RECENT ADVANCES IN THE MODELING AND SIMULATION OF THE MECHANICS OF NANOSCALE MATERIALS

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Table of CONTENTS

Introduction

The workshop "Recent Advances in the Modeling and Simulation of the Mechanics of Nanoscale Materials" was held at the Singh Center for Nanotechnology of the University of Pennsylvania in Philadelphia from August 21-23, 2019. It was a US Association of Computational Mechanics (USACM) thematic workshop under the auspices of the Nanotechnology Technical Thrust Area (TTA), which received financial support from the National Science Foundation.

It brought together experts at the forefront of the modeling and simulation of the mechanics of nanoscale materials, to discuss recent advances in electronic structure calculations, atomistic modeling, continuum approaches for microstructure evolution, scale bridging techniques and applications of machine learning to gain fundamental insight in material behavior. Topics of interest also included the application of these techniques to gain insight into effective material response.

The workshop included the participation of junior and senior faculty members via 32 invited presentations, as well as 19 PhD students and postdocs, who shared their research via poster presentations. The total number of attendees was 64, which enabled vivid discussions among all participants.

The three-day meeting was organized in eleven sessions, which included a session on first principle calculations and quantum properties, a session on plasticity, two sessions dedicated to defects, one session on grain boundaries and interfaces, three sessions focusing on mechanics of materials, one session on phase field models, and it was concluded with two sessions on scale bridging, which included talks on applications of machine learning techniques to aid the same.

Each of the presentations was 30 minutes long including questions. Presenters were encouraged to discuss open challenges in the modeling and simulation of nanoscale phenomena in addition to their recent advances in the field, with the objective of promoting discussions during the workshop.

This report provides a detailed description of the workshop. It includes a summary of all the presentations, following the conference program, as well as a summary of the discussions, identifying important challenges and opportunities for this community. A list of poster presentations is also included. The report concludes with an acknowledgement of all administrative and technical staffs, which were instrumental in the organization, execution and success of this workshop.

Session 1: First Principle Calculations and Quantum Properties

Vikram Gavini: Large-scale real-space electronic structure calculations

Overview and motivation:
About 25% of high performance computing resources for scientific and technological pursuit are dedicated to electronic structure calculations. These calculations, in particular, Density Functional Theory (DFT) have enjoyed great success in the accurate prediction of various phases in materials as well as defect energetics. Despite its success, there are three important challenges:
1. Simulation domain size restrictions: Most simulation codes are based on plane-wave discretization, which require periodic boundary conditions.
2. Pseudo-potential approximation: It has been shown that this may not be transferable for transition metals, or extreme environments like high-pressure conditions.
3. The model exchange-correlation (X-C) functionals (which accounts for all quantum mechanical interactions) do not work for strongly correlated systems.

Background:
The Kohn–Sham (KS) equations (eigenvalue problem) are the governing equations for DFT. The state of the art for solving them can be divided between Fourier space formulations and real space formulations. The former are the most popular. It has spectral convergence and it is very efficient for periodic problems, although it has a uniform resolution (not ideal for defect calculations), and present scalability issues. The other approach is real space formulations. Within this class, FE discretizations of KS-DFT have interesting features, like systematic convergence, can handle complex geometries and boundary conditions, and resolution can be increased where needed. Finally it is based on local basis functions and scales very well on parallel architectures. The main disadvantages are that it requires many basis functions and it results in a generalized eigenvalue problem. First efforts in this direction using linear finite elements appeared to indicate that this method was not tractable. However, higher order finite elements showed a better performance, with close to optimal convergence. Though this does not solve the issues associated with the generalized eigenvalue problem.

Approach and results:

To tackle these challenges, a FE approach based on spectral finite elements is presented, which uses a Gauss-Lobatto-Legendre quadrature rule and a Chebyshev acceleration technique. Benchmark calculations with other open source codes such as Quantum Espresso, indicate much faster calculations for both periodic and non-periodic systems, thanks to its great scalability. These developments are available in an open source code (DFT-FE).

DFT-FE can also handle all-electron calculations although it is not very efficient as compared to using Gaussian basis. To speedup the calculation, an enriched FE basis is proposed, which utilizes results from single atom Kohn-Sham calculations, truncated to maintain local support. This leads to a significantly reduced number of degrees of freedom and reduced spectral width of the Hamiltonian. The speedup achieved is of two orders of magnitude for silicon nanoclusters, and it rapidly becomes faster than NWChem as the system size increases.

Finally, to address the challenge associated with X-C approximations, the following framework was proposed. The idea is to do many body quantum calculations on small scale systems, where these calculations are possible, and then solve the inverse DFT problem i.e. find the X-C functional that would give the same solution. Since the X-C potential and energy is universal, machine learning could be used to systematically improve the description of the X-C potential. However, doing inverse DFT has been a long-standing challenge in computational chemistry. The faced challenges were primarily associated with the fact that the Gaussian basis used are incomplete and have the wrong asymptotics, which leads to spurious oscillations in the solution. A recent breakthrough on this front has been achieved by combining 4 key elements: PDE constrained optimization, a complete higher order FE basis for discretization, cusp correction, and using homogeneous Dirichlet boundary conditions to take care of the far-field asymptotics. This allowed computing the X-C potential to chemical accuracy.

Conclusions:
- Large scale KS DFT calculations were achieved using a real space formulation with higher order FE element basis and Chebyshev filtering.
- Efficient all electron KS-DFT where achieved using FE by using enrichment functions and adaptive quadratures.
- Successfully solved the inverse DFT problem to compute the X-C potential to chemical accuracy.

References:

[1] P. Motamarri et al., "DFT-FE A massively parallel adaptive finite-element code for large-scaledensity functional theory calculations," *Computer Physics Communications* 246 (2020): 106853.

[2] B. Kanungo et al., "Exact exchange-correlation potentials from ground-state electron densities," Nature Communications, 10, 4497, 2019

Amartya Banerjee. Symmetry, deformations and the search for unprecedented materials from first principles.

Overview and motivation:
Symmetries in materials can be thought of as a fundamental concept to motivate the discovery and characterization of new materials. A mathematical framework to characterize materials beyond classical periodic structures (i.e., crystals) is based on the concept of Objective Structures. These are structures in which corresponding atoms see the same environment up to a translation and orthogonal transformation. They are associated with non-periodic symmetries and almost all elements in the periodic table organize themselves in the form of objective structures (e.g., crystals, helical nanotubes, fullerene). Classical Density Functional Theory (DFT) codes are designed for studying periodic crystals and are not suitable for the general class of objective structures. Here, Objective-DFT (i.e., a DFT method for specifically studying Objective Structures) is presented and applied to two classes of objective structures: (i) clusters and molecules, and (ii) helical structures.

Approach and results:
The formulation and implementation of Objective-DFT is presented following a structure that is analogous to classical DFT codes based on the plane wave method (for instance, generalized harmonic analysis is used instead of Fourier transform, and objective/helical waves are used as basis sets instead of plane waves). The resulting formulation enables the use of symmetries to reduce the computational cost of studying the electronic properties of a given structure. Additionally, it enables the electronic structure calculations of nanostructures under non-uniform deformations such as bending and torsion, which are not easy to model using conventional approaches (i.e., employing periodic boundary conditions). Some examples presented include the prediction of the bending modulus of graphene, silicene, germanene and stanenene *ab initio*. Objective DFT also produces cyclic band diagrams which allow one to see the changes in the electronic structure of a nanomaterial as it is bent. Finally, the case of helical symmetry is discussed. As an example, black phosphorus nanotubes undergoing twisting are studied using this method. The twisting stiffness of this structure using Objective DFT can be predicted, and the effects of atomic relaxation can be included. In this case, a helical band diagram is obtained, and this shows a transition from insulator to metal for some nanotubes.

Conclusions:
- Objective DFT is developed as a powerful tool to study objective structures.
- Objective DFT is likely to be instrumental in the discovery and characterization of novel materials.
- Properties of cyclic and helical structures are explored using implementations of Objective DFT, and interesting nanoscale phenomena are discovered and studied.

References:
[1] A. Banerjee et al., "A spectral scheme for Kohn-Sham density functional theory of clusters," Journal of Computational Physics 287 (2015), 226-253.
[2] A. Banerjee et al., "Cyclic density functional theory: A route to the first principles simulation of bending in nanostructures", Journal of Mechanics and Physics of Solids 96 (2016), pp 605-631.

[3] S. Ghosh et al. "Symmetry-adapted real-space density functional theory for cylindrical geometries: Application to large group-IV nanotubes". Physical Review B, 100(12) (2019), 125143.

Mauricio Ponga: How defects affect quantum mechanical properties in crystalline materials.

(Joint work with David Funes, Norman Muller)

This talk was composed of two parts:
Part I: Superconducting radio frequency cavities.
Part II: Framework to predict twinning in 2D materials.

Overview and motivation (part I):
Meissner effect in superconducting radio frequency cavities is a manifestation of exotic quantum behavior: when the temperature is above the critical temperature the magnetic field penetrates the material. However, when the temperature is lower than the critical temperature and it transitions to the superconducting state, the magnetic field is repulsed and the material acts as a magnet. In the presence of defects, the magnetic field can get trapped in the material, which can kill the superconducting state. This problem is of relevance in particle accelerators, where it is observed that thermal treatment has a strong impact in the properties of cavities as it influences the defect pattern.

The goals of the studies presented are to (i) understand the effect of annealing process on dislocation density, (ii) obtain a basic understanding of dislocation climb, and (iii) provide a framework to simulate these phenomena.

A big challenge is the time scale, as the thermal process can take hours or days.

Approach and results (part I):
The tools used to tackle the time scale challenge are accelerated molecular dynamics and discrete dislocation dynamics. Experimental results are also used for validation.

The first process simulated is dislocation climb in Nb, facilitated via vacancies. The vacancy diffusion is modeled using the approach of Venturini and Ortiz to characterize the grand canonical free entropy of the material as a function of the occupation number, and a Fokker-Planck equation, to model the transport process. The code is an add-on to LAMMPS and was used to analyze the climb of edge and screw dislocations in Nb. The annealing of dislocations is then simulated using discrete dislocation dynamics and the results are being validated against experimental results.

Overview and motivation (part II):
Two-dimensional materials exhibit defects such as dislocations, vacancies, holes, grain boundaries, though their interplay has been less studied than in three-dimensional materials.

The precise goal was to explore twinning in 2d materials as a mechanism for achieving new properties in a systematic way via deformation.

