matscipy: materials science at the atomic scale with Python

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Summary

Behaviour of materials is governed by physical phenomena that occur at an extreme range of length and time scales. Computational modelling requires multiscale approaches. Simulation techniques operating on the atomic scale serve as a foundation for such approaches, providing necessary parameters for upper-scale models. The physical models employed for atomic simulations can vary from electronic structure calculations to empirical force fields. However, construction, manipulation and analysis of atomic systems are independent of the given physical model but dependent on the specific application. `matscipy` implements such tools for applications in materials science, including fracture, plasticity, tribology and electrochemistry.

Statement of need

The Python package `matscipy` contains a set of tools for researchers using atomic-scale models in materials science. In atomic-scale modelling, the primary numerical object is a discrete point in three-dimensional space that represents the position of an individual atom. Simulations are often dynamical, where configurations change over time and each atom carries a velocity. Complexity emerges from the interactions of many atoms, and numerical tools are required for generating initial atomic configurations and for analyzing output of such dynamical simulations, most commonly to connect local geometric arrangements of atoms to physical processes. An example, described in more detail below, is the detection of the tip of a crack that moves through a solid body.

We never see individual atoms at macroscopic scales. To understand the behaviour of everyday objects, atomic-scale information needs to be transferred to the continuum scale. This is the

primary objective of multi-scale modelling. `matscipy` focuses on atomic representations of materials, but implements tools for connecting to continuum descriptions in mechanics and transport theory. Each of the application domains described in the following therefore relies on the computation of continuum fields, that is realized through analytic or numerical solutions.

There is no other package that we are aware of, which fills the particular niche of the application domains in the next section. The package addresses the boundary between atomic-scale and continuum modelling in materials with particular emphasis on plasticity, fracture and tribology. The `atomman` atomistic manipulation toolkit (Hale, 2022) and the `atomsk` package (Hirel, 2015) have some overlapping objectives but are restricted to a narrower class of materials systems, principally point defects, stacking faults and dislocations. We target interoperability with the widely used Atomic Simulation Environment (ASE) (Larsen et al., 2017), which offers great flexibility by providing a Python interface to tens of simulation codes implementing different physical models. While ASE's policy is to remain pure Python, we augment some of ASE's functionality with more efficient implementations in C, such as the computation of the neighbour list. Large scale molecular dynamics (MD) simulations are most efficiently performed with optimized codes such as LAMMPS (Thompson et al., 2022), with `matscipy`'s main contribution being to setup input structures and to post-process output trajectories.

The central class in ASE is the `Atoms` class, which is a container that stores atomic positions, velocities and other properties. `Calculators` describe relationships between atoms, and are used for example to compute energies and forces, and can be attached to `Atoms` objects. All other `matscipy` functionality is implemented as functions acting on `Atoms` objects. This is comparable to the design of numpy (Harris et al., 2020) or `scipy` (Virtanen et al., 2020), that are collections of mathematical functions operating on core `array` container objects. In our experience, separating code into functions and containers lowers the barrier to entry for new users and eases testability of the underyling code base.

`matscipy` is a toolbox that enables multi-scale coupling, but it is not a toolbox for actually carrying out two-way coupled calculations. Its target is the construction of atomic domains from continuum information and the extraction of continuum fields from atomic structures. Other packages exist that take care of the actual, two-way coupling. In contrast to `matscipy`, those have a primary focus on handling discretized continuum fields, typically in the form of finite-element meshes, and interpolating nodal or element values between atomic-scale and continuum descriptions. `matscipy` itself has no provisions for handling discrete continuum data, but does implement analytic expressions for continuum fields.

Example implementations of two-way coupling codes are the open-source code `libmultiscale` (Guillaume Anciaux, 2007; G. Anciaux et al., 2018) that explicitly targets atomistic-continuum coupling, or the generic coupling libraries `preCICE` (Chourdakis et al., 2022) or `MpCCI` (Dehning et al., 2015). Another two-way coupling code is `MultiBench` (Miller & Tadmor, 2009), that was specifically designed for benchmarking a wide range of two-way atomistic-continuum coupling schemes. Futhermore, there are specialized multiscale coupling code, such as Green's function molecular dynamics (`GFMD`) (Campañá & Müser, 2006; Pastewka et al., 2012) which targets two-way coupling in contact mechanics and friction simulations. All of these packages have only limited capabilities for constructing atomistic domains. `matscipy` could be combined with these packages for two-way coupled simulation of plasticity, fracture or frictional processes.

