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Atomistic Mechanisms of Pore Collapse and Plasticity in Lithium: A Comparative Molecular Dynamics Study of Classical and Machine-Learning Interatomic Potentials



Project Manager
Aditya Sinha

Principal Investigator
Prof. Dr. rer. nat. Karsten Albe

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Clusters
Lichtenberg II Cluster Darmstadt

Software
LAMMPS, Ovito

JUSTUS-LIEBIG-UNIVERSITÄT GIESSEN
TECHNISCHE UNIVERSITÄT DARMSTADT
UNIKASSEL VERSITÄT
Philipps Universität Marburg

Introduction

This Advanced Research Lab (ARL) project addressed the atomistic modelling of deformation and defect evolution in lithium, a material system of direct relevance to advanced battery technologies. The broader motivation is the development of safer and more reliable energy-storage materials, in which mechanical stability matters as much as electrochemical performance. In such materials, small structural features — nanoscale pores, local loss of contact, or atomic rearrangements — can strongly influence long-term behaviour under pressure or deformation. These processes begin at the atomic scale and are difficult to observe directly in experiments. Molecular dynamics simulation is therefore a valuable complement, because it resolves how individual atoms move and how local structural changes develop during loading. High Performance Computing was essential for this work. The simulations required the repeated evaluation of interatomic interactions for large numbers of atoms over many time steps. In addition, several different systems and loading conditions had to be compared in order to contrast the behaviour of ideal and defect-containing structures, and two classes of interatomic potential had to be evaluated under identical conditions. Machine-learning potentials in particular are considerably more expensive per time step than classical descriptions, which makes systematic comparison impractical on a normal workstation. Access to the Lichtenberg II cluster made it possible to run larger models, perform systematic comparisons, and analyse the material response in a scientifically meaningful way.

Methods

The project used classical molecular dynamics simulations, carried out with LAMMPS, to study the response of lithium model systems under mechanical loading. Atomic structures were first prepared and checked to ensure that the initial configurations were suitable for simulation. Different systems were then constructed, including defect-free reference structures and structures containing controlled nanoscale pores. The prepared systems were subjected to different modes of deformation in order to observe the material response under applied loading. Simulations were submitted to the cluster using job scripts and monitored throughout. Because the runs generated large trajectory files, post-processing and systematic data organisation formed an important part of the workflow. Analysis was performed largely in OVITO and included visualising atomic configurations, tracking structural changes, comparing deformation pathways, and identifying the role of local defects. Classical and machine-learning descriptions of the atomic interactions were compared under otherwise identical simulation conditions, so that differences in the predicted response could be attributed to the potential itself. Specific numerical values and model-specific findings are omitted here, as they remain part of ongoing internal research.

Results

The project produced a working computational workflow for studying atomic-scale deformation in lithium. Several simulation systems were prepared and tested, and deformation simulations were carried out under a range of conditions. The results showed that local structural defects significantly influence how the material responds during mechanical loading: defect-containing systems deformed differently from ideal structures, confirming the importance of atomic-scale features in controlling the overall material response. The simulations also helped reveal how local rearrangements contribute to pore evolution, structural relaxation, and changes in mechanical behaviour. A second important outcome was the comparison between the interatomic interaction models. The predicted response was found to depend strongly on the choice of potential, particularly where local structural changes and deformation mechanisms are involved. This matters beyond the present system, because it shows that computational predictions of this kind must be interpreted carefully and supported by model comparison rather than taken from a single potential. Alongside the scientific results, the project delivered practical outcomes: organised simulation folders, reusable input files, job scripts, analysis routines, and visualisation workflows. These can support future work in the group and be adapted for related materials-modelling studies.

Discussion

The project demonstrated the value of High Performance Computing for atomistic materials research. The available resources allowed the work to move beyond single test calculations towards a systematic understanding of the material behaviour, based on repeated simulations across several systems and modelling approaches. The main challenge was computational cost. Some simulations required long running times, and several trial calculations were needed to identify suitable settings. A second challenge was the volume of data produced: trajectory and output files had to be stored, processed, visualised, and interpreted with care. The work also highlighted a broader challenge in computational materials science, namely that the choice of interatomic potential can itself affect the predicted mechanisms. Model selection and comparison are therefore essential before drawing strong conclusions from simulation results. This is especially relevant for battery materials, where atomic-scale mechanical processes may influence long-term performance and reliability. As an outlook, the developed workflow can be extended to larger systems, more complex defect structures, and more realistic loading conditions, and can support future studies that combine simulation with experimental observation. Overall, the ARL project contributed to a better understanding of how local atomic mechanisms influence the mechanical behaviour of lithium-based energy-storage materials.

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