Approach and results (part II):
Twining is a planar defect whereby the two sides are related to each other via a rotation or shear satisfying the twinning equation. This twinning equation serves as a kinematic framework to explore all possible twin configurations. Interestingly the number of twin possibilities is extremely large, even in 2D, and the low deformation ones were analyzed in further detail. The energy for these selected modes were computed with atomistic and *ab initio* methods. Some of the ones computed for MoS_2 have also been found experimentally. Many of these boundaries have been observed to emerge numerically when deforming the material under uniaxial loading.

Next, the electronic properties of the material were analyzed. Twin boundaries did not change the nature of the material for graphene, but the band gaps were modified for MoS_2. This implies that the electronic behavior and thermal conductivity of the material can be modified by means of defects.

Conclusions:
- Modeling capabilities to link defect and quantum mechanics are still limited.
- The interplay between twinning defects and electronic properties, provides a mechanism for controlling electronic and thermal behavior via mechanical deformations.

References:
[1] D.F. Rojas et al., "Twinning in two-dimensional materials and its application to electronic properties", *Electronic Structure* 96 (2019) 1, 025001.

Session 2: Plasticity

David Rodney: Physical foundation of non-Schmid yield criterion in BCC metals
(Joint work with Emmanuel Clouet, Lisa Ventelon, François Willaime, Lucile Dezerald and Antoine Kraych)

Overview and motivation:
Experimental evidence shows that BCC metals do not follow Schmid law, in which plasticity is controlled by the shear stress along the Burgers vector of the dislocation projected onto the glide plane: (i) they exhibit twinning-antitwinning asymmetry, and (ii) other components of the yield stress are shown to affect the plastic behavior.

To characterize this non-Schmidt effect, authors have used a generalized yield criterion, in which stresses that affect dislocation glide are combined linearly with phenomenological parameters (one parameter, a_1, for twinning/antitwinning asymmetry, and two more parameters for non-glide effects). These parameters are often identified using atomistic simulations, using a fitting procedure. However, there is no complete understanding on the physical origins of these parameters, and it is also unclear why such a linear combination works so well. Answering these questions (for screw dislocations) is precisely the goal of this presentation.

Approach and results:
Detailed studies on the twinning-antitwinning asymmetry reveal that there are deviations in the dislocation path with respect to the glide plane when going from one well to the next. This therefore implies that the driving force on the dislocation has to be projected on the actual trajectory. Approximating the path as piecewise linear, a modified Schmid law was written that depends on the deviation angle (α). This angle is material dependent and can be computed from DFT. This simple correction qualitatively reproduces experimental data and quantitatively reproduces results from DFT calculations. Interestingly, using trigonometric identities, the functional form previously proposed on phenomenological grounds is recovered, with an explicit dependence of the parameter a_1 on alpha.

Non-glide effects are then studied using DFT by applying pure shear perpendicular to the Burgers vector of the dislocation. As expected the Peierls barrier depends on the shear stress. This has been qualitatively explained by Vitek, is based on the fact that the displacement field perpendicular to the dislocation is dilatational and that there is a coupling between the external field and the dilatational field. To understand this quantitatively, it is proposed to model the dislocation core as an Eshelby inclusion, and use the eigenstrain approach of Mura to model the coupling, namely, how internal stresses change along the Peierls barrier. The resulting predictions fall right on top of the DFT data, both with and without resolved shear stress.

Both of the above effects can then be put together to have a model for the enthalpy of the dislocation that recovers twinning/antitwinning asymmetry and non-glide effects. Furthermore a generalized yield criterion can be obtained by noting that, at the Peirels barrier, the first and second derivative of the enthalpy of the dislocation must vanish. The resulting yield criteria has the classical functional form previously utilized, where now the parameters have a quantified physical meaning and depend on α and the eigenstrain via relaxation volumes. It is important to note that all the parameters that characterize non-glide behavior can be computed from the zero stress Peierls barrier.

Conclusions:

- Twinning/antitwinning asymmetry is related to deviations of the dislocation path away from the glide plane
- Non-glide effects are due to the deformation of the dislocation core that can be modeled using an Eshelby inclusion approach.
- Future work includes non-glide effects on twinning and extension to finite temperatures.

References:
[1] L. Dezerald et al. "Plastic anisotropy and dislocation trajectory in BCC metals." *Nature Communications* 7 (2016): 11695.

Eugen Rabkin. The microstructural origins of size effect in strength of metal nanoparticles.

(Joint work with Tyler Flanagan, Oleg Kovalenko, Seok-Woo Lee)

Overview and motivation:

The paradigm "Smaller is stronger" is now 10 years old, and it has its origins primarily in compression experiments on focused ion beam (FIB) machined micro and nanopillars. Data form these experiments approximately follows a master curve which describes the power law behavior of normalized resolved shear stress on the diameter of the pillar, and the exponent is about -2/3. However, the fabrication technique for these nanopillars introduces many defects, primarily at the surface layer, which can harden the surface thus making the pillars stronger as the size is reduced.

Other experimental methods via etching have enabled to fabricate micropillars without FIB and compression experiments on these reveal no size effect. It was then speculated that the plasticity could be nucleation controlled. However, other deficiencies have also been pointed out for this fabrication method: the pillars resulting from the etching process are a solid solution, with solute atoms at a distance smaller than pillar diameter.

This work aims at understanding the origin of the size effect of gold nanoparticles under compression and explaining some of the discrepancies that exist between experiments and theory.

Approach and results:

Dewetting of thin films on a substrate is proposed as an alternative method to fabricate nanostructures, namely, faceted nanoparticles, which form driven by the decrease of the total surface/interface energy. The resulting particles are believed to be defect free, so it is suitable to study nucleation controlled plasticity.

The load displacement curves for faceted Au micro-particles exhibit an elastic region followed by a sudden particle collapse. This critical stress for collapse is given by the nucleation of dislocations, which then proceed in avalanches leading to the sudden deformation. The compressive stress at which the collapse occurs approaches the theoretical strength of Au (several GPa) and a trend of "smaller is stronger" with an exponent of 0.77 is observed. These findings were also supported by MD simulations, where the exponent found there was very similar to the experimental exponent.

The above results were very satisfying. However later experiments on faceted Ni microparticles obtained by solid state dewetting depicted different exponents for the experiments and simulations (more than double in experiments). Further experiments on Mo nanoparticles showed that while rounded particles exhibited no size dependence, faceted particles exhibit an unusually high exponent of about 1.

In view of these inconsistencies, further experiments on Au were performed. For larger particles, the previous results were recovered, whereas smaller particle sizes showed some trend of saturation. TEM analyses of the particles showed that small Au particles are defect-free while larger particles have dislocations. This probably determines the size effect. This was modeled using the truncated source model using the dislocation density from experiments. This model gave results similar to that of the experiments with saturation

occurring for smaller particles. This model was also able to quantitatively predict the size effect of Au pillars.

Experimentally, large particles are probably large because they initially have defects that enable their growth during the dewetting process, and this also induces size effects under compression test.

Conclusions:
- Small metal particles obtained by solid state dewetting are defect-free and achieve the theoretical strength.
- Large particles are large because they contain defects
- Defects are responsible for the artificial size effect in strength.

References:
[1] A. Sharma et al. "Nickel nanoparticles set a new record of strength." *Nature Communications* 9, 4102 (2018).
[2] T.J. Flanagan et al. "The effect of defects on strength of gold microparticles." *Scripta Materialia* 171 (2019): 83-86.

John Bassani: Non-associative plastic flow: insights from multiscale simulations

Overview and motivation:
Non-associative plastic flow is related to non-Schmid effects in crystals, though it not only happens in crystals, but also in granular solids and amorphous materials. In crystals, dislocation cores may not be confined to the slip planes, leading to a dependence of the Peierls stress on the full stress state (not only shear stresses). In disordered systems, the sources of plastic deformations are the so-called shear transformation zones (STZs), which can shear under the application of stresses. In both cases, the jerky flow is observed, which seems to be a characteristic of non-associative flow, much like slip-stick in frictional materials.

Historically, Schmid law was predominantly thinking of basal slip in hexagonal closed-packed materials. But, as noted by Cottrell, for too long, fcc has been taken as the model for plastic behavior, while it really is the exception rather than the norm (dislocations in fcc materials have very planar cores). Prager and Drucker started already thinking about non-associative flow, as they recognized that friction was a model for plastic type behavior.

It is here conjectured that non-associated flow is the appropriate plasticity theory for most materials, both crystalline and disordered, and that leads to significant effects.

Approach and results:
A simple mechanism displaying non-associated plastic-flow behavior is friction. In this case, the yield function (F) depends on the shear (S) as well as the normal force (N). Because the slip is not in the direction of the normal force, the flow potential (G) is a different function. As a simple example, G can be taken to just be S, although, in general, it can depend on both S and N. The resulting dissipation is positive but there is a second order work, which could be negative and that could lead to a highly destabilizing behavior.

Mathematically, non-associated flow (i.e., F and G different) leads to incremental equilibrium equations that are not self-adjoint, and therefore one does not have nice variational principles as for self-adjoint systems.

Vitek and Groger studied the core structure under stress of screw dislocations in Mo using a bond order potential and a strong discrepancy was found with respect to Schmid law. Based on these results, a modified yield criteria was formulated, where the effective yield stress depends not only on the Schmid stress, but also on the other components. The resulting yield surface exhibits tension-compression asymmetry. Furthermore, the active slip systems can actually be different in tension and compression. Building upon this, single crystal plasticity calculations were done, as well as predictions of the yield and flow functions for a random polycrystal using a Taylor model. Interestingly, the flow potential is just the Von Mises function.

Various applications were then explored: cavitation, sheet necking, stretching of thin sheets, which were shown to significantly depend on the non-associated behavior. Correlations were found between low values of the second-order work with strain bursts.

In conclusion, non-associated flow has it origins in non-planar core dislocation structures in crystalline materials, and in friction in granular materials, and its effects are now widely found.

Conclusions:
- The existence of non-planar core structures of screw dislocations leads to significant effects of non-glide stresses on plastic flow in single crystals that persist in the effective behavior of polycrystals, leading to non-associated plastic flow continuum models at all levels.
- Effects of friction in granular solids, will lead to dependence of the structure of STZs on the full state of stresses and thus lead to non-associated flow.
- Paraphrasing Cottrell: associated plastic flow constitutive behavior is the exception rather than the rule.
- Macroscopic deformation and failure modes can be significantly affected by non-associated flow.

Session 3: Defects I

David McDowell. Some challenges in length and time scaling for modeling dislocations.

