Ting-Ju Wei

Computational Materials Scientist | AI-Driven Multiscale Modeling

Ph.D., Civil Engineering (AI for Engineering Applications), National Taiwan University

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Personal Website Google Scholar

PROFILE

Computational-materials researcher specializing in **crystal plasticity (CPFEM)**, multiscale microstructure modeling, and **AI-based surrogate models** for metallic and heterogeneous materials. I build physics-informed models that link **polycrystalline microstructure**—grain orientation, texture evolution, and dislocation-mediated plasticity—to macroscopic mechanical response, reaching **sub-1% accuracy** with **1000×+ speedups** over FFT-based crystal-plasticity solvers (DAMASK). The same framework transfers directly to **recrystallization, dislocation, and precipitation** behavior in alloy heat treatment and processing. First-author work in *CMAME* and *Materials & Design*. Seeking to apply microstructure simulation and AI modeling to **alloy design and high-cleanliness metal process development**.

EDUCATION

Ph.D., Civil Engineering — AI for Engineering Applications 2023 – 2026

National Taiwan University

Thesis: Deep Material Networks for Microstructure Learning in Multiscale Simulations.

- Proposed **ODMN** (orientation-aware deep material network), a semi-analytical crystal-plasticity surrogate for polycrystals capturing grain orientation, texture evolution, and dislocation-mediated hardening; **trained on linear-elastic data only**, it predicts the full **nonlinear** mechanical response at **under 1% error** with **over 1000× speedup** over DAMASK (published in *CMAME*).
- Proposed domain-specific **foundation models** for short-fiber composites and FCC polycrystals; transfer learning maps microstructure to surrogate parameters and generalizes across manufacturing-induced microstructural variation.
- Built a **piezoelectric deep material network (PDMN)** for nonlinear electromechanical homogenization of piezoelectric composites.

M.Sc., Civil Engineering — Computer-Aided Engineering 2021 – 2023

National Taiwan University

Thesis: Bubble Generation during Root Canal Treatment — Numerical Modeling and Experimental Validation.

- Ran **molecular-dynamics** simulations of CoCrFeMnNi high-entropy alloys and developed planar-defect (stacking-fault and dislocation) identification algorithms (published in *Materials Chemistry and Physics*).
- Proposed **dimensionless parameters** and a **CFD computational framework** to predict root-canal irrigation efficiency and cavitation-bubble formation; validated experimentally with NTU Hospital.

B.Sc., Civil Engineering 2013 – 2017

National Chung Hsing University

TECHNICAL SKILLS

Computational Materials	Crystal plasticity & CPFEM; multiscale homogenization; polycrystalline microstructure & texture-evolution modeling; microstructure–property linkage; high-entropy alloys (molecular dynamics).
AI / ML for Materials	Physics-informed surrogate & reduced-order modeling; deep material networks; foundation models & transfer learning; data-driven microstructure-to-property prediction.
Simulation & Modeling	Multiphysics coupling (mechanical, thermal, electromechanical); total-Lagrangian nonlinear finite element methods; eigenerosion-based fracture modeling.
Programming	Python, C/C++, Fortran, MATLAB; numerical algorithm development; scientific computing; software design patterns.
Software & Tools	DAMASK (crystal plasticity / FFT); Abaqus, ANSYS (commercial FEM); LAMMPS (atomistics); PyTorch (deep learning); in-house nonlinear FEM solver development.
Languages	Mandarin Chinese (native); English (IELTS 7.0); Taiwanese Hokkien (intermediate).

SELECTED PROJECTS

AI-Driven Virtual Materials Development Platform 2026
Doctoral research

- Ported the **DAMASK** crystal-plasticity solver into the **ODMN** framework to enhance predictive fidelity and scale the surrogate to industrial forming problems.
- Ran concurrent **two-scale (macro–micro)** simulations on industrial benchmarks — sheet-metal **deep drawing** and an **L-shape thermomechanical** part.
- Demonstrated a fast, high-fidelity pipeline as a foundation for **industrial digital twins**, linking microstructure directly to product performance.

Piezoelectric Deep Material Network (PDMN) 2025 – 2026
Doctoral research

- Extended the deep material network to **nonlinear electromechanical homogenization** of piezoelectric composites, capturing coupled mechanical–electrical response.

Foundation Models for Materials Microstructures 2024 – 2026
Doctoral research

- Developed transfer-learning **foundation models** for short-fiber composites and FCC polycrystals: microstructure reconstruction plus stiffness and nonlinear-behavior prediction.
- Generalized across manufacturing-induced microstructural variation, reducing per-material retraining cost (published in *Materials & Design*).

Orientation-Aware Deep Material Network (ODMN) for Crystal Plasticity 2023 – 2025
Doctoral research • published in *CMAME*

- Proposed **ODMN**, a semi-analytical crystal-plasticity surrogate for polycrystals capturing grain orientation, texture evolution, and dislocation-mediated hardening.
- **Trained on linear-elastic data only**, yet predicts the full **nonlinear** mechanical response at **under 1% error** with **over 1000× speedup** vs. the FFT-based DAMASK solver.

NASA Space Apps Challenge — Global Winner, Best Use of Science 2022
Carrington Event — space-weather challenge

- Built a science-driven solution for NASA's **Carrington Event** challenge on extreme space weather (geomagnetic storms), recognized worldwide for rigorous use of scientific data.
- Ranked **1st of 5,300+ teams** globally; project page.

SELECTED PUBLICATIONS

Author name in **bold**. Full list on Google Scholar.

Journal Articles

[1] **T.-J. Wei**, Y.-M. Lu, and C.-S. Chen, "Deep material network for homogenization of piezoelectric composites," *arXiv preprint arXiv:2606.22566*, 2026.

