# Takahiro Shimada

## List of Publications by Year in Descending Order

**Source:** https://exaly.com/author-pdf/6417295/takahiro-shimada-publications-by-year.pdf
**Version:** 2024-04-25

This document has been generated based on the publications and citations recorded by exaly.com. For the latest version of this publication list, visit the link given above.
The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

| | | | |
|---|---|---|---|
| 167 papers | 1,715 citations | 23 h-index | 32 g-index |
| 177 ext. papers | 1,994 ext. citations | 4.1 avg, IF | 4.98 L-index |

| # | Paper | IF | Citations |
|---|---|---|---|
| 167 | Thermomechanical conversion in high-rate plastic deformation of nanotwinned polycrystalline copper. *Journal of Thermal Stresses*, **2022**, 45, 65-80 | 2.2 | |
| 166 | Atomistic investigation on the conversion of plastic work to heat in high-rate shear deformation. *International Journal of Plasticity*, **2022**, 149, 103158 | 7.6 | 0 |
| 165 | A unified atomic energy release rate criterion for nonlinear brittle fracture in graphene nanoribbons. *International Journal of Solids and Structures*, **2022**, 234-235, 111260 | 3.1 | |
| 164 | Flexoelectric properties of multilayer two-dimensional material MoS2. *Journal Physics D: Applied Physics*, **2022**, 55, 125302 | 3 | 1 |
| 163 | Abnormal Electromechanical Property of Nonlinearly Graded Lead-Free Ferroelectric Thin Films. *Advanced Theory and Simulations*, **2021**, 2100370 | 3.5 | 1 |
| 162 | The rectilinear motion of the individual asymmetrical skyrmion driven by temperature gradients. *Acta Materialia*, **2021**, 221, 117383 | 8.4 | 1 |
| 161 | Electrocaloric effect enhancement in compositionally graded ferroelectric thin films driven by a needle-to-vortex domain structure transition. *Journal Physics D: Applied Physics*, **2021**, 54, 255307 | 3 | 5 |
| 160 | Shock response and defect evolution of copper single crystals at room and elevated temperatures. *Modelling and Simulation in Materials Science and Engineering*, **2021**, 29, 045006 | 2 | 1 |
| 159 | Prediction of tunable magnetoelectric properties in compositionally graded ferroelectric/ferromagnetic laminated nanocomposites. *Applied Physics Letters*, **2021**, 118, 052905 | 3.4 | 2 |
| 158 | Energy storage and dissipation of elastic-plastic deformation under shock compression: Simulation and Analysis. *Mechanics of Materials*, **2021**, 158, 103876 | 3.3 | 3 |
| 157 | Interlaminar Fracture Toughness Measurement of Multilayered 2D Thermoelectric Materials Bi2Te3 by a Tapered Cantilever Bending Experiment. *Experimental Mechanics*, **2021**, 1 | 2.6 | 1 |
| 156 | Reversible control of intrinsic shear strength of a ZnO single crystal through electron-beam-induced hole state. *Journal of Materials Research*, **2021**, 1 | 2.5 | 1 |
| 155 | Linear-superelastic Ti-Nb nanocomposite alloys with ultralow modulus via high-throughput phase-field design and machine learning. *Npj Computational Materials*, **2021**, 7, | 10.9 | 2 |
| 154 | An Atomic-Level Unified Criterion for Brittle Fracture. *Structural Integrity*, **2020**, 334-336 | 0.2 | |
| 153 | Ferrotoroidic polarons in antiferrodistortive SrTiO3. *Physical Review B*, **2020**, 101, | 3.3 | 2 |
| 152 | Atomic investigation of effects of coating and confinement layer on laser shock peening. *Optics and Laser Technology*, **2020**, 131, 106409 | 4.2 | 7 |
| 151 | Electron-beam irradiation alters bond strength in zinc oxide single crystal. *Applied Physics Letters*, **2020**, 116, 111902 | 3.4 | 5 |

| | | | |
|---|---|---|---|