Overview and motivation (challenge 1):
One of the big challenges is to model the gulf that exists between atomistic scale and mesoscales of crystal plasticity. Multiple methods currently exist for bridging the intermediate scales, such as coarse-grained atomistics, microscopic phase field models, discrete dislocation dynamics or statistical dislocation models. Further strategies include Coupled Atomistics and Discrete Dislocation (CADD) method, quasi-continuum method and the domain decomposition method.

Approach and results (challenge 1):
A method with attractive features for predictive mesoscale modeling is the Concurrent Atomistic-Continuum method (CAC). It has fully resolved atomistics and uses the same governing equations and interatomic potentials in both atomistic and coarse-grained domains. In this modeling strategy, dislocations can travel seemingly between fully resolved atomistic regions and coarse-grained regions.

CAC enables to study systems without periodic boundary conditions and reach time scales and loading conditions which are much more realistic than classical periodic molecular dynamic simulations. Examples of interest include interactions of dislocations with multiple surfaces and defects such as dislocation pile-ups, grain boundaries, voids, and impenetrable obstacles. It is worth noting that these sorts of interactions would be hard to simulate with discrete dislocation dynamics where assumptions would have to be made regarding these interactions.

Overview and motivation (challenge 2):
A second, but related challenge in the modeling of dislocations, is the thermally assisted obstacle bypass of dislocations. Most simulations have been performed in the overdriven regime, where universal scaling relations apply.

Approach and results (challenge 2):
A strategy followed here is to use Nudged Elastic Band (NEB) (CAC can actually also be used for NEB calculations) and an attempt frequency that goes inversely with the length of the dislocation segment. It turns out that the long-range dislocation interactions are critical to model this process, and that random array of obstacles offer less resistance than a periodic array of obstacles.

It is important to note that many body dislocation problems lie away from equilibrium and are entropically stabilized. This implies that the entropic prefactor is important to characterize in TST.

Overview and motivation (challenge 3):
Finally, a third challenge or gap in the modeling of dislocations is the uncertainty in bridging atomistics and experiments to the mesoscale and reconciling information coming from different sources. An application considered is the coordinated kink pair formation in BCC alpha iron with the objective of informing the parameters of the Kocks-Ashby-Argon Flow Rule. The resulting parameters of a bottom-up approach are however not within the 95% confidence interval of the experiments.

Approach and results (challenge 3):
The approach considered to overcome this initial disagreement is that of constrained likelihood, where the bottom-up information is used to penalize parameters estimation that are based on top-down modeling, based on surrogate models. This results in a good compromise between the inherent approximations that exist in interatomic potentials and the uncertainties that exist in experimental observations.

A more recent approach consists on augmenting the previously used top-down and bottom-up likelihood functions with an inter-scale discrepancy layer. This achieved a lower calibration variance.

Conclusions:
- CAC is a powerful method for mesoscale modeling, although the time scale challenge still remains largely unsolved.
- Reconciling information from simulations and experiments is important, for which a couple of strategies have been proposed.

References:
[1] S. Xu et al. "A quasistatic implementation of the concurrent atomistic-continuum method for FCC crystals." *International Journal of Plasticity* 72 (2015): 91-126.
[2] C. Sobie et al. "Scale transition using dislocation dynamics and the nudged elastic band method." *Journal of the Mechanics and Physics of Solids* 105 (2017): 161-178.
[3] S. Foiles et al. "Preface for focus issue on uncertainty quantification in materials modeling." *Modelling and Simulation in Materials Science and Engineering* 27 (2019).

Michael Ortiz. Atomistic simulation of hydrogen storage in Pd nanoparticles.
(Joint work with M.P Ariza, J.P. Mendez, X. Sun, M. Ponga, K.G. Wang)

Overview and motivation:
There are many examples for which one requires atomistic and diffuse time scales such as lithiation of silicon, the evolution of the microstructure for alloys or corrosion. All of these are out of the scope of molecular dynamics in views of the large gap in space and time, even with the advent of exascale computing. Coarse-graining strategies are thus required. The strategy presented is diffusive molecular dynamics (DMD), which combines a statistical description of atomistic fluctuations, Onsager type empirical kinetic relations, and quasi-continuum for the spatial coarse-graining (although this last part is not described here).

Approach and results:
The approach presented adopts a grand canonical representation of sites (note that these are not atoms, but sites), where the state of each site is characterized by its position, momenta and occupancy. The axiom of maximum entropy is then applied to obtain the grand canonical probability distribution as a function of the mean field of the atoms (expected position, momenta, energy and occupancy). The resulting grand canonical partition function provides the grand canonical free entropy and the local equilibrium relations, which reduce to conventional statistical mechanics for the case uniform temperature and chemical potential.

Calculations of the partition function are however complicated. Here, a convenient trial Hamiltonian (harmonic) is used instead of the exact one to obtain an approximation of the entropy function and the mesoscopic dynamics. The variables of the trial Hamiltonian can actually be optimized, leading to an additional equation.

Closure relations are needed to characterize the evolution of the temperature and chemical potential. Here, these are modeled using Onsager theory, that is, using a discrete Fourier law and a discrete Fick's law. There is currently work in progress to derive the kinetic relations consistently from Liouville equation and a Galerkin reduction (though this is not possible to do yet for the grand-canonical ensemble, as the Liouville type equation is unknown for this case).

The approach is applied to the process of hydrogen absorption and desorption in Pd nanostructures, which exhibit two phases. Interestingly, applying DMD to nanowires delivers a sharp phase boundary that propagates, and the velocity propagation comes from the model. For Pd nanoparticles, the misfit strains between the two phases leads to the appearance of misfit dislocations. These defects relax the energy, but also pin down the interface, and thus slow down the absorption of H. This interplay between morphology and kinetics may thus be studied as a function of particle shapes.

Conclusions:
- DMD is a useful paradigm for transport phenomena with atomistic fidelity.
- Useful in understanding hydrogen absorption in nanoparticles.

References:
[1] G. Venturini et al. "Atomistic long-term simulation of heat and mass transport." *Journal of the Mechanics and Physics of Solids* 73 (2014): 242-268.
[2] X. Sun et al. "Atomistic modeling and analysis of hydride phase transformation in palladium nanoparticles." *Journal of the Mechanics and Physics of Solids* 125 (2019): 360-383.

Emmanuel Clouet. Secondary slip of screw dislocations in hcp zirconium.
 (Joint work with Emile Maras)

Overview and motivation:
Zr is a transition metal with hcp structure, where plasticity is controlled at low temperature by the mobility of screw dislocations, where the principal glide planes occur in the prismatic planes. However, at sufficiently high temperatures it can also cross-slip to glide on basal and pyramidal planes.

The core structure of screw dislocations can be obtained using *ab-initio* calculations, which show that the most stable configuration is dissociated into two partials in the prismatic plane, although other structures also exist in the pyramidal plane, and in both prismatic and pyramidal. The energy barriers can also be computed versus the reaction coordinate. From it, it can be inferred that there is easy glide in the prismatic plane and energy barriers in the pyramidal planes. Glide in the basal slip is examined here.

Approach and results:
Ab initio calculations were used to test whether screw dislocations can glide in the basal plane. Specifically, NEB calculations were performed which indicated the presence of an intermediate configuration. The trajectory evolves through a combination of prismatic and pyramidal glides, which leads to an average basal glide. According to these results, the basal slip is a composite glide rather than elementary one. However, this is in contradiction with experiments, which show evidence of elementary basal slip.

The above simulations assumed that dislocations were straight. To overcome this limitation, molecular dynamic simulations were performed to study the glide of screw dislocations in the basal plane as a function of temperature and stress. It is observed that the dislocation moves via the nucleation and propagation of kinks, and the average velocity is strongly

dependent on stress and temperature, as expected. A detailed analysis of the position in space and time shows jumps in the pyramidal planes leading again to basal slip only on average, in contradiction with experimental observations. However, this can be a result of the MD set up, as the basal plane is the maximum resolved shear stress in the simulation. In addition, the stress rates in molecular dynamics are much larger than in experiments due to the time scale limitations.

Further NEB calculations were then performed, taking now into account the nucleation and propagation of kinks. Two regimes were identified corresponding to low and high stresses. The shape of critical kink pair was then extracted from MD as a function of applied stress and it was observed that it slightly widens with increasing stress in the slow stress regime, while it widens at a much higher rate with a decrease in the height in the high stress regime. This information can then be used to get the activation volume (first derivative of the activation enthalpy as a function of the applied stress), which exhibits a discontinuity with stress. Reasonable fits can be obtained with analytical expressions. The trajectory can be extracted from the NEB calculations, showing a pure basal slip for low stresses, and a combined prismatic and pyramidal slip for high stresses. The results from NEB and molecular dynamics are in good agreement for the high stress regime, which is the one accessible to MD.

Conclusions:
- Basal and pyramidal glide are competing mechanisms with the first one being favored at low stresses (in the experimental range), and the latter at high stresses (in agreement with MD simulations).

References:
[1] E. Clouet et al "Dislocation locking versus easy glide in titanium and zirconium." *Nature Materials* 14 (2015): 931-936.
[2] P. Kwasniak et al, "Basal slip of <a> screw dislocations in hexagonal titanium", *Scripta Materialia* 162 (2019) 296-299.

Session 4: Defects II

Jaime Marian. Simulating dynamic strain aging in body-centered cubic metals on diffusive timescales
(Joint work with: Yue Zhao, Lucile Dezerald)

Overview and motivation:
Plasticity in BCC materials, such as W, is governed by straight screw dislocation segments that move in a jerky or continuous fashion. Typical of BCC materials, the flow stress of high purity single crystal W exhibits a very strong temperature dependence, which can be understood with the aid of various models for the different regimes present (line tension model, elastic interaction model, kink-diffusion model). If solutes are added (e.g. Re as substitutional solute), the thermal dependence of the flow stress can lead to combined softening and hardening effects. The question addressed is how to add solute atoms (both substitutional and interstitial) to the standard plasticity picture of BCC metals. Some of the challenges are (i) elementary screw dislocation motion and solute jumps are atomistic in size, yet dislocation motion and solute diffusion occurs at mesoscopic time scales. (ii)

both motions are strongly thermally activated and (iii) BCC plasticity displays a number of anomalies (as compared to fcc).

Approach and results:
A mesoscopic approach is presented to model BCC alloys, building up on a previous framework for pure W. In such framework, kinetic Monte Carlo is used for the evolution of dislocations, (as it is strongly thermally activated), kink-pair nucleations are modeled as rare events whose rate depend on temperature and stresses (this follows original ideas by Srolovitz and Bulatov) and non-Schmid effects (twinning/anti-twinning asymmetry and non-glide effects) follow the framework of Vitek, Groger and Bassani. The various parameters involved are computed using quantum simulations and atomistic simulations. The resulting velocity of the dislocation as a function of length follows a linear relationship at low stress and temperature. Under extreme conditions though, a lot of debris is produced that is induced from self-pinning, a phenomena that has been observed experimentally in some systems.

