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

CONTACT INFORMATION

• Administrator
  Kelly Chu - Administrative Associate
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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

2022-23
• Computational Engineering: ME 123 (Spr)
• The Science and the Practice of Metal 3D Printing: ME 349 (Win)

2021-22
• Computational Engineering: ME 123 (Spr)
• Introduction to Statistical Mechanics: ME 346A (Win)

2020-21
• Computational Engineering: ME 123 (Aut)
• Introduction to Molecular Simulations: ME 346B (Spr)
• Introduction to Statistical Mechanics: ME 346A (Win)

2019-20
• Introduction to Statistical Mechanics: ME 346A (Spr)
• Mechanical Analysis in Design: ME 329 (Win)
• Mechanics of Materials: ME 80 (Aut)
• Seminar in Solid Mechanics: ME 395 (Aut, Win)

STANFORD ADVISEES

Doctoral Dissertation Reader (AC)
David Doan, Saisneha Koppaka

Postdoctoral Faculty Sponsor
Rasool Ahmad, Wurong Jian

Doctoral Dissertation Advisor (AC)
Shaswat Mohanty

Doctoral Dissertation Co-Advisor (AC)
Sara Ha

Master's Program Advisor
Renee Nguyen, Saketh Pemmasani

Doctoral (Program)
Amitesh Jayaraman

Publications

PUBLICATIONS

• 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** *ADDITIONAL 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. *ADDITIONAL 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., Clarke, D. R.  
  2020; 50: 437–64

- Phase-field investigation of the stages in radial growth of core-shell Ge/Ge1-xSnx nanowires. *Nanoscale*
  Wang, Y., Meng, A. C., McIntyre, P. C., Cai, W.  
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- 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  
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- GPU-accelerated dislocation dynamics using subcycling time-integration. *MODELLING AND SIMULATION IN MATERIALS SCIENCE AND ENGINEERING*
  Bertin, N., Aubry, S., Arsenlis, A., Cai, W.  
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- 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.  
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- 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/Ge1-xSnx nanowire light emitters. *Materials Today Nano*
  Meng, A. C.  
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- 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.  
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- 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.  
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• 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., Woytowitz, 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.
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• 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.
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• Computation of virtual X-ray diffraction patterns from discrete dislocation structures *COMPUTATIONAL MATERIALS SCIENCE*
  Bertin, N., Cai, W.
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• 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.
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• 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*
  Ramachandranmoorthy, 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.
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• 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-Gagné, S., Park, J., Schroeder, et al
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• Stability of Eshelby dislocations in FCC crystalline nanowires *INTERNATIONAL JOURNAL OF PLASTICITY*
  Ryu, S., Cai, W.
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• 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.
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  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.
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• 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.
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- Spontaneous, Defect-Free Kinking via Capillary Instability during Vapor-Liquid-Solid Nanowire Growth. *Nano letters*
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  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.
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- Anisotropic Size-Dependent Plasticity in Face-Centered Cubic Micropillars Under Torsion *JOM*
  Ryu, I., Cai, W., Nix, W. D., Gao, H.
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- 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.
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- Shape-Controlled, Self-Wrapped Carbon Nanotube 3D Electronics. *Advanced science (Weinheim, Baden-Wurttemberg, Germany)*
  Wang, H., Wang, Y., Tee, B. C., Kim, K., Lopez, J., Cai, W., Bao, Z.
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- 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.
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- 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.
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- Ideal Shear Strength of a Quantum Crystal *PHYSICAL REVIEW LETTERS*
  Landinez Borda, E. J., Cai, W., de Koning, M.
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- 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.
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• 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.
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• 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.
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• Zipping, 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*
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• Atomistic simulations of grain boundary segregation in nanocrystalline yttria-stabilized zirconia and gadolinia-doped ceria solid oxide electrolytes  *Acta Materialia*
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  Ryu, I., Nix, W. D., Cai, W.
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• Zipping, 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.
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• Modeling Dislocation Mechanisms of the Acoustic Nonlinearity in Metallic Crystals  *9th International Workshop on Structural Health Monitoring (IWSHM)*
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• Modelling plasticity of BCC micro-pillars using dislocation dynamics  *Acta Materialia*
  Ryu, I., Nix, William, D., Cai, W.
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• 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.
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  Filletier, T., Ryu, S., Kang, K., Yin, J., Bernal, R. A., Sohn, K., Li, S., Huang, J., Cai, W., Espinosa, H. D.
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• 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.
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• 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.
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• 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.
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• 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.
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• Contribution of dislocation dipole structures to the acoustic nonlinearity. *JOURNAL OF APPLIED PHYSICS*
  CASH, W. D., Cai, W.
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• Stress-driven migration of simple low-angle mixed grain boundaries. *ACTA MATERIALIA*
  Lim, A. T., Haataja, M., Cai, W., Srolovitz, D. J.
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• Plasticity of metal nanowires. *JOURNAL OF MATERIALS CHEMISTRY*
  Weinberger, C. R., Cai, W.
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• Molecular Dynamics. *Comprehensive Nuclear Materials*
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• Equilibrium shape of dislocation shear loops in anisotropic alpha-Fe. *MODELLING AND SIMULATION IN MATERIALS SCIENCE AND ENGINEERING*
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• Predicting the dislocation nucleation rate as a function of temperature and stress. *JOURNAL OF MATERIALS RESEARCH*
  Ryu, S., Kang, K., Cai, W.
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• Molecular dynamics simulations of gold-catalyzed growth of silicon bulk crystals and nanowires. *JOURNAL OF MATERIALS RESEARCH*
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• The stability of Lomer-Cottrell jogs in nanopillars. *SCRIPTA MATERIALIA*
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  Lee, E., Prinz, F. B., Cai, W.
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  Cash, W. D., Cai, W.
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• Entropic Effect on the Rate of Dislocation Nucleation
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• Nanoscale patterning controls inorganic-membrane interface structure. *Nanoscale*
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• Analysis of the elastic strain energy driving force for grain boundary migration using phase field simulation. *Scripta Materialia*
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• Size and temperature effects on the fracture mechanisms of silicon nanowires: Molecular dynamics simulations. *International Journal of Plasticity*
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• Numerical tests of nucleation theories for the Ising models. *Physical Review E*
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• 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.
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• Atomistic simulations of surface segregation of defects in solid oxide electrolytes. *Acta Materialia*
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• Kinetic Monte Carlo simulations of oxygen vacancy diffusion in a solid electrolyte: Computing the electrical impedance using the fluctuation-dissipation theorem. *Electrochemistry Communications*
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• Orientation-Dependent Plasticity in Metal Nanowires under Torsion: Twist Boundary Formation and Eshelby Twist. *Nano Letters*
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