| 150 | In situ TEM observation of nanodomain mechanics in barium titanate under external loads. *Physical Review Materials*, **2020**, 4, | 3.2 | 2 |
| 149 | Defect engineering for nontrivial multiferroic orders in SrTiO3. *Physical Review Materials*, **2020**, 4, | 3.2 | 2 |
| 148 | Ferroelectric critical size of SnTe nanoribbon and its mechanical strain engineering. *Transactions of the JSME (in Japanese)*, **2020**, 86, 19-00430-19-00430 | 0.2 | |
| 147 | Ferroelectric control of magnetic skyrmions in multiferroic heterostructures. *Physical Review B*, **2020**, 102, | 3.3 | 7 |
| 146 | Deformation mode dependence of an exothermic chemical reaction in Ti/Si multilayered nanofilms. *Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing* , **2020**, 796, 140021 | 5.3 | |
| 145 | Beyond conventional nonlinear fracture mechanics in graphene nanoribbons. *Nanoscale*, **2020**, 12, 18363-18370 | 7.7 | 9 |
| 144 | An experimental study on atomic-level unified criterion for brittle fracture. *International Journal of Solids and Structures*, **2020**, 206, 1-8 | 3.1 | 3 |
| 143 | Two-dimensional polar metal of a PbTe monolayer by electrostatic doping. *Nanoscale Horizons*, **2020**, 5, 1400-1406 | 10.8 | 2 |
| 142 | Enhancement of electromechanical properties in (0□3) lead-free ferroelectric nanocomposites with multiphase coexistence. *Composites Communications*, **2020**, 22, 100540 | 6.7 | 4 |
| 141 | Selective excitation of two-wave structure depending on crystal orientation under shock compression. *Science China: Physics, Mechanics and Astronomy*, **2020**, 63, 1 | 3.6 | 5 |
| 140 | Asymmetric flux-closure domains in compositionally graded nanoscale ferroelectrics and unusual switching of toroidal ordering by an irrotational electric field. *Acta Materialia*, **2019**, 179, 215-223 | 8.4 | 10 |
| 139 | Deterministic Switching of Polarization Vortices in Compositionally Graded Ferroelectrics Using a Mechanical Field. *Physical Review Applied*, **2019**, 11, | 4.3 | 13 |
| 138 | Electron engineering of metallic multiferroic polarons in epitaxial BaTiO3. *Npj Computational Materials*, **2019**, 5, | 10.9 | 8 |
| 137 | Ultrasoft silicon nanomembranes: thickness-dependent effective elastic modulus. *Nanoscale*, **2019**, 11, 15184-15194 | 7.7 | 7 |
| 136 | Periodically-arrayed ferroelectric nanostructures induced by strain concentration in SrTiO3. *Transactions of the JSME (in Japanese)*, **2019**, 85, 19-00175-19-00175 | 0.2 | |
| 135 | Lifetime prediction of thermoelectric devices under thermal cycling. *Journal of Power Sources*, **2019** , 437, 226861 | 8.9 | 7 |
| 134 | Strain energy density approach for brittle fracture from nano to macroscale and breakdown of continuum theory. *Theoretical and Applied Fracture Mechanics*, **2019**, 103, 102300 | 3.7 | 12 |
| 133 | Effect of the oxygen vacancy on the ferroelectricity of 90□domain wall structure in PbTiO3: A density functional theory study. *Journal of Applied Physics*, **2019**, 126, 174107 | 2.5 | 4 |

| | | | |
|---|---|---|---|
| 132 | Periodically-arrayed ferroelectric nanostructures induced by dislocation structures in strontium titanate. *Physical Chemistry Chemical Physics*, **2019**, 21, 22756-22762 | 3.6 | 3 |
| 131 | Investigation into the Breakdown of Continuum Fracture Mechanics at the Nanoscale: Synthesis of Recent Results on Silicon. *Structural Integrity*, **2019**, 205-210 | 0.2 | 3 |
| 130 | Topological ferroelectric nanostructures induced by mechanical strain in strontium titanate. *Physical Chemistry Chemical Physics*, **2019**, 21, 22420-22428 | 3.6 | 1 |