Application domains

Within materials science, the package has different application domains:

- **Elasticity.** Solids respond to small external loads through a reversible elastic response. The strength of the response is characterized by the elastic moduli. `matscipy.elasticity` implements functions for computing elastic moduli from small deformation that consider potential symmetries of the underlying atomic system, in particular for crystals. The implementation also includes estimates of uncertainty on elastic moduli - either from

a least-squares error, or from a Bayesian treatment if stress uncertainty is supplied. `matscipy` also implements analytic calculation of elastic moduli for some interatomic potentials, described in more detail below. The computation of elastic moduli is a prerequisite for multi-scale modelling of materials, as they are the most basic parameters of continuum material models. `matscipy` was used to study finite-pressure elastic constants and structural stability in crystals (Grießer, Frérot, et al., 2023) and glasses (Grießer, Moras, et al., 2023).

- **Plasticity.** For large loads, solids can respond with irreversible deformation. One form of irreversibility is plasticity, that is carried by extended defects, the dislocations, in crystals. The module `matscipy.dislocation` implements tools for studying structure and movement of dislocations. Construction and analysis of model atomic systems is implemented for compact and dissociated screw, as well as edge dislocations in cubic crystals. The implementation supports ideal straight as well as kinked dislocations. Some of the dislocation functionality requires the `atomman` and/or `OVITO` packages as optional dependencies (Hale, 2022; Stukowski, 2009). The toolkit can be applied to a wide range of single- and multi-component ordered systems, and could be used as an initial starting point for modelling dislocations in systems with chemical disorder. The module was employed in a study of interaction of impurities with screw dislocations in tungsten (Grigorev et al., 2020, 2023).

- **Fracture mechanics.** Cracking is the process of generating new surface area by splitting the material apart. The module `matscipy.fracture_mechanics` provides functionality for calculating continuum linear elastic displacement fields near crack tips, including support for anisotropy in the elastic response (Sih et al., 1965). The module also implements generation of atomic structures that are deformed according to this near-tip field. This functionality has been used to quantify lattice trapping, which is the pinning of cracks due to the discreteness of the atomic lattice, and to compare simulations with experimental measurements of crack speeds in silicon (Kermode et al., 2015). There is also support for flexible boundary conditions in fracture simulations using the formalism proposed by Sinclair (Sinclair, 1975), where the finite atomistic domain is coupled to an infinite elastic continuum. Finally, we provide an extension of this approach to give a flexible boundary scheme that uses numerical continuation to obtain full solution paths for cracks (Buze & Kermode, 2021).

- **Tribology.** Tribology is the study of two interfaces sliding relative to one another, as encountered in frictional sliding or adhesion. Molecular dynamics simulations of representative volume elements of tribological interfaces are routinely used to gain insights into the atomistic mechanisms underlying friction and wear. The module `matscipy.pressurecoupling` provides tools to perform such simulations under a constant normal load and sliding velocity. It includes an implementation of the pressure coupling algorithm described by Pastewka et al. (2010). By dynamically adjusting the distance between the two sliding surfaces according to the local pressure, the algorithm ensures mechanical boundary conditions that account for the inertia of the bulk material which is not explicitly included in the simulation. This algorithm was used to study friction (Seidl et al., 2021) and wear (G. Moras et al., 2011; Gianpietro Moras et al., 2018; Pastewka et al., 2011; Peguiron et al., 2016; Reichenbach et al., 2021).