The addition of solutes, such as Re (substitutional solute) in W (it is a commercial alloy), can increase the ductility (this is the case for W). To model this, the KMC model is augmented by adding interaction with solutes in two ways: (i) effect of stress field of dislocations on solute diffusion (this can be characterized by the activation volume tensor using DFT) (ii) and the effect of solute atoms on dislocation structure (the long range effect is simply an elastic dilatation effect, while the short range effects are inelastic and need to be computed using, for instance, DFT). This interaction is more complex in BCC metals than FCC ones, as solutes can interact with both edge and screw segments and the nature of the interaction is quite different.

There are three key processes in the motion of dislocations in these alloys: kink-pair nucleation, kink de-trapping and solute diffusion. Quantifying the rates of these events as a function of temperature and stress, delivers that diffusion does not play an important role as could be expected.

The resulting dislocation velocities can be equated to an equivalent flow stress, and it is observed that the flow stresses slightly decreases with concentration for low values, and then increases at higher concentrations, with a square root type of hardening that is consistent with experimental observations. Physically, at low concentrations, kink-pairs are easily nucleated, while the blocking due to solutes is minimal. As the concentration goes up though, kink blocking dominates. A map may then be drawn that separates solute softening from solute hardening as a function of temperature and concentration.

Moving next to BCC interstitial solid solutions, the existence of unstable flow is well documented. Here, diffusion of solute is going to be prevalent. In particular O in W is studied and it is found that tetrahedral sites are lower energy as compared to octahedral interstitial sites. Tetrahedral-tetrahedral diffusion is then studied by means of NEB DFT calculations as a function of stresses. Short-range inelastic interactions are also studied in detail, and two stable configurations are found (easy core and hard core). A stress temperature map was developed for this case for a given concentration (0.2% O) where three different regimes are identified:
1. At high temperatures, intermediate stress conditions, solute diffusion/trapping dominates over kink-pair nucleation (called solute decoration of the dislocation).

2. At intermediate temperatures and intermediate stress conditions, both solute and dislocation interact on similar time scales, leading to jerky flow.
3. At low temperatures and intermediate stresses, the solute effectively does not move and kink nucleation dominates, which leads to solute hardening.

This information can be mapped to a strain rate, temperature map, where the three regimes are also clearly visualized.

Conclusions:
- KMC allows to simulate diffusive timescales for dislocation motion.
- Proposed a solute chemo-mechanical coupling via DFT calculation.
- Developed a substitutional solid solution interaction model that predicts softening-to-hardening in W-Re.
- Developed an interstitial solid solution interaction model that predicts jerky flow regime in W-O.

References:
[1] Y. Zhao and J. Marian. "Direct prediction of the solute softening-to-hardening transition in W–Re alloys using stochastic simulations of screw dislocation motion." *Modelling and Simulation in Materials Science and Engineering* 26 (2018): 045002.
[2] Y. Zhao et al. "Electronic structure calculations of oxygen atom transport energetics in the presence of screw dislocations in tungsten." *Metals* 9 (2019): 252.

Anter El-Azab. A continuum theory for defects and microstructure evolution under irradiation.

Overview and motivation:
Nuclear materials are often subjected to extreme environments of temperature, pressure and irradiation. These adverse environments lead to a wide range of defects and microstructures depending on irradiation temperature, such as atomic disorder, stacking fault tetrahedral, dislocation loops, dislocation networks, voids and bubbles. The various responses can be categorized as microstructure evolution, composition evolution, or phase change, which lead at the engineering scale to swelling and growth, creep, hardening, and corrosion. For each of these three categories, there is a wide range of individual modeling strategies. There is currently a lack of a grand theory of irradiation effects in materials, particularly for alloys. Here, this science gap is being addressed through the use of continuum mechanics and non-equilibrium thermodynamics.

Approach and results:
The proposed framework integrates the usual continuum mechanics with kinetics of solutes and defects and thermodynamics, with the latter providing constitutive closures. Defects (e.g. dislocations, point defects) are incorporated into the continuum mechanics framework via incompatible inelastic deformations. (The total deformation is often decomposed into an elastic and an inelastic part, both of which are generally incompatible.) The stresses may then be related to the elastic deformation via Hooke's law, for instance, and the total deformation directly links to the displacement field. The mechanics problem is then governed by the equilibrium equation while additional equations are required for defect and microstructure evolution. These are obtained by invoking a linear constitutive

postulate compatible with energy conservation and the second law of thermodynamics. This framework has been applied to study void nucleation and growth under Frenkel pair production, as well as swelling, using a diffuse interface approach.

Conclusions:
- A field theoretic framework for irradiation effects can be established using the framework of continuum mechanics and thermodynamics.

Session 5: Grain boundaries and interfaces

Yashashree Kulkarni. Mechanistic insights into crystalline interfaces via thermal fluctuations

Overview and motivation:
Membranes even if appear flat or smooth, microscopically, due to thermal vibrations, they will exhibit fluctuations. These fluctuations have important implications in biological membranes (physiological processes) and 2D materials, like graphene (morphology, mechanical and electronic properties). The question raised here is: what are there implications of thermal fluctuations on crystalline interfaces, such as grain boundaries and twin boundaries?

Crystalline interfaces may be considered as interfaces separating two phases. The also exhibit fluctuations, although of the order of 1 or 2 lattice spacings (and a few picoseconds), in contrast with lipid membranes where fluctuations are of tens of nanometers. The advantage of these small fluctuations is that they are amenable to study via molecular dynamics simulations.

Thermal fluctuations are here used to study the stiffness and mobility of grain and twin boundaries, i.e. both equilibrium and non-equilibrium properties.

Approach and results:
The talk is divided into three parts:

1. Kinetics of twin boundaries via thermal fluctuations.
Energetic parameters such as stiffness may be obtained form interface fluctuations using statistical mechanics. Specifically, assuming for simplicity that fluctuations only exist in one direction, the interfacial height can be expanded in Fourier space. One can then write the energy of the membrane and invoke equipartition of energy to write an expression of the variance of the Fourier coefficients as a function of the wave number. This dependence will depend on the energy expression. These expressions can be used to derive stiffness (or other parameters appearing in the energy expression) after the fluctuations are evaluated via MD simulations. For twin boundary a slope of -1 is observed in the variance versus wavenumber in logarithmic scale. Karma *et al.* obtained a -1 slope as well for low angle grain boundaries, and attributed this slope to shear-coupled GB motion. Similar mechanisms exist for twin boundaries. Other grain boundaries exhibit -2 slope due to surface stretching, i.e., a different mechanism.

2. Entropic interactions between fluctuating twin boundaries.

There have been numerous studies of entropic interactions in lipid membranes, where it was observed that there are repulsive forces between nearby interfaces resulting in suppression of fluctuations of small wavelengths. For a grain boundary with -2 slope, low wavelength fluctuations also got reduced, while for twin boundaries, they were enhanced. Analytical studies using elasticity theory confirmed that indeed there was an attractive force. However, the amplitude is quite small, and it is unclear what its implications are.

3. Mobility of grain boundaries via thermal fluctuations

Migration of grain boundaries is governed by the grain boundary mobility. Karma and others came up with the idea that the normal motion of the mean position of fluctuating grain boundary can be treated as a 1D Brownian motion, which enables to obtain the mobility coefficient via mean square displacement. Many previous studies focused on high temperature where a linear dependence with time is clearly observed. However, studies on grain boundaries at lower temperatures showed a different behavior, which is expected, as the linear dependence in time is only valid for time scales that are larger, and not accessible from molecular dynamics simulations. Taking into account the additional analytical terms that are often neglected for long time scales, the mobility can still be extracted using Green-Kubo type of relations, where the velocity autocorrelations can be obtained from MD.

Conclusions:
- Fluctuations can be used to study equilibrium and non-equilibrium properties of interfaces.

References:
[1] D. Chen and Y. Kulkarni. "Thermal fluctuations as a computational microscope for studying crystalline interfaces: A mechanistic perspective." *Journal of Applied Mechanics* 84 (2017): 121001.
[2] D. Chen and Y. Kulkarni. "Atomistic modeling of grain boundary motion as a random walk." *Physical Review Materials* 2 (2018): 093605.

Nikhil Admal. Polycrystal plasticity with anisotropic grain boundary evolution
(Joint work with Jaime Marian, Javier Segurado, Giacomo Po, Matt Jacobs, Stanley Osher)

Overview and motivation

Polycrystalline plasticity to grain boundary evolution is important, for instance, for dynamic recrystallization (DRX). It occurs in a wide variety of processes, such as welding. The overarching goal of the work presented is to predict microstructure evolution during dynamic loading, in particular, to capture deformation, microstructure evolution and predict nucleation of defect-free grains. It should also take into account grain boundary migration mechanisms into account, and it should be computationally scalable to large polycrystals.

Approach and results:

Shearing of bycrystals leads to normal motion of grain boundaries, and this is characterized by the so-called coupling factor. This factor was long thought to be a geometric factor, though recent results clearly show that it depends on the boundary conditions and the need

to ensure compatibility. Consequently, the coupling factor is not a grain boundary property that can be used as a fundamental quantity in continuum models, but rather, it should be an outcome of the simulation. This motivates the need to couple grain microstructure models and crystal plasticity.

Existing grain microstructure models (they do not account for deformation) include diffuse and sharp interface models. Among the diffuse models, the Kobayashi-Warren-Carter model serves as an inspiration for the present work, and it is explained in further detail. The KWC energy functional is based on two parameters, phi (indicates disorder) and theta (indicates misorientation), and the associated Euler Lagrange equation allows the modeling of grain shrinkage and rotation.

However KWC model is phenomenological in nature. Yet, it lends itself very nicely to include crystal plasticity in it. A crystal plasticity free energy is thus proposed as a function of phi (similar to KWC), the elastic deformation and the dislocation density tensor. It is composed of an elastic energy and a grain boundary energy inspired by KWC, where theta is replaced by the dislocation density. The resulting model allows simulating grain shrinkage, rotation and sliding. Here, the coupling factor is an outcome of the model depending on slip systems allowed in the model. The model also has the capability to predict grain nucleation via agglomeration of dislocations.