| 129 | Intrinsic and extrinsic effects on the electrotoroidic switching in a ferroelectric notched nanodot by a homogeneous electric field. *Physical Chemistry Chemical Physics*, **2019**, 21, 25011-25022 | 3.6 | 2 |
| 128 | Continuum thermodynamics of unusual domain evolution-induced toughening effect in nanocracked strontium titanate. *Engineering Fracture Mechanics*, **2018**, 190, 232-244 | 4.2 | 4 |
| 127 | Effect of geometric configuration on the electrocaloric properties of nanoscale ferroelectric materials. *Journal of Applied Physics*, **2018**, 123, 124103 | 2.5 | 11 |
| 126 | Ferroelectric critical size and vortex domain structures of PbTiO3 nanodots: A density functional theory study. *Journal of Applied Physics*, **2018**, 123, 114101 | 2.5 | 9 |
| 125 | Challenge toward nanometer scale fracture mechanics. *Engineering Fracture Mechanics*, **2018**, 187, 33-44 | 4.2 | 13 |
| 124 | Giant magnetoelectric effect at the graphone/ferroelectric interface. *Scientific Reports*, **2018**, 8, 12448 | 4.9 | 5 |
| 123 | Phase field simulations on domain switching-induced toughening in ferromagnetic materials. *European Journal of Mechanics, A/Solids*, **2017**, 65, 205-211 | 3.7 | 2 |
| 122 | Multiferroic Phases and Transitions in Ferroelectric Lead Titanate Nanodots. *Scientific Reports*, **2017**, 7, 45373 | 4.9 | 4 |
| 121 | Griffith Criterion for Nanoscale Stress Singularity in Brittle Silicon. *ACS Nano*, **2017**, 11, 6271-6276 | 16.7 | 30 |
| 120 | Multiferroic Dislocations in Ferroelectric PbTiO. *Nano Letters*, **2017**, 17, 2674-2680 | 11.5 | 17 |
| 119 | Multilevel hysteresis loop engineered with ferroelectric nano-metamaterials. *Acta Materialia*, **2017**, 125, 202-209 | 8.4 | 20 |
| 118 | Self-ordering of nontrivial topological polarization structures in nanoporous ferroelectrics. *Nanoscale*, **2017**, 9, 15525-15533 | 7.7 | 18 |
| 117 | Switching the chirality of a ferroelectric vortex in designed nanostructures by a homogeneous electric field. *Physical Review B*, **2017**, 96, | 3.3 | 26 |
| 116 | A unified and universal Griffith-based criterion for brittle fracture. *International Journal of Solids and Structures*, **2017**, 128, 67-72 | 3.1 | 23 |
| 115 | Strain-induced ferroelectricity and lattice coupling in BaSnO and SrSnO. *Physical Chemistry Chemical Physics*, **2017**, 19, 26047-26055 | 3.6 | 14 |

| | | | |
|---|---|---|---|
| 114 | Unusual Metallic Multiferroic Transitions in Electron-Doped PbTiO3. *Advanced Electronic Materials*, **2017**, 3, 1700134 | 6.4 | 6 |
| 113 | Ferroelectricity in Ruddlesden-Popper Chalcogenide Perovskites for Photovoltaic Application: The Role of Tolerance Factor. *Journal of Physical Chemistry Letters*, **2017**, 8, 5834-5839 | 6.4 | 27 |
| 112 | Strain-induced improper ferroelectricity in Ruddlesden-Popper perovskite halides. *Physical Review B*, **2017**, 96, | 3.3 | 8 |
| 111 | Multiphysics in Nanostructures. *Nanostructure Science and Technology*, **2017**, | 0.9 | 5 |
| 110 | Ferroelectric Nanostructures. *Nanostructure Science and Technology*, **2017**, 97-139 | 0.9 | |
| 109 | Methodology of Quantum Mechanics/Atomic Simulations. *Nanostructure Science and Technology*, **2017**, 5-34 | 0.9 | |
| 108 | Multiferroic Nanostructures. *Nanostructure Science and Technology*, **2017**, 165-192 | 0.9 | |
| 107 | Strain Engineering on Nanosemiconductors. *Nanostructure Science and Technology*, **2017**, 67-96 | 0.9 | |
| 106 | Magnetism in Nanostructures. *Nanostructure Science and Technology*, **2017**, 141-164 | 0.9 | |
| 105 | Ideal Strength in Low-Dimensional Nanostructures. *Nanostructure Science and Technology*, **2017**, 35-66 | 0.9 | |