- **Electrochemistry.** Electrochemistry describes the motion and spatial distribution of charged atoms and molecules (ions) within an external electric field. Classical treatment of charged systems leads to continuous fields that describe mean concentration distributions, while true atomic systems consist of discrete particles with fixed charges. Neither do continuum models account for structured layering of ions in a polar solvent like water nor do they describe finite size effects at high concentrations such as densely packed monolayers. Sampling discrete particle positions from smooth distributions may, however, yield good initial configurations that accelerate equilibration in atomistic calculations. The `matscipy.electrochemistry` module provides tools that statistically sample discrete

coordinate sets from continuum fields and apply steric corrections (Martinez et al., 2009) to avoid overlap of finite size species. To generate continuum concentration distributions, the package also contains a control-volume solver (Selberherr, 1984) for the one-dimensional Poisson–Nernst–Planck equations (Bazant et al., 2006), as well as an interface to the finite-element solver FEniCS (Logg et al., 2012).

All-purpose atomic analysis tools

As well as these domain-specific tools, `matscipy` contains general utility functionality which is widely applicable:

- **Neighbour list.** An efficient linear-scaling neighbour list implemented in C delivers orders-of-magnitude faster performance for large systems than the pure Python implementation in ASE (Larsen et al., 2017), see Figure 1. The neighbour list is stored in a data structure comparable to coordinate (COO) sparse matrix storage format (Saad, 1990), where two arrays contain the indices of the neighbouring atoms and further arrays store distance vectors, absolute distances, and other properties associated with an atomic pair. This allows compact code for evaluating properties that depend on pairs, such as pair-distribution function or interatomic potential energies and forces. Most of the tools described in the following rely on this neighbour list format. The neighbour list is becoming widely used for post-processing and structural analysis of the trajectories resulting from molecular dynamics simulations, and even to accelerate next-generation message passing neural networks such as MACE (Batatia, Kovacs, et al., 2022; Batatia, Batzner, et al., 2022).
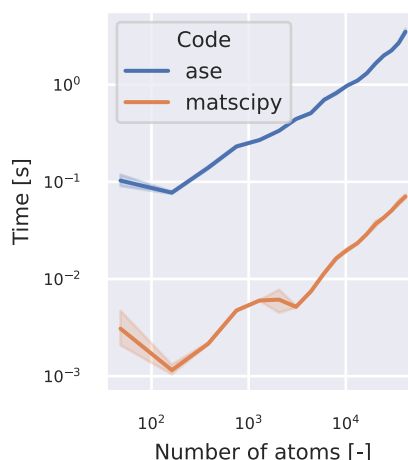

Figure 1: Execution time of the computation of the neighbour list in ASE and Matscipy. These results were obtained on a single core of an Intel i7-1260P processor on the ASE master branch (git hash 52a8e783).

- **Atomic strain.** Continuum mechanics is formulated in terms of strains, which characterizes the fractional shape changes of small volumes. Strains are typically only well defined if averaged over sufficiently large volumes, and extracting strain fields from atomic-scale calculations is notoriously difficult. `matscipy` implements calculations of strain by observing changes in local atomic neighbourhoods across trajectories. It fits a per-atom displacement gradient that minimizes the error in displacement between two configurations as described by M. L. Falk & Langer (1998). The error resulting from this fit quantifies the non-affine contribution ot the overall displacement and is known as D^2_{min}. We used this analysis to quantify local strain in the deformation of crystals (Gola et al., 2019, 2020) and glasses (Jana & Pastewka, 2019).

- **Radial, spatial and angular correlation functions.** Topological order in atomic-scale systems is often characterized by statistical measures of the local atomic environment. The simplest one is the pair-distribution or radial-distribution function, that gives the probability $g_2(r)$ of finding an atom at distance r. For three atoms, we can define a probability of finding a specific angle, yielding the angular correlation functions. `matscipy` has utility function for computing these correlation functions to large distances, including the correlation of arbitrary additional per-atom properties such as per-atom strains.

- **Ring analysis.** Topological order in network glasses can be characterized by statistics of shortest-path rings (Franzblau, 1991). `matscipy` implements calculations of these rings using a backtracking algorithm in C. We regularly use `matscipy` to charactize shortest-path rings in amorphous carbon (Jana & Pastewka, 2019; Pastewka et al., 2008).