The model has some limitations: (i) it is specialized to only misorientation angle dependence (a generalization to 3D is needed), (ii) the KWC functional form places restrictions on the dependence of the GB energy on misorientation, (iii), there is no consideration of symmetry, (iv) it is numerically inefficient, and (v) the sign of coupling factor is pre-decided. The first four limitations can be overcome. A generalization to 3D is proposed. As for the numerics, inspiration is drawn from thresholding methods, which are extremely fast compared to phase field models. Preliminary results indeed indicate great computational advantages.

Conclusions:
- Integrated KWC model for microstructure evolution to crystal plasticity.
- Generalized to 3D and improved numerical efficiency with thresholding methods.

References:
[1] N.C. Admal et al. "A unified framework for polycrystal plasticity with grain boundary evolution." *International Journal of Plasticity* 106 (2018): 1-30.
[2] N.C. Admal et al. "A three-dimensional misorientation axis-and inclination-dependent Kobayashi–Warren–Carter grain boundary model." *Journal of the Mechanics and Physics of Solids* 128 (2019): 32-53.

Brandon Runnels. Unifying mechanisms of grain boundary migration through a continuum thermodynamic framework.

Overview and motivation:
It is commonly believed that disconnections are carriers of shear coupling in grain boundary mobility. Disconnections are defects with both a burgers vector and a step height (they can be interpreted as dislocations of dislocations). In contrast to grain boundary

energetics, data for grain boundary mobility does not exhibit such clear patterns with grain boundary character. Coupling factors can be positive and negative and can act very differently depending on loading conditions. An important question thus emerges: what are the intrinsic properties governing grain boundary mobility?

Approach and results:
Here, grain boundary motion is interpreted as crystal plasticity with a clear map in terminology (e.g., mobility -> yield, thermal motion -> thermal softening, disconnection modes -> slip systems, shear coupling -> normality flow rule, etc.).

Grain boundary motion can be understood at the continuum setting as a permanent deformation F_{GB}. From an atomistic perspective, there are infinite numbers of transformation modes, each with an associated disconnection mode. From a continuum perspective though, F_{GB} has to be isochoric and has to satisfy Hadamard condition, which thus limits it to pure shear. In addition, the energy landscape is non-convex, which will likely result in strain localization and fine phase mixtures. It is suggested that grain boundary structures, disconnection and mode switching are actually manifestations of this non-convexity.

The model used to describe GB motion is a variational model based on minimum dissipation (it includes a free energy and a dissipation energy), where interface position is an internal variable. As an ansatz for mode selection, a minimization is performed over grain boundary modes. It is suggested that the dissipation energy is the sought after intrinsic property and three methods are suggested for its calculation.

Method 1: Upper bound for dissipation energy using optimal transport.
The energy versus reaction coordinate is smoother than expected, but the dissipation energy versus tilt angles displays some interesting results, namely mode switching. However there is a systematic overestimation of the dissipation energy.

Method 2: Dissipation energy extracted form area under the stress-strain curve.
Dissipation energy is proportional to plastic work, and it is here computed for two conditions (displacement driven shear and synthetic driving force) giving consistent results. Additionally there are cusps like structures. The obtained dissipation is only as good as the simulated boundaries, and results are currently limited to 0K.

Method 3: Continuum grain boundary migration model
The continuum model is based on energy minimization for the elastic response and an evolution equation for F_{GB}. Its application to various examples show some interesting fluctuations that look like disconnections.

Conclusions:
- Minimum dissipation potential formalism is useful for the modeling of grain boundary migration.
- Dissipation for each mode are suggested to be intrinsic properties.
- Mode switching is due to non-convexity of the strain energy density.

References:
[1] I. Chesser et al. "A continuum thermodynamic framework for grain boundary motion." *Journal of the Mechanics and Physics of Solids* (2019): 103827.

Session 6: Mechanics of Materials I

Garritt Tucker. Implementing higher-order descriptors to unravel competing deformation effects at an atomic scale

Overview and motivation:
In nanocrystalline materials, both experiments and computational studies show a transition point where the flow stress peaks versus grain diameter. Some of the observations from the literature note that: (i) there is a transition from dislocation to grain boundary driven deformation as grain size is reduced, (ii) the maximum strength grain size has been qualitatively observed to occur near this transition. The goal here is to quantify these observations by quantifying the role of defects (grain boundaries and dislocations) during strain accommodation, and how these correlate with the macroscopic material behavior. In addition, grain boundary structure and behavior will be analyzed using higher-order descriptors (atomistic shape moment).

Approach and results:
Nanocrystalline atomistic simulation boxes are generated for various grain sizes from phase field generated microstructures. Mechanical deformation is then performed on these, and the results are post-processed to understand deformation mechanisms. As previously discussed, the flow stress peaks with grain size.

To quantify the individual mechanisms and their role in strain accommodation, the atomic deformation gradient tensor, atomic micro-rotation vector and atomic strain vector are computed and combined with classical metrics such as common neighbor analysis and slip vectors. These enable to distinguish dislocations, grain boundaries and twinning, and to quantify the strain and strain fractions due to these mechanisms as a function of grain size. The results match very well with the different regimes highlighted by the flow stress versus grain size. Low grain size is grain boundary dominated (inverse Hall-Petch regime), large grain size is grain dominant (Hall-Petch regime), and the peak corresponds to an equal competition. The hypothesis regarding the flow stress peak was thus quantified to be true.

An interesting question then emerges as to whether the flow stress peak can be moved to a different grain size by affecting these mechanisms. A study of nanocrystalline alloys, namely Ni-P using a hybrid Monte Carlo/MD approach, reveals that indeed the solute affects position of that peak. A more detailed study of the distribution of the solute within grain boundaries indicates that it is very inhomogeneous, with more solute in high-energy grain boundaries, though data shows large scattering. To this, it is noted that microscopic degrees of freedom (even for the same macroscopic degrees of freedom) vastly influence the mechanical properties. A question is therefore whether there are better grain boundary descriptors. They considered shape descriptors based on spherical harmonics to characterize local atomic environment. These are tested over various grain boundary structures as well as to analyze grain boundary migration. The goal is to connect these descriptors to material behavior.

Conclusions:
- Transition from dislocation to GB driven plasticity in nanocrystalline materials was quantified using metrics for strain contributions from the different mechanisms.
- New grain boundary descriptors are proposed to characterize grain boundary structure and behavior.

Timothy Rupert. Probing nanoscale complexion transformations with computational techniques that complement experiments.

(Joint work with Zhiliang Pan and Vlad Turlo)

Overview and motivation:
An overarching goal is to tailor defects to control material properties. A good example of this is the stabilization of grain boundaries in nanocrystalline materials, which has been widely studied. Here, changes in grain boundary structure are targeted. In particular, amorphous intergranular films (AIF) are added to grain boundaries, to lead a nanolayer GB complexion.

Approach and results:
Experimental results show that AIF can toughen nanocrystalline materials and make them more ductile. It also increases the stability of the nanostructural material at high temperatures and speeds up the consolidation of powder during sintering.

AIFs are formed experimentally by pre-melting the grain boundaries and quickly cooling the system down. However, the distribution is heterogeneous in thickness over the sample. Atomistic simulations can be used to understand and characterize the structure, topology and statistics of these complexions.

Hybrid Monte Carlo/molecular dynamics modeling is used to analyze the grain boundary structure at a resolution that is inaccessible to experiments. Looking at the radial distribution functions, the interiors of these layers look like a bulk phase, and small differences are found near the amorphous-crystalline interfaces. There is actually a further transition region that differs from bulk amorphous phases, which is independent of film thickness at high temperatures. Also at high temperatures, the nearby crystals have less of an effect on how the transition regions look like.

The distribution of the thickness is hard to quantify experimentally, as it is very sensitive on how those boundaries are imaged, and there is a bias towards thicker more visible films. Atomistic simulations with varied doping show that there are huge variations in GB composition, which explains the variation in GB thickness.

Finally, atomistic models are also important for alloy design. They can guide experiments, by identifying the correct temperature and compositions.

Conclusions:
- Short-range order can be used to identify local structural variations within amorphous complexions. A transition region is identified.

- Local grain boundary composition can vary widely in a polycrystal. This variation is responsible for the thickness variation of AIFs.
- Alloy choices are important for complexion structures.

References:
[1] Z Pan and TJ Rupert, "Spatial variation of short-range order in amorphous intergranular complexions", Computational Materials Science 131 (2017): 62-68
[2] V Turlo and TJ Rupert, "Prediction of a wide variety of linear complexions in face centered cubic alloys", Acta Materialia 185 (2020): 129-141

Jun Lou. Quantitative in-situ nanomechanical study of low dimensional materials.

This talk is composed of two parts
Part I. Metal plasticity at small length scales (Au nanowires).
Part II. Fracture toughness and toughening of 2D materials, such as Graphene.

Overview and motivation (Part I):
Mechanical properties are well known to be size-dependent. For nanocrystals, one has a pseudo Hall-Petch relationship, where the relevant scale is the diameter of the metallic nanowire. For sizes below ~10 nm, there is a transition of deformation mechanism, whereby surface dominates the plastic behavior, with dislocations being nucleated at the surface.

Approach and results (Part I):
Lou's group is capable of synthesizing nanowires with diameters from a few nanometers to a few hundred of nanometers, all single crystals, to focus on surface effects. Observations and measurements of the deformation of these nanowires are then analyzed using in situ TEM, where the clamping is done via cold-welding (automatic fusing of nanowires, when in contact, to form a single defect-free nanowire). Uniaxial tests of Au nanowires reveal that plastic deformation occurs by nucleation of partial dislocations at the surface that quickly slip through the crystal, ultimately leading to necking till a single atomic chain. However, repeated experiments on Au nanowires, reveal that some of them exhibit a brittle-like fracture. In this case, twin structures develop perpendicular to the tensile axis, becoming weak point where fracture can initiate and quickly propagate through the cross section. The cause of this very distinct behavior was solved in collaboration with a theoretical group, and it was discovered that the cause was a misalignment issue when performing the tensile tests. For larger misalignments (>~10 degrees), twins activate first which leads to brittle failure, whereas partial dislocation nucleation at the surface dominates for small orientations.

Overview and motivation (Part II):
Graphene has very interesting properties like extremely high mobility and mechanical properties, and holds promise for applications such as flexible electronics and functional nanocomposites.

The mechanical properties of graphene have been previously investigated via nanoindentation. However, considering the small area probed for such experiments, it is possible that such area is defect free leading to results close to the theoretical strength.

Approach and results (Part II):
The mechanical properties of graphene drastically change in the presence of defects. This is important, as applications will have to deal with large surfaces of graphene, which necessarily contain defects. An important property is then fracture toughness. Experimental measurements of the fracture toughness reveal a very small value (like a ceramic). A natural question is then whether the grain structure allows changing such value. However, numerical simulations indicated that little gain could be achieved in this manner (about 10%). We then considered rebar graphene, which consists of a grapheme sheet reinforced with nanonwires, which resulted in an increase of about 50% of the fracture toughness.