| 104 | Ferroic Nanometamaterials and Composites. *Nanostructure Science and Technology*, **2017**, 193-214 | 0.9 | |
| 103 | Critical dimensional limit of continuum fracture mechanics for dislocation emission. *Engineering Fracture Mechanics*, **2016**, 163, 108-116 | 4.2 | 3 |
| 102 | Multiferroic nature of intrinsic point defects in BiFeO3: A hybrid Hartree-Fock density functional study. *Physical Review B*, **2016**, 93, | 3.3 | 32 |
| 101 | Unusual Multiferroic Phase Transitions in PbTiO Nanowires. *Nano Letters*, **2016**, 16, 6774-6779 | 11.5 | 7 |
| 100 | Multiferroic Transitions and Misfit Phase Diagram in Oxygen-Deficient Epitaxial (111) PbTiO3. *Advanced Electronic Materials*, **2016**, 2, 1600113 | 6.4 | 3 |
| 99 | Polar Superhelices in Ferroelectric Chiral Nanosprings. *Scientific Reports*, **2016**, 6, 35199 | 4.9 | 10 |
| 98 | Modulation of Gas Adsorption and Magnetic Properties of Monolayer-MoS2 by Antisite Defect and Strain. *Journal of Physical Chemistry C*, **2016**, 120, 14113-14121 | 3.8 | 51 |
| 97 | Multiferroic Domain Walls in Ferroelectric PbTiO3 with Oxygen Deficiency. *Nano Letters*, **2016**, 16, 454-8 | 11.5 | 36 |

| | | | |
|---|---|---|---|
| 96 | One-dimensional atomic multiferroics by dislocation cores in nonmagnetic ferroelectric PbTiO3. *The Proceedings of the Materials and Mechanics Conference*, **2016**, 2016, OS11-16 | 0 | |
| 95 | Antiferroelectric and antiferrodistortive phase transitions in Ruddlesden-Popper Pb2TiO4from First-Principles. *Multiscale and Multiphysics Mechanics*, **2016**, 1, 233-244 | | |
| 94 | Mechanics of Fibrous Biological Materials With Hierarchical Chirality. *Journal of Applied Mechanics, Transactions ASME*, **2016**, 83, | 2.7 | 8 |
| 93 | An I-integral method for crack-tip intensity factor variation due to domain switching in ferroelectric single-crystals. *Journal of the Mechanics and Physics of Solids*, **2016**, 94, 207-229 | 5 | 19 |
| 92 | Instability criterion for ferroelectrics under mechanical/electric multi-fields: Ginzburg-Landau theory based modeling. *Acta Materialia*, **2016**, 112, 1-10 | 8.4 | 16 |
| 91 | Polar and toroidal electromechanical properties designed by ferroelectric nano-metamaterials. *Acta Materialia*, **2016**, 113, 81-89 | 8.4 | 24 |
| 90 | Hybrid improper ferroelectricity in SrZrO3/BaZrO3 superlattice. *Physical Chemistry Chemical Physics* , **2016**, 18, 24024-32 | 3.6 | 6 |
| 89 | Breakdown of continuum fracture mechanics at the nanoscale. *Scientific Reports*, **2015**, 5, 8596 | 4.9 | 53 |
| 88 | Magnetic instability criterion for spin□attice systems. *Computational Materials Science*, **2015**, 97, 216-221 | 3.2 | 9 |
| 87 | Interplay of coupling between strain and rotation in ferroelectric SrZrO3/SrTiO3 superlattices. *Journal of Physics Condensed Matter*, **2015**, 27, 385901 | 1.8 | 1 |
| 86 | Mechanical control of magnetism in oxygen deficient perovskite SrTiO3. *Physical Chemistry Chemical Physics*, **2015**, 17, 27136-44 | 3.6 | 21 |
| 85 | Defect-strain engineering for multiferroic and magnetoelectric properties in epitaxial (110) ferroelectric lead titanate. *Physical Review B*, **2015**, 92, | 3.3 | 13 |
| 84 | Multiferroic grain boundaries in oxygen-deficient ferroelectric lead titanate. *Nano Letters*, **2015**, 15, 27-33 | 11.5 | 23 |
| 83 | Hybrid functional study on the ferroelectricity of domain walls with O-vacancies in PbTiO3. *Mechanical Engineering Journal*, **2015**, 2, 15-00037-15-00037 | 0.5 | 2 |
| 82 | Multiferroic Vacancies at Ferroelectric PbTiO(3) Surfaces. *Physical Review Letters*, **2015**, 115, 107202 | 7.4 | 16 |