- **Topology building for non-reactive MD simulations.** Non-reactive force fields for MD simulations consist of non-bonded and bonded interaction terms (Jorgensen et al., 1996). The latter require an explicit specification of the interatomic bonding topology, i.e. which atoms are involved in bond, angle and dihedral interactions. `matscipy` provides efficient tools to generate this topology for an atomic structure based on matscipy's neighbour list, and then assign the relevant force field parameters to each interaction term. Input and output routines for reading and writing the corresponding control files for LAMMPS (Thompson et al., 2022) are also available. We used this functionality in various studies on tribology, wetting and nanoscale rheology (K. Falk et al., 2020, 2022; Goeldel et al., 2021; Mayrhofer et al., 2016; Reichenbach et al., 2020)

Interatomic potentials and other calculators

Besides generating and analysing atomic-scale configurations, `matscipy` implements specific interatomic potentials (Müser et al., 2023). The goal here is not to provide the most efficient implementation of computing interatomic forces. We rather aim to provide simple implementations for testing new functional forms, or testing new features such as the computation of derivatives of second order.

- **Interatomic potentials.** The module `matscipy.calculators` has implementations of classical pair-potentials, Coulomb interactions, the embedded-atom method (EAM) (Daw & Baskes, 1984) and other many-body potentials (e.g. Stillinger & Weber, 1985; Tersoff, 1989).

- **Second-order derivatives.** The thermodynamic and elastic properties of solid materials are closely connected to the Hessian of the overall system, which contains the second derivatives of the total energy with respect to position and macroscopic strains. `matscipy` implements analytic second-order potential derivatives for pair-potentials (Lennard-Jones, 1931), EAM potentials (Daw & Baskes, 1984), bond-order potentials (Brenner, 1990; Kumagai et al., 2007; Tersoff, 1989), cluster potentials (Stillinger & Weber, 1985) and electrostatic interaction (Van Beest et al., 1990). This is achieved through a generic mathematical formulation of the manybody total energy (Grießer, Frérot, et al., 2023; Müser et al., 2023) in `matscipy.calculators.manybody`. The module `matscipy.numerical` additionally provides routines for the numerical (finite-differences) evaluation of these properties. These analytic second-order derivatives allow a fast and accurate computation of the aforementioned properties in crystals, polymers and amorphous solids, even for unstable configurations where numerical methods are not applicable.

- **Quantum mechanics/molecular mechanics.** The module `matscipy.calculators.mcfm` implements a generalised force-mixing potential (Bernstein et al., 2009) with support for multiple concurrent QM clusters, named MultiClusterForceMixing (MCFM). It has been

applied to model failure of graphene-nanotube composites (Gołębiowski et al., 2018, 2020).

- **Committee models.** The module `matscipy.calculators.committee` provides support for committees of interatomic potentials with the same functional form but differing parameters, in order to allow the effect of the uncertainty in parameters on model predictions to be estimated. This is typically used with machine learning interatomic potentials (MLIPs). The implementation follows the approach of (Musil et al., 2019) where the ensemble of models is generated by training models on different subsets of a common overall training database.

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References

Anciaux, Guillaume. (2007). *Simulation multi-échelles des solides par une approche couplée dynamique moléculaire/éléments finis. De la modélisation à la simulation haute performance.* [Theses, Université Sciences et Technologies - Bordeaux I]. https://theses.hal.science/tel-00263816

Anciaux, G., Junge, T., Hodapp, M., Cho, J., Molinari, J.-F., & Curtin, W. A. (2018). The Coupled Atomistic/Discrete-Dislocation method in 3d part i: Concept and algorithms. *J. Mech. Phys. Solids*, *118*, 152–171. https://doi.org/10.1016/j.jmps.2018.05.004

Batatia, I., Batzner, S., Kovács, D. P., Musaelian, A., Simm, G. N. C., Drautz, R., Ortner, C., Kozinsky, B., & Csányi, G. (2022). *The design space of E(3)-equivariant atom-centered interatomic potentials* (No. arXiv:2205.06643). https://doi.org/10.48550/arXiv.2205.06643

Batatia, I., Kovacs, D. P., Simm, G. N. C., Ortner, C., & Csanyi, G. (2022). MACE: Higher order equivariant message passing neural networks for fast and accurate force fields. In A. H. Oh, A. Agarwal, D. Belgrave, & K. Cho (Eds.), *Advances in neural information processing systems*. https://openreview.net/forum?id=YPpSngE-ZU