Conclusions:
   * Theory needs to complement experiments.
   * There are a lot of opportunities for two dimensional materials.

References:
[1] Y Liu et al, "Cold welding of ultrathin gold nanowires", Nature Nanotechnology, 5 (2010): 218-224.
[2] EF Hacopian et al, "Toughening graphene by integrating carbon nanotubes", ACS Nano 12 (2018): 7901-7910.

Mitra Taheri. Toward the tailoring of materials properties far from equilibrium: convergence of microscopy, data Science, and theory

Overview and motivation:
Microscopy has a long history of successes and failures going through the development of optical microscopy, transmission electron microscopy (TEM), aberration correction TEM (ACTEM). Upcoming developments include on the fly studies to look at non-equilibrium events, and intelligent microscopy that combines theory, machine learning and experimental techniques.

Approach and results:
A grand challenge is the understanding of materials far from equilibrium, such as strongly correlated systems or extreme thermal events, which requires high spatio-temporal and energy resolution. Also, chemical order is becoming increasingly important, for instance, in the analysis of grain boundaries or high entropy alloys. New tools to push the boundary of electron microscopy in several of these fronts were presented, leading to a paradigm shift in microscopy and spectroscopy. Some specific advances include improved DQE (detective quantum efficiency) to highly increase the signal to noise ratio.

As a result of the large spatio-temporal resolution, data is collected at a massive rate, which therefore requires on-the-fly processing. Here, machine learning tools can enable the identification of defects, for instance, from very noisy data.

Some of the applications studied with these tools include
- The understanding of non-equilibrium geometries in grain boundaries during irradiation, with the goal of building radiation tolerant materials. Aspects studied include grain size effects, effects of local strains, grain boundaries degrees of freedom, and their correlations with defect absorption.
- Grain boundary dislocation densities and geometrically necessary dislocations. The approach taken combines precision electron diffraction with automated crystallographic orientation mapping to look at the Nye tensor, which subsequently can give the geometrically necessary dislocation (GND) density.
- New techniques that provide synchrotron level data in TEM to spatially resolve the local order at GBs are also presented. These techniques combined with characterizations of the GNDs show that sink efficiency depends on the microscopic degrees of freedom of the GBs (even between boundaries with identical macroscopic degrees of freedom). Simulations by David Srolovitz further supported this.
- The above results raise the question of whether GB equilibrium is just a microstate. The answer is yes. Experiments and simulations on equilibrium GBs and disordered or non-equilibrium GBs show that they have different sink efficiency.

Overall, the tools developed enable a high resolution in space, time and energy. However, interactions with theory and simulation are crucial to answer fundamental questions regarding the role of preexisting dislocations, the role of highly dislocated grain boundaries and their evolution to understand sink efficiency and radiation tolerance.

Open questions include dislocation and point defect interaction, absorption at grain boundaries, dislocation defect drag, and dislocation defect highways.

Conclusions
- New high-resolution techniques enable to visualize and quantify GB dislocation content and local order.
- A lot more is needed on the theory side to understand GB structure and its evolution.

References
[1] G.A. Vetterick et al. "Achieving radiation tolerance through non-equilibrium grain boundary structures." *Scientific reports* 7 (2017): 12275.
[2] J.L. Hart et al. "A Synchrotron in the TEM: Spatially Resolved Fine Structure Spectra at High Energies." arXiv preprint arXiv:1909.06323 (2019).

Session 7: Mechanics of Materials II

Ryan Elliott. A framework for the interpretation of modulated martensites in shape memory alloys
(Joint work with Vincent Jusuf)

Overview and motivation:
Shape memory alloys are materials that undergo reversible martensitic phase transformations (they are first-order diffusionless, solid-to-solid phase transformations) under thermal or mechanical loading. They are related to changes in the crystal structure of

the alloy. From a continuum perspective these transformations corresponds to changes in the free energy landscape and its (single or multiple) minima as a function of load or temperature.

A key feature discovered in the last decade is that the strain of transformation between the martensite and austenite phases measured by a deformation gradient can tell a lot about the macroscopic properties of these structures. In particular, the minimum eigenvalue of the stress tensor has been shown to relate to the level of hysteresis, and thus reversibility and damage.

In addition, some shape memory alloys have modulated microstructures (MMs), which often require a much larger unit cell to describe the martensite phase. However, first principle calculations show that the small unit cell martensite is the lowest energy phase. It thus remains an open question why modulated microstructures are observed experimentally. There are basically two existent theories for the experimental observation of MMs, both of which are based on kinematic arguments without looking at the energy: (i) adaptive martensite hypothesis: MMs as nano-twinning of ground state (ii) periodic zig-zag of closed-packed planes and thinking of different stacking sequences to build different MMs. Understanding these structures from an energetic perspective is precisely the focus of this work.

Approach and results:
In 2011 Elliott developed a model for base martensite (non-modulated martensite). In particular, he developed an effective interatomic potential that allowed him to do atomistic statics and look at the bifurcation problem to explore all possible phases predicted by the model. The model was able to predict the existence of various structures and phase transitions.

There is hope that it can also predict modulated structures, as bifurcations correspond to different wave vectors becoming unstable. Indeed it was possible to find these structures, and they thus are natural features of the energy landscape. The resulting MMs phases are quite stable and close to the base martensite phase, and they are much more compatible than the base martensite. Actually, when kinematic compatibility is enforced as a constraint, MMs become the energy minimizing phases.

It was observed that all the modulated structures found with the atomistic model consisted of stacking of four different types of planes associated with two base martensite phases. Based on this observation, a Modulated Martensite Mixture Model (M^4) was developed, where a simple rule of mixture was used for the deformation of the MMs. This gave very good prediction for the properties of the real MMs (better than predictions based on previous models). Then, the rule of mixtures was used to try to find a more compatible structure than those found via previous atomistic calculations. Such a MM was indeed found and this was confirmed by atomistic model that it was more compatible than what was previously found before. The model thus had a predictive capability.

Conclusions
- MMs are energy minimizing phases when enforcing kinematic compatibility.
- MMs can be interpreted as mixtures of two phases.

- A simple mixture rule allows predicting a new structure that is more compatible than previously identified ones.

References
[1] D. B. Ghosh et al. "Structural phase transition path-following and stable phase scouting through a coupled DFT–BFB algorithm." *Modelling and Simulation in Materials Science and Engineering* 19 (2011): 085007.

Prashant Purohit. Interactions and assembly of inclusions on lipid membranes.
 (Joint work with Xinyu Liao)

Overview and motivation:
Cell membranes are lipid bilayers that, mechanically speaking, act as a fluid in the plane. These lipid membranes can have embedded protein molecules that can diffuse around, a process that is important for viral infections. Most of the studies of these processes are made using coarse-grained molecular simulations, although some experiments also exist. In this diffusion process, thermal fluctuations are an important component, and are here modeled using a continuum mechanics approach combined with statistical mechanics analysis.

Approach and results:
Lipid membranes are modeled as a flat membrane using the Helfrich model, where the energy accounts for the mean curvature and hydrostatic tension (Gauss curvature is not important). A triangular finite element discretization is then used, where each triangle is assumed to remain flat during the deformation. The energy then adopts a quadratic form, which is easily amenable to statistical mechanical analysis to compute the partition function and the free energy. Simple thermodynamic relations can then be used to compute the change of projected area with tension, and the entropy, resulting in good approximations of the analytical solution of Helfrich as the number of finite elements increases.

Inclusions are then modeled as rigid inclusions within the finite element discretization. Additionally, the angle between the inclusions and the membranes at the point of contact is imposed using a penalty method. The free energy may then be computed as a function of the distance between two inclusions to understand whether there is an interaction force. The energetic and entropic contributions are computed separately and recover the functional form previously proposed. The energetic and entropic terms are competing terms, which lead to a maximum free energy at an optimal separation distance. Inclusion clusters may then be analyzed, for which there is no analytical solution, and again in this case, there is an optimal distance.

Next, the diffusion of these inclusions is modeled using overdamped Langevin dynamics and associated Fokker-Plank equation, where the drag comes from the fluid nature of the membrane and is modeled using the Saffman-Delbruck formula, and the potential is the previously computed one by means of statistical mechanics. First the diffusion of a single protein is analyzed under the presence of a second inclusion that is considered fixed. Under reflecting boundary conditions, the Fokker-Plank equation delivers the Boltzmann distribution at equilibrium. The first passage time can also be computed for various boundary conditions. For self-assembly conditions, the passage time is an order of

magnitude smaller than what was seen in experiments but the membrane that can be simulated is much smaller in the model and hence the results are not unreasonable.

For a more detailed analysis, the hydrodynamics interactions between inclusions have to be considered. A way to account these interactions is through the Oseen tensor. It is observed that hydrodynamic interactions speed up the self-assembly process.

Conclusions
- Proposed a time-efficient approach from statistical mechanics to compute the free energy of a thermally fluctuating membrane with inclusions.
- This allows studying the self-assembly process of inclusions.

References
[1] X. Liao and P.K. Purohit. "Self-assembly on a lipid membrane viewed as a first passage time problem." *Journal of the Mechanics and Physics of Solids* 135 (2020): 103787.

Andrej Kosmrlj. Statistical mechanics of microscopically thin thermalized structures.

Overview and motivation:
Thin solid shells and structures can now be fabricated at very small scales where thermal fluctuations become important. The main question here discussed is how do thermal fluctuations affect their mechanical properties? This is discussed in the context of flat sheets, spherical shells and cylindrical shells, using tools from renormalization group calculations and molecular dynamic simulations.

Approach and results (free standing flat sheets):
The material is assumed linear elastic, though deformations can be considerable (i.e. nonlinear kinematics). Actually, these nonlinearities are responsible for many of the interesting results here shown.