| 81 | Hierarchical ferroelectric and ferrotoroidic polarizations coexistent in nano-metamaterials. *Scientific Reports*, **2015**, 5, 14653 | 4.9 | 25 |
| 80 | Colossal magnetoelectric effect in 3-1 multiferroic nanocomposites originating from ultrafine nanodomain structures. *Applied Physics Letters*, **2015**, 107, 232904 | 3.4 | 19 |
| 79 | Anomalous toughening in nanoscale ferroelectrics with polarization vortices. *Acta Materialia*, **2015**, 88, 147-155 | 8.4 | 31 |

| | | | |
|---|---|---|---|
| 78 | Fracture Mechanics at Atomic Scales. *Advanced Structured Materials*, **2015**, 379-396 | 0.6 | 3 |
| 77 | Disappearance of ferroelectric critical thickness in epitaxial ultrathin BaZrO3 films. *Physical Review B*, **2014**, 90, | 3.3 | 15 |
| 76 | Strain-mediated multilevel ferroelectric random access memory operating through a magnetic field. *RSC Advances*, **2014**, 4, 45382-45388 | 3.7 | 7 |
| 75 | Ab initio study of multiferroic BiFeO3 (110) surfaces. *Physical Review B*, **2014**, 89, | 3.3 | 16 |
| 74 | Self-shaping of bioinspired chiral composites. *Acta Mechanica Sinica/Lixue Xuebao*, **2014**, 30, 533-539 | 2 | 7 |
| 73 | Effects of chirality and surface stresses on the bending and buckling of chiral nanowires. *Journal Physics D: Applied Physics*, **2014**, 47, 015302 | 3 | 5 |
| 72 | Strain tunable ferroelectric and dielectric properties of BaZrO3. *Journal of Applied Physics*, **2014**, 115, 224107 | 2.5 | 19 |
| 71 | Multi-physics properties in ferroelectric nanostructure. *Mechanical Engineering Reviews*, **2014**, 1, SMM0009-SMM0009 | 1.7 | 11 |
| 70 | First-Principles Study of Ferroelectric-Ferromagnetic Coupling in Multiferroic BiFeO3. *Zairyo/Journal of the Society of Materials Science, Japan*, **2014**, 63, 168-173 | 0.1 | 1 |
| 69 | Strain-induced polarity switching of magnetic vortex in Fe1−xGax alloys with different compositions. *Journal of Applied Physics*, **2014**, 115, 203911 | 2.5 | 5 |
| 68 | Large electrocaloric effect induced by the multi-domain to mono-domain transition in ferroelectrics. *Journal of Applied Physics*, **2014**, 115, 164102 | 2.5 | 32 |
| 67 | Unusual winding of helices under tension. *Applied Physics Letters*, **2014**, 105, 043702 | 3.4 | 12 |
| 66 | Chiral selectivity of improper ferroelectricity in single-wall PbTiO3 nanotubes. *Physical Review B*, **2014**, 89, | 3.3 | 9 |
| 65 | Multi-physics analysis of nano-structured ferroelectrics by first-principles simulations. *Acta Mechanica*, **2013**, 224, 1261-1270 | 2.1 | 2 |
| 64 | Role of grain orientation distribution in the ferroelectric and ferroelastic domain switching of ferroelectric polycrystals. *Acta Materialia*, **2013**, 61, 6037-6049 | 8.4 | 38 |
| 63 | Unusual domain evolution in semiconducting ferroelectrics: A phase field study. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2013**, 377, 1643-1648 | 2.3 | 3 |
| 62 | Control of the polarity of magnetization vortex by torsion. *Applied Physics Letters*, **2013**, 103, 242413 | 3.4 | 19 |
| 61 | Direct approach for flexoelectricity from first-principles calculations: cases for SrTiO3 and BaTiO3. *Journal of Physics Condensed Matter*, **2013**, 25, 415901 | 1.8 | 25 |

| | | | |
|---|---|---|---|
| 60 | Effect of strain on the evolution of magnetic multi-vortices in ferromagnetic nano-platelets. *Journal of Physics Condensed Matter*, **2013**, 25, 226002 | 1.8 | 12 |
| 59 | Ferroelectricity at a junction structure of a 180° domain wall and a (001) surface in PbTiO3: A density functional theory study. *Physica B: Condensed Matter*, **2013**, 410, 22-27 | 2.8 | 5 |