Bazant, M. Z., Chu, K. T., & Bayly, B. J. (2006). Current-voltage relations for electrochemical thin films. *SIAM J. Appl. Math.*, *65*(5), 1463–1484. https://doi.org/10.1137/040609938

Bernstein, N., Kermode, J. R., & Csányi, G. (2009). Hybrid atomistic simulation methods for materials systems. *Rep. Prog. Phys.*, *72*(2), 026501. https://doi.org/10.1088/0034-4885/72/2/026501

Brenner, D. W. (1990). Empirical potential for hydrocarbons for use in simulating chemical vapor deposition of diamond films. *Phys. Rev. B*, *42*(15), 9458–9471.

Buze, M., & Kermode, J. R. (2021). Numerical-continuation-enhanced flexible boundary condition scheme applied to mode-I and mode-III fracture. *Phys. Rev. E*, *103*(3), 033002. https://doi.org/10.1103/PhysRevE.103.033002

Campañá, C., & Müser, M. H. (2006). Practical green's function approach to the simulation of elastic semi-infinite solids. *Phys. Rev. B*, *74*(7), 075420. https://doi.org/10.1103/

PhysRevB.74.075420

Chourdakis, G., Davis, K., Rodenberg, B., Schulte, M., Simonis, F., Uekermann, B., Abrams, G., Bungartz, H., Cheung Yau, L., Desai, I., Eder, K., Hertrich, R., Lindner, F., Rusch, A., Sashko, D., Schneider, D., Totounferoush, A., Volland, D., Vollmer, P., & Koseomur, O. (2022). preCICE v2: A sustainable and user-friendly coupling library [version 2; peer review: 2 approved]. *Open Research Europe*, *2*(51). https://doi.org/10.12688/openreseurope.14445.2

Daw, M. S., & Baskes, M. I. (1984). Embedded-atom method: Derivation and application to impurities, surfaces, and other defects in metals. *Phys. Rev. B*, *29*, 6443–6453. https://doi.org/10.1103/PhysRevB.29.6443

Dehning, C., Bierwisch, C., & Kraft, T. (2015). Co-simulations of discrete and finite element codes. In M. Griebel & M. A. Schweitzer (Eds.), *Meshfree methods for partial differential equations VII* (pp. 61–79). Springer. https://doi.org/10.1007/978-3-319-06898-5_4

Falk, K., Reichenbach, T., Gkagkas, K., Moseler, M., & Moras, G. (2022). Relating dry friction to interdigitation of surface passivation species: A molecular dynamics study on amorphous carbon. *Materials*, *15*(9), 3247. https://doi.org/10.3390/ma15093247

Falk, K., Savio, D., & Moseler, M. (2020). Nonempirical free volume viscosity model for alkane lubricants under severe pressures. *Phys. Rev. Lett.*, *124*, 105501. https://doi.org/10.1103/PhysRevLett.124.105501

Falk, M. L., & Langer, J. S. (1998). Dynamics of viscoplastic deformation in amorphous solids. *Phys. Rev. E*, *57*(6), 7192–7205. https://doi.org/10.1103/PhysRevE.57.7192

Franzblau, D. S. (1991). Computation of ring statistics for network models of solids. *Phys. Rev. B*, *44*(10), 4925–4930. https://doi.org/10.1103/PhysRevB.44.4925

Goeldel, S. von, Reichenbach, T., Konig, F., Mayrhofer, L., Moras, G., Jacobs, G., & Moseler, M. (2021). A combined experimental and atomistic investigation of PTFE double transfer film formation and lubrication in rolling point contacts. *Tribol. Lett.*, *69*, 136. https://doi.org/10.1007/s11249-021-01508-9

Gola, A., Schwaiger, R., Gumbsch, P., & Pastewka, L. (2020). Pattern formation during deformation of metallic nanolaminates. *Phys. Rev. Mater.*, *4*(1), 013603. https://doi.org/10.1103/PhysRevMaterials.4.013603

Gola, A., Zhang, G.-P., Pastewka, L., & Schwaiger, R. (2019). Surface flaws control strain localization in the deformation of Cu|Au nanolaminate pillars. *MRS Commun.*, *9*(3), 1067–1071. https://doi.org/10.1557/mrc.2019.93