[2] **T.-J. Wei**, T.-H. Su, and C.-S. Chen, "A parametric multiscale surrogate framework based on texture-generalizable deep material networks for polycrystal modeling," *arXiv preprint arXiv:2512.06779v2*, 2026, Under Review.

[3] **T.-J. Wei**, W.-N. Wan, and C.-S. Chen, "Deep material network: Overview, applications, and current directions," *Multiscale Science and Engineering*, pp. 1–19, 2026.

[4] **T.-J. Wei** and C.-S. Chen, "Foundation model for composite microstructures: Reconstruction, stiffness, and nonlinear behavior prediction," *Materials & Design*, vol. 257, p. 114 397, 2025.

[5] **T.-J. Wei** and C.-S. Chen, "Foundation model for polycrystalline material informatics," *arXiv preprint arXiv:2512.06770*, 2025, Under Review.

[6] **T.-J. Wei**, T.-H. Su, and C.-S. Chen, "Orientation-aware interaction-based deep material network in polycrystalline materials modeling," *Computer Methods in Applied Mechanics and Engineering*, vol. 441, p. 117 977, 2025, ISSN: 0045-7825.

[7] W.-N. Wan, **T.-J. Wei**, T.-H. Su, and C.-S. Chen, "Decoding material networks: Exploring performance of deep material network and interaction-based material networks," *Journal of Mechanics*, vol. 40, pp. 796–807, 2024, ISSN: 1811-8216.

[8] K.-T. Chen, **T.-J. Wei**, G.-C. Li, M.-Y. Chen, Y.-S. Chen, S.-W. Chang, H.-W. Yen, and C.-S. Chen, "Mechanical properties and deformation mechanisms in CoCrFeMnNi high entropy alloys: A molecular dynamics study," *Materials Chemistry and Physics*, vol. 271, p. 124 912, 2021, ISSN: 0254-0584.

Selected Conference Presentations

[9] **T.-J. Wei** and C.-S. Chen, "Deep material networks for homogenization of heterogeneous piezoelectric materials," in *The 17th World Congress on Computational Mechanics (WCCM) and the 10th European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS)*, July 19–24, Munich, Germany, 2026.

[10] **T.-J. Wei** and C.-S. Chen, "Deep material networks for nonlinear electromechanical homogenization of piezoelectric composites," in *AI-Empowered Simulations and CAE Applications via Engineering Software 2.0 and 3.0 (AESCAPE 2026)*, September 8–11, Dallas, Texas, USA, 2026.

[11] **T.-J. Wei** and C.-S. Chen, "Generalizable deep material networks for polycrystalline and composite materials: Incorporating graph neural networks and foundation models," in *The 9th Asian Pacific Congress on Computational Mechanics (APCOM) and the 7th Australasian Conference on Computational Mechanics (ACCM)*, December 7–10, Brisbane, Australia, 2025.

[12] **T.-J. Wei**, W.-N. Wan, and C.-S. Chen, "Orientation-aware interaction-based deep material network for polycrystalline materials with diverse microstructures," in *The XVIII International Conference on Computational Plasticity (COMPLAS)*, September 2–5, Barcelona, Spain, 2025.

[13] **T.-J. Wei** and C.-S. Chen, "Advancing multiscale modeling in polycrystalline materials: A novel deep material network approach," in *The 16th World Congress on Computational Mechanics (WCCM) and the 4th Pan American Congress on Computational Mechanics (PANACM)*, July 21–26, Vancouver, Canada, 2024.

[14] **T.-J. Wei**, T.-H. Su, and C.-S. Chen, "Graph-enhanced ODMN: A unified model for advanced polycrystalline material modeling," in *Association of Computational Mechanics Taiwan (ACMT 2024) and the 15th Workshop on Boundary Element Methods (TWBEM 15)*, October 5–6, 2024.

[15] **T.-J. Wei**, Y.-Y. Chen, C.-C. Lin, W.-W. Liu, A.-B. Wang, and J.-S. Chen, "Simulating an irrigation flow in root canal: Predicting the likelihood of the cavitation bubble formation," in *Association of Computational Mechanics Taiwan (ACMT 2023) Annual Meeting*, October 28–29, Taipei, Taiwan, 2023.

HONORS & AWARDS

Dean's Award for Graduate Students 2026
College of Engineering, National Taiwan University

Honorable Mention — Walsin Lihwa × NTU Engineering Research Competition 2026
AI-Driven Virtual Materials Development and Intelligent Manufacturing Decision Platform

Saxon Student Mobility Scholarship 2025
Saxon Ministry for Science, Culture and Tourism — research stay at TU Dresden

Ministry of Education Doctoral Scholarship (AY 113) 2024
National Taiwan University

Xin-Miao Technology Doctoral Scholarship 2023
Xin-Miao Educational Foundation — 5 doctoral students university-wide per year

2nd Place, Taipei City — NASA Space Apps Challenge 2023
NASA

Global Winner, Best Use of Science — NASA Space Apps Challenge 2022
1st of 5,300+ teams worldwide • *project page*

PROFESSIONAL EXPERIENCE

Contractor's Professional Engineer 2022 – 2026
Rong-Hua Construction Co., Ltd.

- Provided licensed technical consultation, design review, and engineering certification for construction projects.

Contractor's Professional Engineer 2021 – 2022
Feng-Ya Construction Co., Ltd.

- Delivered professional review and engineering certification for construction contracts.

Associate Technical Specialist 2017 – 2021
Experimental Forest, National Taiwan University

- Managed engineering procurement, contract preparation, subcontractor coordination, construction documentation, and contract performance.

CERTIFICATION

Professional Engineer (PE), Civil Engineering 2021
Public Construction Commission — Credential ID 017987