| 58 | Chiral selectivity of unusual helimagnetic transition in iron nanotubes: chirality makes quantum helimagnets. *Nano Letters*, **2013**, 13, 2792-7 | 11.5 | 10 |
| 57 | Hybrid Hartree-Fock density functional study of charged point defects in ferroelectric PbTiO3. *Physical Review B*, **2013**, 87, | 3.3 | 55 |
| 56 | OS1206 Ab-initio Study of Emergence of Helimagnetism and Its Chiral Selectivity in Single-wall Iron Nanotubes. *The Proceedings of the Materials and Mechanics Conference*, **2013**, 2013, _OS1206-1_-_OS1206-3_ | 0 | |
| 55 | Criterion of mechanical instabilities for dislocation structures. *Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing*, **2012**, 534, 681-687 | 5.3 | 8 |
| 54 | Ab initio study of shear strain effects on ferroelectricity at PbTiO3 thin films. *Surface Science*, **2012**, 606, 1331-1339 | 1.8 | 3 |
| 53 | Emergence of ferromagnetism at a vacancy on a non-magnetic ferroelectric PbTiO3 surface: A first-principles study. *Acta Materialia*, **2012**, 60, 6322-6330 | 8.4 | 20 |
| 52 | Strain-induced phase transitions in multiferroic BiFeO3 . *Physics Letters, Section A: General, Atomic and Solid State Physics*, **2012**, 376, 3368-3371 | 2.3 | 5 |
| 51 | Local suppression of ferroelectricity at PbTiO3 surface steps: a density functional theory study. *Journal of Physics Condensed Matter*, **2012**, 24, 045903 | 1.8 | 8 |
| 50 | Vacancy-driven ferromagnetism in ferroelectric PbTiO3. *Applied Physics Letters*, **2012**, 100, 162901 | 3.4 | 52 |
| 49 | First-principles study of nanometer-sharp domain walls in ferromagnetic Fe monolayers under in-plane strain. *Journal of Physics Condensed Matter*, **2012**, 24, 095303 | 1.8 | 3 |
| 48 | Ab initio study of spin-spiral noncollinear magnetism in a free-standing Fe(110) monolayer under in-plane strain. *Physical Review B*, **2012**, 85, | 3.3 | 15 |
| 47 | Absence of ferroelectric critical size in ultrathin PbTiO3 nanotubes: a density-functional theory study. *Physical Review Letters*, **2012**, 108, 067601 | 7.4 | 34 |
| 46 | Critical Thickness for Formation of Fatigue Dislocation Structures: A Discrete Dislocation Dynamics Study. *Nihon Kikai Gakkai Ronbunshu, A Hen/Transactions of the Japan Society of Mechanical Engineers, Part A*, **2012**, 78, 1242-1249 | | 2 |
| 45 | Development of Multi-Physics Instability Criterion for Atomic Structures and Application to Domain Switching in Ferroelectrics under External Electric Field. *Zairyo/Journal of the Society of Materials Science, Japan*, **2012**, 61, 155-161 | 0.1 | 4 |
| 44 | 318 A first-principles study of a nano-scale magnetic domain wall in an iron monolayer and the effect of in-plane strain. *The Proceedings of Conference of Kansai Branch*, **2012**, 2012.87, _3-29_ | 0 | |
| 43 | Coexistence of rectilinear and vortex polarizations at twist boundaries in ferroelectric PbTiO3 from first principles. *Physical Review B*, **2011**, 83, | 3.3 | 20 |

| | | | |
|---|---|---|---|
| 42 | Ab initio study of ferromagnetic single-wall nickel nanotubes. *Physical Review B*, **2011**, 84, | 3.3 | 15 |
| 41 | First-principles study of the interplay between grain boundaries and domain walls in ferroelectric PbTiO3. *Physical Review B*, **2011**, 83, | 3.3 | 27 |
| 40 | Ab initio study of ferromagnetism in edged iron nanowires under axial strain. *Physical Review B*, **2011**, 84, | 3.3 | 11 |
| 39 | OS1607 Development of magnetic instability criterion for atomic structures and its applications. *The Proceedings of the Materials and Mechanics Conference*, **2011**, 2011, _OS1607-1_-_OS1607-3_ | 0 | |