Gołębiowski, J. R., Kermode, J. R., Haynes, P. D., & Mostofi, A. A. (2020). Atomistic QM/MM simulations of the strength of covalent interfaces in carbon nanotube-polymer composites. *Phys. Chem. Chem. Phys.*, *22*(21), 12007–12014. https://doi.org/10.1039/d0cp01841d

Gołębiowski, J. R., Kermode, J. R., Mostofi, A. A., & Haynes, P. D. (2018). Multiscale simulations of critical interfacial failure in carbon nanotube-polymer composites. *J. Chem. Phys.*, *149*(22), 224102. https://doi.org/10.1063/1.5035508

Grießer, J., Frérot, L., Oldenstaedt, J. A., Müser, M. H., & Pastewka, L. (2023). Analytic elastic constants in molecular calculations: Finite strain, non-affine displacements, and many-body interatomic potentials. *Phys. Rev. Mater.*, *7*(7), 073603. https://doi.org/10.1103/PhysRevMaterials.7.073603

Grießer, J., Moras, G., & Pastewka, L. (2023). Yielding under compression and the polyamorphic transition in silicon. *Phys. Rev. Mater.*, *7*(5), 055601. https://doi.org/10.1103/PhysRevMaterials.7.055601

Grigorev, P., Goryaeva, A. M., Marinica, M.-C., Kermode, J. R., & Swinburne, T. D. (2023). Calculation of dislocation binding to helium-vacancy defects in tungsten using hybrid ab initio-machine learning methods. *Acta Mater.*, *247*, 118734. https://doi.org/10.1016/j.actamat.2023.118734

Grigorev, P., Swinburne, T. D., & Kermode, J. R. (2020). Hybrid quantum/classical study of hydrogen-decorated screw dislocations in tungsten: Ultrafast pipe diffusion, core reconstruction, and effects on glide mechanism. *Phys. Rev. Mater.*, *4*, 023601. https://doi.org/10.1103/PhysRevMaterials.4.023601

Hale, L. (2022). https://github.com/usnistgov/atomman

Harris, C. R., Millman, K. J., Walt, S. J. van der, Gommers, R., Virtanen, P., Cournapeau, D., Wieser, E., Taylor, J., Berg, S., Smith, N. J., Kern, R., Picus, M., Hoyer, S., Kerkwijk, M. H. van, Brett, M., Haldane, A., Río, J. F. del, Wiebe, M., Peterson, P., … Oliphant, T. E. (2020). Array programming with NumPy. *Nature*, *585*(7825), 357–362. https://doi.org/10.1038/s41586-020-2649-2

Hirel, P. (2015). Atomsk: A tool for manipulating and converting atomic data files. *Comput. Phys. Commun.*, *197*, 212–219. https://doi.org/10.1016/j.cpc.2015.07.012

Jana, R., & Pastewka, L. (2019). Correlations of non-affine displacements in metallic glasses through the yield transition. *J. Phys. Mater.*, *2*, 045006. https://doi.org/10.1088/2515-7639/ab36ed

Jorgensen, W. L., Maxwell, D. S., & Tirado-Rives, J. (1996). Development and testing of the OPLS all-atom force field on conformational energetics and properties of organic liquids. *J. Am. Chem. Soc.*, *118*(45), 11225–11236. https://doi.org/10.1021/ja9621760

Kermode, J. R., Gleizer, A., Kovel, G., Pastewka, L., Csányi, G., Sherman, D., & De Vita, A. (2015). Low speed crack propagation via kink formation and advance on the silicon (110) cleavage plane. *Phys. Rev. Lett.*, *115*(13), 135501. https://doi.org/10.1103/PhysRevLett.115.135501

Kumagai, T., Izumi, S., Hara, S., & Sakai, S. (2007). Development of bond-order potentials that can reproduce the elastic constants and melting point of silicon for classical molecular dynamics simulation. *Comp. Mater. Sci.*, *39*(2), 457–464. https://doi.org/10.1016/j.commatsci.2006.07.013