A useful analogy to understand the behavior of thermally fluctuating flat sheets can be found in the mechanics of crumpled sheets. When the amplitude of the quenched ripples (induced by crumpling) is larger than the thickness of the sheets, the bending of crumpled sheets becomes harder, while stretch/shear becomes easier. Qualitatively, similar mechanical behavior is induced by thermal fluctuations when the magnitude of height fluctuation becomes larger than the thickness of the sheet, which is defined as the square root of the ratio of the bending modulus and the Young's modulus in 2D materials. Since the magnitude of height fluctuations increases with temperature and with the size of the sheet, we can introduce a characteristic length scale $l_{thermal}$ at which the magnitude of height fluctuations becomes comparable to the sheet thickness. For a regular sheet of paper the thermal length scale is gigantic and thus thermal fluctuations are irrelevant. However, for 2D materials such as graphene, the thermal length scale at room temperature is of the order of nanometers, and thus the effect of thermal fluctuations become important. Beyond the characteristic thermal length scale, thermal fluctuations effectively renormalize bending rigidity and Young's modulus and make them scale dependent with universal power law exponents. These different exponents are related to each other due to the rotational

invariance, and they can be estimated with the renormalization group theory and atomistic or Monte Carlo simulations.

The projected area of the sheets is also temperature dependent. The thermal expansion coefficient has two contributions: one that is positive is induced from the thermal expansion of atomic bonds, and a second entropic contribution, which is negative, is induced by height fluctuations. As a consequence, fluctuating membranes can have negative thermal expansion coefficients.

External tensile stress suppresses the height of the fluctuations. This effect dominates at scales larger than a length scale l_{stress}, which is inversely proportional to the magnitude of applied tensile stress. The relative value of the various length scales and the system size L defines three domains: (i) for L < l_{stress}, the projected area increases linearly with the applied stresses with the slope corresponding to the renormalized bulk modulus; (ii) for $l_{thermal}$ < l_{stress} < L, nonlinear stress-strain behavior is observed with a universal power law exponent, and (iii) for l_{stress} < $l_{thermal}$, thermal effects are completely suppressed and classical mechanics is recovered.

Under compression, the sheet may buckle. Interestingly, analyses reveal that thermal fluctuations increase the critical buckling load for sheets that are larger than the thermal length scale. The increased critical buckling load is directly related to the thermal stiffening of the bending rigidity, which is also verified with MD simulations.

The analyses above all pertain to isotropic sheets. For anisotropic sheets, the thermal fluctuations depend on the full tensor of elastic constants. However, at large lengths scales, due to thermal fluctuations, the anisotropic sheets behave like isotropic sheets.

Approach and results (spherical shells):
Due to the shell curvature, the strain tensor contains an additional term, which couples bending and stretching deformations. As a consequence, the magnitude of radial fluctuations is suppressed at large length scales. In this case, the magnitude of the fluctuations doesn't increase with the system size, but rather with a new elastic length scale, that is given by the square root of the radius and the thickness of the shell. When this elastic length scale is larger than the thermal length scale, then thermal fluctuations become important. Similarly, to the flat sheet case, thermal fluctuations lead to an increase in the renormalized bending rigidity and a decrease of the normalized Young's modulus. In addition, thermal fluctuations generate an effective entropic compressive stress (analogous to some external pressure) that reduces the critical buckling pressure of the shell. At sufficiently large temperatures the effective compressive stress can induce the spontaneous collapse of the spherical shell even in the absence of external pressure.

Approach and results (cylindrical shells):
Cylindrical shells also contain additional terms in the kinematics induced by curvature. Similar to spherical shells, thermal fluctuations become relevant beyond the characteristic elastic length scale, and the renormalized Young's modulus (bending rigidity) decreases (increases) with the same power law exponents as that of flat sheets. Different from spherical shells, the critical buckling load is non-monotonic with temperature. The critical buckling load is initially reduced due to thermal kicks over the activation barrier, but at high temperatures the critical buckling load increases due to the renormalization of elastic constants.

Conclusions
- Thermal fluctuation can become important at small scales.
- Thermal fluctuations can lead to unusual and surprising mechanical behavior.

References
[1] A. Košmrlj and D.R. Nelson. "Statistical mechanics of thin spherical shells." *Physical Review X* 7 (2017): 011002.
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Session 8: Mechanics of Materials III

Pradeep Sharma. Flexoelectricity and Electrets

Overview and motivation:
Piezolectricity deals with the coupling of electrical signals and mechanical deformation, so that one can induce the other and vice versa. Applications are very varied (e.g. tennis rackets, wireless sensors, robotic arms) with energy harvesting being of marked interest. However the energy scale is low which reduces applications to small devices, and there are currently many efforts to engineer high piezoelectricity.

Approach and results:
In centrosymmetric crystals the center of positive and negative charges coincide (even after uniform deformation) and there is consequently, no polarization. In non-centrosymmetric crystals though, charge separation can be achieved with deformation, and can thus be piezoelectric. The number of piezoelectric materials is therefore given by their structure for uniform deformations, and there are a limited number of them. However, for non-uniform strains, it is possible to develop an asymmetry, even for centrosymmetric crystals (non piezoelectric). This phenomenon is denoted as flexoelectricity and it has been demonstrated experimentally.

It is possible to obtain an apparent piezoelectric behavior at the nanoscale without using piezoelectric materials, by incorporating an inclusion. The inclusion will lead to local deformations, which by flexoelectricty, will generate a polarization. If, on average, these polarizations don't average out to zero, a net piezoelectric effect will be achieved. The recipe thus consists on having high elastic and dielectric constants, small size (to induce large strain-gradients), non-centrosymmetric shape and optimum volume fraction.

Numerical calculations on BTO and graphene sheets with triangular holes show that a polarization can be achieved for small holes for an optimal volume fraction. These results have also been verified experimentally on other systems.

An important open issue in this field is the lack of a rigorous homogenization theory. Also, determining flexoelectric properties numerically and experimentally is challenging, though DFT efforts by Vikram Gavini and Amartya Banerjee will certainly greatly help in this endeavor.

Since strain and strain gradients scale with the inverse of the elastic moduli, large strain gradients are easier to achieve in soft materials. Also, soft materials are of interest for applications in soft robotics, biological applications and stretchable electronics.

Although many soft materials are not piezoelectric, they can become electromechanically active via the so-called Maxwell stress, which is present in all dielectric materials. More specifically, an electric field can deform the material (these deformations may be large), but there is no converse effect (cannot be used for energy harvesting). Also the Maxwell stress effect is nonlinear, it requires a very high voltage and it is not reversible.

An idea is to embed massless charges in a soft material to create piezoelectric materials. This type of materials exists and is called electrets. Their measured piezoelectricity is much higher than that of one of the best piezoelectric materials.

Work in progress includes flexoelectricity in soft materials, where current results are very encouraging, and comparisons with experimental investigations are pending.

Also, using two-scale asymptotics, Liu and Sharma homogenized electrets and found that there is a true effective piezoelectric property and an emergent piezoelectricity. Interestingly, several exact relations were obtained, which is rare in homogenization theory.

Finally, it was noted that fleoxelectricity plays an important role in biology, and is responsible, for instance, for our hearing capabilities.

Conclusions

Open issues in electrets include (i) the combination of electrets with flexoelectricity to exploit size effects, (ii) charge stability at high temperatures (they leak after some time), (iii) making electrets out of really soft materials.

References

[1] S. Krichen and P. Sharma. "Flexoelectricity: A perspective on an unusual electromechanical coupling." *Journal of Applied Mechanics* 83.3 (2016): 030801.
[2] Q. Deng et al. "Electrets in soft materials: Nonlinearity, size effects, and giant electromechanical coupling." *Physical Review E* 90 (2014): 012603.

Kaushik Dayal. Electromechanics and statistical mechanics of dielectric elastomers

Overview and motivation:

Dielectric elastomers show promise for many applications (e.g. soft robotics, biomedical devices), but they are not so used in real settings, as very high fields would be required (even close to electrical breakdown). It is also worth mentioning that dielectric elastomers may not necessarily be seen as passive elements that deform under the application of the electric field, but their microstructure and electromechanical coupling can be optimized.

Approach and results:

Sequences of models (monomer, single chain and polymer network) are proposed to understand the behavior of dielectric elastomers.

The monomer model follows standard literature with energetic contributions that include (strain energy, bond energy –small-, dipole strain, electrostatic term, and external electric field energy). Simplifying assumptions are made for the various terms. In particular, interaction energies between monomers are neglected (using a two scale approach).

To construct the chain model, monomers are assumed to not stretch, and their orientation can thus be characterized via a probability distribution over the sphere. Statistical mechanics is then used to compute the partition function and free energy. Results in closed form are obtained in two limits (small strain case, and very large strain) and these are compared with numerical experiments at various values of the electric field, exhibiting a good agreement.

Arruda and Boyce approach is then used to get to the network model. It is assumed for simplicity that the chains are uniformly oriented on the sphere, and the integration over the sphere is approximated by integrating over eight specific chains, which are the ones resulting from connecting the center of a cube with its eight corners. This sort of procedure works very well as can be observed for instance by comparing to more accurate quadrature rules.

The resulting behavior is analyzed for two thought experiments. The first once consists on simultaneously applying a voltage (that induces a compression) and a traction that precisely balances out the deformation. This allows observing the non-naïve behavior of the material. A significant deformation is observed as a result of the electric field, even without having optimized the microstructure in any way. The second thought experiment consists of a simultaneous shear and a voltage. It is observed that the electric field can further induce a shear, thus breaking the symmetry in material behavior. Both of these results can be interpreted at the continuum level.

Conclusions
- There are additional contributions to the Maxwell stresses (estimated ~15%).
- Overall incompressibility implies that chains must stretch if they rotate. Also, chains rotate to align with the field. These give rise to an unexpected coupling between electric field and deformations.

References
[1] N. Cohen et al. "Electroelasticity of polymer networks." *Journal of the Mechanics and Physics of Solids* 92 (2016): 105-126.

Pedro Ponte-Castaneda. Macroscopic instabilities and domain formation in elastometric composites

Overview and motivation:
Elastomeric composites with periodic microstructure may develop microscopic or macroscopic instabilities. An example of microscopic instability is given by a porous elastomer consisting of 2D periodic systems with circular holes, when subjected to compression or tension. Another more interesting example which develops microscopic instabilities is that of periodic rigidly reinforced composites, where depending on the

loading conditions, different patterns (wavelength of the instability) develop, including long wave length instabilities.

In the context of random composites, elastomeric composites can only develop macroscopic instabilities (the concept of microscopic instabilities does not really make sense). Examples of these have been shown by Ponte Castañeda.

What happens after a macroscopic instability (which corresponds to loss of ellipticity)? Loss of ellipticity in metals is associated with shear localization, which eventually leads to cracks and failure. In these elastomers the behavior is different and results in domain formation, to relax the stresses. There is a mathematical procedure for computing these microstructures, which is called quasi-convexification. This methodology has been previously applied for a class of reinforced elastomers leading first to a microscopic or a macroscopic instability depending on the concentration of the reinforcing phase. Experimental investigations on similar systems exhibit chevron (double laminar) microstructures.