| 38 | Ab initio study of magnetism at iron surfaces under epitaxial in-plane strain. *Physical Review B*, **2010**, 81, | 3.3 | 23 |
| 37 | Dislocation nucleation in a thin Cu film from molecular dynamics simulations: Instability activation by thermal fluctuations. *Physical Review B*, **2010**, 82, | 3.3 | 12 |
| 36 | Stone-Wales transformations triggered by intrinsic localized modes in carbon nanotubes. *Physical Review B*, **2010**, 81, | 3.3 | 52 |
| 35 | First-principles study on ferroelectricity at PbTiO3 surface steps. *Journal of Physics Condensed Matter*, **2010**, 22, 355901 | 1.8 | 18 |
| 34 | Ab initio study of ferroelectric closure domains in ultrathin PbTiO3 films. *Physical Review B*, **2010**, 81, | 3.3 | 48 |
| 33 | Simplified Analysis of Mechanical Instability in Three-dimensional Atomic Components and Its Application to Nanoscale Crack. *Journal of Solid Mechanics and Materials Engineering*, **2010**, 4, 1071-1082 | | 1 |
| 32 | Mechanical Instability Criterion of Dislocation Structures Based on Discrete Dislocation Dynamics. *Nihon Kikai Gakkai Ronbunshu, A Hen/Transactions of the Japan Society of Mechanical Engineers, Part A*, **2010**, 76, 1721-1728 | | 1 |
| 31 | Influence of nonlinear atomic interaction on excitation of intrinsic localized modes in carbon nanotubes. *Physica D: Nonlinear Phenomena*, **2010**, 239, 407-413 | 3.3 | 16 |
| 30 | 1016 Ab initio study of ferroelectricity at twist boundary in PbTiO_3 and effect of strain. *The Proceedings of the Computational Mechanics Conference*, **2010**, 2010.23, 524-525 | 0 | |
| 29 | 105 Ab initio study of magnetism in edged Fe nanowires under axial tension. *The Proceedings of Conference of Kansai Branch*, **2010**, 2010.85, _1-5_ | 0 | |
| 28 | 1511 Molecular dynamics simulations on local defect nucleation triggered in carbon nanotubes by intrinsic localized modes. *The Proceedings of the Materials and Mechanics Conference*, **2010**, 2010, 99-101 | 0 | |
| 27 | Ab initio study of ferroelectricity in edged PbTiO3 nanowires under axial tension. *Physical Review B*, **2009**, 79, | 3.3 | 47 |
| 26 | First-principles Investigation of Edged Ferroelectric PbTiO3 Nanowires and the Role of Axial Strain. *Materials Research Society Symposia Proceedings*, **2009**, 1199, 147 | | |
| 25 | Simplified evaluation of mechanical instability in large-scale atomic structures. *Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing*, **2009**, 513-514, 166-171 | 5.3 | 14 |

| | | | |
|---|---|---|---|
| 24 | Development of Efficient Instability Analysis Method for Atomic Structures Using Linear Elements and Its Application to Amorphous Metal. *Journal of Solid Mechanics and Materials Engineering*, **2009**, 3, 807-818 | | 3 |
| 23 | Fracture Nano-Mechanics : 1st Report, Interface Strength of Nano-Components(Thermal and Mechanical Reliability of Electronic Device and Mechanical Engineering). *Nihon Kikai Gakkai Ronbunshu, A Hen/Transactions of the Japan Society of Mechanical Engineers, Part A*, **2009**, 75, 778-783 | | |
| 22 | Instability Mode Analysis of Dislocation Nucleation from Notch Based on Atomistic Model : Instability Activation Mechanism under Finite Temperature. *Nihon Kikai Gakkai Ronbunshu, A Hen/Transactions of the Japan Society of Mechanical Engineers, Part A*, **2009**, 75, 1247-1254 | | 1 |
| 21 | Fracture Nano-Mechanics : 2nd Report, Strength of Nano-Elements(Thermal and Mechanical Reliability of Electronic Device and Mechanical Engineering). *Nihon Kikai Gakkai Ronbunshu, A Hen/Transactions of the Japan Society of Mechanical Engineers, Part A*, **2009**, 75, 784-791 | | |