Larsen, A. H., Mortensen, J. J., Blomqvist, J., Castelli, I. E., Christensen, R., Dułak, M., Friis, J., Groves, M. N., Hammer, B., Hargus, C., Hermes, E. D., Jennings, P. C., Jensen, P. B., Kermode, J., Kitchin, J. R., Kolsbjerg, E. L., Kubal, J., Kaasbjerg, K., Lysgaard, S., … Jacobsen, K. W. (2017). The atomic simulation environment - a Python library for working with atoms. *J. Phys. Condens. Matter*, *29*(27), 273002. https://doi.org/10.1088/1361-648x/aa680e

Lennard-Jones, J. E. (1931). Cohesion. *Proc. Phys. Soc.*, *43*(5), 461–482. https://doi.org/10.1088/0959-5309/43/5/301

Logg, A., Mardal, K.-A., Wells, G. N., & others. (2012). *Automated solution of differential equations by the finite element method* (A. Logg, K.-A. Mardal, & G. N. Wells, Eds.). Springer. https://doi.org/10.1007/978-3-642-23099-8

Martinez, L., Andrade, R., Birgin, E. G., & Martínez, J. M. (2009). PACKMOL: A package for building initial configurations for molecular dynamics simulations. *J. Comput. Chem.*, *30*(13), 2157–2164. https://doi.org/10.1002/jcc.21224

Mayrhofer, L., Moras, G., Mulakaluri, N., Rajagopalan, S., Stevens, P. A., & Moseler, M. (2016). Fluorine-terminated diamond surfaces as dense dipole lattices: The electrostatic origin of polar hydrophobicity. *J. Am. Chem. Soc.*, *138*, 4018–4028. https://doi.org/10.1021/jacs.5b04073

Miller, R. E., & Tadmor, E. B. (2009). A unified framework and performance benchmark of fourteen multiscale atomistic/continuum coupling methods. *Modell. Simul. Mater. Sci. Eng.*, *17*(5), 053001. https://doi.org/10.1088/0965-0393/17/5/053001

Moras, Gianpietro, Klemenz, A., Reichenbach, T., Gola, A., Uetsuka, H., Moseler, M., & Pastewka, L. (2018). Shear melting of silicon and diamond and the disappearance of the polyamorphic transition under shear. *Phys. Rev. Mater.*, *2*(8), 083601. https://doi.org/10.1103/PhysRevMaterials.2.083601

Moras, G., Pastewka, L., Gumbsch, P., & Moseler, M. (2011). Formation and oxidation of linear carbon chains and their role in the wear of carbon materials. *Tribol. Lett.*, *44*, 355. https://doi.org/10.1007/s11249-011-9864-9

Müser, M. H., Sukhomlinov, S. V., & Pastewka, L. (2023). Interatomic potentials: Achievements and challenges. *Adv. Phys. X*, *8*(1), 2093129. https://doi.org/10.1080/23746149.2022.2093129

Musil, F., Willatt, M. J., Langovoy, M. A., & Ceriotti, M. (2019). Fast and accurate uncertainty estimation in chemical machine learning. *J. Chem. Theory Comput.*, *15*(2), 906–915. https://doi.org/10.1021/acs.jctc.8b00959

Pastewka, L., Moser, S., Gumbsch, P., & Moseler, M. (2011). Anisotropic mechanical amorphization drives wear in diamond. *Nat. Mater.*, *10*(1), 34–38. https://doi.org/10.1038/nmat2902

Pastewka, L., Moser, S., & Moseler, M. (2010). Atomistic insights into the running-in, lubrication, and failure of hydrogenated diamond-like carbon coatings. *Tribol. Lett.*, *39*(1), 49–61. https://doi.org/10.1007/s11249-009-9566-8

Pastewka, L., Pou, P., Pérez, R., Gumbsch, P., & Moseler, M. (2008). Describing bond-breaking processes by reactive potentials: Importance of an environment-dependent interaction range. *Phys. Rev. B*, *78*(16), 161402(R). https://doi.org/10.1103/PhysRevB.78.161402

Pastewka, L., Sharp, T. A., & Robbins, M. O. (2012). Seamless elastic boundaries for atomistic calculations. *Phys. Rev. B*, *86*, 075459. https://doi.org/10.1103/PhysRevB.86.075459

