., Cai, W., Chang, J., Yip, S.
2001; A: 220-233
 - **Atomistic and Mesoscale Modeling of Dislocation Mobility** *PhD Thesis*
Cai, W.
Massachusetts Institute of Technology.2001
 - **Periodic Boundary Conditions for Dislocation Dynamics Simulations in Three Dimensions**
Bulatov, V. V., Rhee, M., Cai, W.
2001
 - **Minimizing boundary reflections in coupled-domain simulations** *PHYSICAL REVIEW LETTERS*
Cai, W., de Koning, M., Bulatov, V. V., Yip, S.
2000; 85 (15): 3213-3216
 - **Efficient free-energy calculations by the simulation of nonequilibrium processes** *COMPUTING IN SCIENCE & ENGINEERING*
de Koning, M., Cai, W., Antonelli, A., Yip, S.
2000; 2 (3): 88-96
 - **Intrinsic mobility of a dissociated Dislocation in silicon** *PHYSICAL REVIEW LETTERS*
Cai, W., Bulatov, V. V., Justo, J. F., Argon, A. S., Yip, S.
2000; 84 (15): 3346-3349
 - **Vacancy interaction with dislocations in silicon: The shuffle-glide competition** *PHYSICAL REVIEW LETTERS*
Justo, J. F., de Koning, M., Cai, W., Bulatov, V. V.
2000; 84 (10): 2172-2175

- **Efficient Free-Energy Calculations by the Simulation of Nonequilibrium Processes** *Computing in Science and Engineering*
de Koning, M., Cai, W., Antonelli, A., Yip, S.
2000; 2: 88
- **Dynamics of dissociated dislocations in Si: A micro-meso simulation methodology** *Symposium on Multiscale Modelling of Materials, at the 1998 MRS Fall Meeting*
Cai, W., Bulatov, V. V., Justo, J. F., Yip, S., Argon, A. S.
MATERIALS RESEARCH SOCIETY.1999: 69–75
- **Kinetic Monte Carlo method for dislocation glide in silicon** *5th International Conference on Advanced Materials (IUMRS)*
Cai, W., Bulatov, V. V., Yip, S.
SPRINGER.1999: 175–83
- **Kink asymmetry and multiplicity in dislocation cores** *PHYSICAL REVIEW LETTERS*
Bulatov, V. V., Justo, J. F., Cai, W., Yip, S.
1997; 79 (25): 5042-5045