| 20 | M2-2 Multi-physics Analysis on Ferroelectric PbTiO_3 Nanowires from First-principles (M2 MaterialCharacterization). *The Proceedings of the Symposium on Micro-Nano Science and Technology*, **2009**, 2009.1, 37-38 | 0 | |
| 19 | T0301-2-5 Development of Evaluation Method for Mechanical Instability Using Linear Elements and Its Application to Cracked Atomic Strcuture. *The Proceedings of the JSME Annual Meeting*, **2009**, 2009.8, 53-54 | | |
| 18 | 1034 Ab initio study of multi-physics properties between magnetism and mechanical strain at Fe (001) thin films. *The Proceedings of the Computational Mechanics Conference*, **2009**, 2009.22, 300-301 | 0 | |
| 17 | 1030 Ab initio study of ferroelectricity at PbTiO_3 surface step. *The Proceedings of the Computational Mechanics Conference*, **2009**, 2009.22, 292-293 | 0 | |
| 16 | Ab initio study of stress-induced domain switching in PbTiO3. *Physical Review B*, **2008**, 77, | 3.3 | 41 |
| 15 | Shell model potential for PbTiO3and its applicability to surfaces and domain walls. *Journal of Physics Condensed Matter*, **2008**, 20, 325225 | 1.8 | 35 |
| 14 | Development of Efficient Instability Analysis Method for Atomic Structures Using Linear Elements and Its Application to Amorphous Metal. *Nihon Kikai Gakkai Ronbunshu, A Hen/Transactions of the Japan Society of Mechanical Engineers, Part A*, **2008**, 74, 1328-1335 | | 3 |
| 13 | OS1203 First-principles Investigation on Domain Switching Mechanism in Lead Titanate. *The Proceedings of the Materials and Mechanics Conference*, **2008**, 2008, _OS1203-1_-_OS1203-2_ | 0 | |
| 12 | 236 Development of Efficient Instability Analysis Method for Atomic Structures Using Linear Elements and Its Application to Amorphous Metal. *The Proceedings of the Computational Mechanics Conference*, **2008**, 2008.21, 456-457 | 0 | |
| 11 | OS0418 Ab initio study of ferroelectricity in edged PbTiO_3 nanowires under axial strain. *The Proceedings of the Materials and Mechanics Conference*, **2008**, 2008, _OS0418-1_-_OS0418-2_ | 0 | |
| 10 | 210 Development of Shell Model Potential for PbTiO_3 and Applicability to Surfaces and Domain Walls. *The Proceedings of the Computational Mechanics Conference*, **2008**, 2008.21, 149-150 | 0 | |
| 9 | 632 Ab initio study of stress-induced domain switching in PbTiO_3. *The Proceedings of the Materials and Mechanics Conference*, **2007**, 2007, 489-490 | 0 | |
| 8 | Development of Interatomic Potential for Pb(Zr, Ti)O3 Based on Shell model. *Journal of Solid Mechanics and Materials Engineering*, **2007**, 1, 1423-1431 | | 13 |
| 7 | 811 Development of Interatomic Potential for PbTiO_3 Based on Shell model. *The Proceedings of the Computational Mechanics Conference*, **2007**, 2007.20, 263-264 | 0 | |

| | | | |
|---|---|---|---|
| 6 | Ab initio density functional theory study of strain effects on ferroelectricity at PbTiO3 surfaces. *Physical Review B*, **2006**, 74, | 3.3 | 37 |
| 5 | Development of Interatomic Potential for Pb(Zr,Ti)O3 Based on Shell Model. *Nihon Kikai Gakkai Ronbunshu, A Hen/Transactions of the Japan Society of Mechanical Engineers, Part A*, **2006**, 72, 817-822 | | 2 |
| 4 | 272 Ab initio study of strain effects on ferroelectricity at PbTiO_3 surface. *The Proceedings of the Computational Mechanics Conference*, **2006**, 2006.19, 629-630 | 0 | |
| 3 | 516 Development of Interatomic Potential for Pb(Zr,Ti)O_3 Based on Shell model. *The Proceedings of Conference of Kansai Branch*, **2005**, 2005.80, _5-37_-_5-38_ | 0 | |
| 2 | Fracture Nanomechanics | | 9 |
| 1 | Fracture Nanomechanics | | 10 |