Peguiron, A., Moras, G., Walter, M., Uetsuka, H., Pastewka, L., & Moseler, M. (2016). Activation and mechanochemical breaking of C−C bonds initiate wear of diamond (110) surfaces in contact with silica. *Carbon*, *98*, 474–483. https://doi.org/10.1016/j.carbon.2015.10.098

Reichenbach, T., Mayrhofer, L., Kuwahara, T., Moseler, M., & Moras, G. (2020). Steric effects control dry friction of h- and f-terminated carbon surfaces. *ACS Appl. Mater. Interf.*, *12*, 8805–8816. https://doi.org/10.1021/acsami.9b18019

Reichenbach, T., Moras, G., Pastewka, L., & Moseler, M. (2021). Solid-phase silicon homoepitaxy via shear-induced amorphization and recrystallization. *Phys. Rev. Lett.*, *127*(12), 126101. https://doi.org/10.1103/PhysRevLett.127.126101

Saad, Y. (1990). *SPARSKIT: A basic tool kit for sparse matrix computations* (NAS 1.26:185876). ntrs.nasa.gov.

Seidl, C., Hörmann, J. L., & Pastewka, L. (2021). Molecular simulations of electrotunable lubrication: Viscosity and wall slip in aqueous electrolytes. *Tribol. Lett.*, *69*(1), 22. https://doi.org/10.1007/s11249-020-01395-6

Selberherr, S. (1984). *Analysis and simulation of semiconductor devices*. Springer Science & Business Media. https://doi.org/10.1007/978-3-7091-8752-4

Sih, G. C., Paris, P. C., & Irwin, G. R. (1965). On cracks in rectilinearly anisotropic bodies. *Int. J. Fract. Mech.*, *1*(3), 189–203. https://doi.org/10.1007/BF00186854

Sinclair, J. E. (1975). The influence of the interatomic force law and of kinks on the propagation of brittle cracks. *Philos. Mag.*, *31*, 647–671. https://doi.org/10.1080/14786437508226544

Stillinger, F. H., & Weber, T. A. (1985). Computer simulation of local order in condensed phases of silicon. *Phys. Rev. B*, *31*(8), 5262. https://doi.org/10.1103/PhysRevB.31.5262

Stukowski, A. (2009). Visualization and analysis of atomistic simulation data with OVITO–the open visualization tool. *Modell. Simul. Mater. Sci. Eng.*, *18*(1), 015012. https://doi.org/10.1088/0965-0393/18/1/015012

Tersoff, J. (1989). Modeling solid-state chemistry: Interatomic potentials for multicomponent systems. *Phys. Rev. B*, *39*(8), 5566(R). https://doi.org/10.1103/PhysRevB.39.5566

Thompson, A. P., Aktulga, H. M., Berger, R., Bolintineanu, D. S., Brown, W. M., Crozier, P. S., in 't Veld, P. J., Kohlmeyer, A., Moore, S. G., Nguyen, T. D., Shan, R., Stevens, M. J., Tranchida, J., Trott, C., & Plimpton, S. J. (2022). LAMMPS - a flexible simulation tool for particle-based materials modeling at the atomic, meso, and continuum scale. *Comp. Phys. Commun.*, *271*, 108171. https://doi.org/10.1016/j.cpc.2021.108171

Van Beest, B., Kramer, G. J., & Van Santen, R. (1990). Force fields for silicas and aluminophosphates based on ab initio calculations. *Phys. Rev. Lett.*, *64*(16), 1955. https://doi.org/10.1103/PhysRevLett.64.1955

Virtanen, P., Gommers, R., Oliphant, T. E., Haberland, M., Reddy, T., Cournapeau, D., Burovski, E., Peterson, P., Weckesser, W., Bright, J., Walt, S. J. van der, Brett, M., Wilson, J., Millman, K. J., Mayorov, N., Nelson, A. R. J., Jones, E., Kern, R., Larson, E., … Vázquez-Baeza, Y. (2020). SciPy 1.0: Fundamental algorithms for scientific computing in Python. *Nat. Methods*, *17*(3), 261–272. https://doi.org/10.1038/s41592-019-0686-2