Approach and results:
For a periodic microstructure, the homogenized behavior is given by considering the energy under affine boundary conditions associated with all possible combinations of the unit cells (could be over one or several unit cells depending on the wavelength of the instability). Before the onset of any instability the composite is described by the so-called principal solution, which is the one-cell periodic solution. The resulting energy is quasi-convex, and therefore rank-one convex but not necessarily strictly rank-one convex.

To characterize the behavior beyond the instability point the following strategy is used. The idea is that the homogenized energy is, by construction lower than the principal solution, and consequently, by taking the quasi-convex envelope on both sides, lower than the quasi-convexification of the principal solution (in some cases it may be equal).

Although the quasi-convex envelope is in general hard to compute, there are other notions of convexification, and relations of these via inequalities that allow generating estimates. In particular, if the rank one envelope is quasi-convex, it must correspond to the quasi-convex envelope. Thankfully the rank-one envelope is easy to compute (using Kohn-Strang formula).

The results indicate that there are three regimes or phases depending on the deformation. One of these is the principal solution, which is observed for large deformations. The other two correspond to one lamination and 2 laminations.

An interesting outcome of this example is that loss of global rank-one convexity and loss of ellipticity do not always coincide. In general, loss of global rank-one convexity takes place before loss of ellipticity (loss of local rank-1 convexity).

Conclusions
- Macroscopic instabilities are followed by domain formation.
- Loss of rank-one convexity generally takes place before loss of ellipticity.
- Does relaxation via principal solution always work?

References
[1] R. Avazmohammadi, and P. Ponte Castañeda "Macroscopic constitutive relations for elastomers reinforced with short aligned fibers: Instabilities and post-bifurcation response." *Journal of the Mechanics and Physics of Solids* 97 (2016): 37-67.
[2] J. Furer and P. Ponte Castañeda. "Reinforced elastomers: Homogenization, macroscopic stability and relaxation." *Journal of the Mechanics and Physics of Solids* (2019): 103689.

Session 9: Phase Field Model

Peter Voorhees. The morphology and topology of nanoporous metals

Peter Voorhees was absent due to medial reasons and the presentation was therefore not given.

Katsuyo Thornton. Nanoscale simulations using phase-field crystal models

Overview and motivation:
Continuum models including phase field models are useful in predicting many aspects of material behavior. However, in some cases, neglecting the description of atoms leads to crucial loss of information, for instance, when defects are considered.

Phase field crystal (PFC) is a promising method to simulate atomistic details at diffusive scales, and has been applied to many systems, such as formation of strain induced compositional domains, epitaxy or defect structure and energetics. Here, the method retains dynamic information via the probability distribution. PFC free energy can in fact be derived from classical density functional theory, under suitable assumptions, and it thus has physical foundations with approximations. A big question in the community is whether the method can be parameterized to specific materials to provide quantitative predictions.

This talk focused on two topics: (i) identifying low energy grain boundary structures and metastable ones, and (ii) modeling of 2D materials.

Approach and results (applications to grain boundaries):
Identification of grain boundary structures is often done in molecular statics by sliding one crystal with respect to the other. This is however a tedious process and sometimes it does not find the lowest energy state. The approach taken here to identify grain boundary structure and its energetics is by having two crystals that are initially separated, and these are allowed to grow. This can be done for different orientations and shifts in order to identify the lowest-energy grain boundary structure. These are often characterized by less diffusive peaks which are indicative of lower atom mobilities, as could be expected. The results obtained are compared with grain boundary structures predicted by genetic algorithm, showing a remarkable agreement. Such comparisons were done for various GB, even some exhibiting nanofaceting. Consequently, PFC can be used a surrogate model that could be used for instance, to inform initial conditions for atomistic models.

Approach and results (applications 2D materials):
2D materials are a promising application for PFC. Most previous studies are however confined to two dimensions. Here, the goal is to develop a three-dimensional model of these

2D materials to examine buckling under compression for triangular and honeycomb lattice. Simulation results were presented to demonstrate the new model.

Conclusions
- PFC provides atomistic description over diffusive time scales and naturally incorporates elasticity.
- PFC can identify grain boundary structures. It can be a useful coarse-grained model.
- Developed a 3D model for 2D materials.

Martin Diehl. Coupling crystal plasticity and phase field methods: the future of integrated computational materials engineering?

(Joint work with P. Shanthraj, P. Eisenlohr, F. Roters, D. Raabe)

Overview and motivation:
Integrated Computational Materials Engineering (ICME) "entails integration of information across length and time scales for all relevant material phenomena and enables concurrent analysis of manufacturing, design and materials within a holistic system" [1]. The goal is to connect processing, microstructure and properties, which is the holy grail of computational material science and engineering.

The above goal is however far from reach. This talk is thus much narrower and focuses on the continuum modeling of polycrystalline materials (physics based models) at engineering time and length scales, integrating all relevant phenomena. Phenomena besides plasticity that are discussed included fracture, twinning and chemomechanics.

Approach and results:
Continuum modeling of crystal plasticity is typically based on the kinematic decomposition of the deformation gradient between the elastic and plastic part, where the plastic velocity gradient is written as function of the shear rate along the various slip systems. The shear rates depend on the critical resolved shear stress, which evolve during the deformation (hardening). The constitutive models for the shear rates are either phenomenological or physics based. Here, a physics-based approach developed and implemented together with Jaime Marian and David Cereceda is presented. This model integrates DFT, atomistic simulations and kMC results and accounts for non-Schmid effects. This leads to a continuum models that is fully parameterized with by results from atomistic simulations and that results in yield stresses that compare very well to experiments, which is quite remarkable. For hardening, one can use a generalized Taylor law, where the parameters can be obtained from discrete dislocation dynamics (DDD).

Fracture may be modeled using the phase field method, where the phase field parameter is a damage parameter. This approach is used to understand fracture in cast Al alloys, whose microstructure in the form of voids has been characterized experimentally, although the crystallographic orientation is unknown. The behavior is shown to be strongly dependent on the geometry of the voids as well as crystal orientation.

Twining can also be modeled using a phase field approach, which allows to simulate twinning evolution and its coupling with dislocation density. Various examples simulated showed microstructures, which strongly resemble experimental images.

Regarding chemomechanics, precipitation is modeled as a spherical inclusion with an eigenstrain (Eshelby problem), and the matrix is considered to have composition dependent elastic constants. Simulations are carried out on the codes DAMASK and OpenPhase and compared to each other. Chemomechanical coupling strongly affects the precipitation kinetics.

Conclusions:
- Recrystallization is a very important problem for steel manufacturing, which would be great to model in combination with crystal plasticity. Possible approaches include (i) cellular automata approach, (ii) KWC approach (e.g. Admal and Marian), (iii) multi-phase field.

References:
[1] J. Allison et al. "Integrated computational materials engineering: a new paradigm for the global materials profession." *JOM* 58.11 (2006): 25-27.

Session 10: Scale Bridging I

Jarek Knap. Accelerating Scale Bridging via Surrogate Modeling
(Joint work with Ting Wang, Kenneth W. Leiter, Petr Plechac)

Overview and motivation:
Multiscale modeling is a systematic approach for constructing high-fidelity material models by combining physics of relevant scales. Scale bridging is however computationally challenging. This is the case, for instance, of the modeling of energetic materials, such as RDX, where the coupling between chemical composition and mechanical deformations is notoriously complicated: a multiscale strategy that combines FEM and DPD-E LAMMPS, without including chemistry is already computationally intractable. Consequently there is a need to reduce the computational cost of the lower scale model, which is here pursued via surrogate models.

Approach and results:
Gaussian process regression is a common approach for surrogate modeling. It provides predictions and uncertainties on non-simulated data. However, it requires inverting a large matrix (the covariance matrix), which can also lead to large computational costs. The approach suggested here is to do adaptive online Gaussian process regression (local surrogate models). This approach highly reduces the computational cost, however global continuity and smoothness is lost. A global approach can be obtained with hierarchical Cholesky decomposition. It is a multiresolution approach, it gives smoothness and continuity, and it significantly reduces the computational cost.

The goal is to apply these strategies to the simulation of energetic materials, incorporating chemistry. Simulations of scaled thermal explosion experiments are currently work in progress.

Conclusions:
- Multiscale modeling can produce high-fidelity models, but can be computationally impractical.
- Surrogate modeling can reduce computational cost. Examples are, Gaussian process regression and hierarchical Cholesky decomposition.

Yuri Mishin. Physcally-informed artificial neural networks for atomistic modeling of materials
(Joint with J. Hickman, G..Purja Pun, V.I. Yamakov)

Overview and motivation:
Atomistic simulations of materials rely on interatomic potential to characterize forces between atoms, and consequently, potentials are the most critical ingredient. Classical potentials express energy and forces as a function of atomic coordinates. The functional form is often motivated by physical/chemical intuition, and parameters are optimized with experimental or DFT data. The resulting potentials can be simple or complex, they are very fast and can be used for multiple purposes (e.g., mechanical behavior, diffusion kinetics, thermodynamic properties). An important drawback though is that they are specific to certain classes of materials (e.g. metals with EAM potentials, covalent with Tersoff or SW), which poses difficulties for simulating mixed materials. In addition, since there are only a few parameters, they tend to be inaccurate, and they cannot be improved systematically. The development is also difficult and slow process.

Over the past 10-15 years a new approach appeared whereby interatomic potentials were developed using machine learning approaches. Here, instead of atomic positions, it considers local structure fingerprints that capture the environment of every atom, and this is mapped to energetics with nonlinear regression strategies that use a wide range of parameters. The resulting models are extremely accurate (DFT level), much faster than DFT, applicable to any type of bonding, and can be improved systematically with more DFT data. However, they are a pure mathematical interpolation with no guidance from physics or chemistry, and, as a result, they can only interpolate, and not extrapolate. In addition, they require massive DFT calculations for their parameterization and they are much slower than traditional interatomic potentials.

Approach and results:
Physically-informed NN (PINN) potentials are proposed, with the goal of getting the best from both worlds. The idea here is to use traditional potentials with parameters that can be adjusted on the fly (every atom in the simulation has its own set of parameters) by means of structural fingerprints and a neural network. Extrapolation and transferability outside of the training domain is then improved.

In order to not focus on a specific class of materials, a more general interatomic potential is considered, namely an (empirical) analytical bond order potential. It includes short-range repulsion, bond order, bond angle dependence and bond screening by neighbors, it has 8 parameters, and it is applicable to metallic and covalent materials.

The result, as demonstrated for instance for Al and Si, is a physically meaningful interatomic potential, even under extrapolation, while having the same accuracy as NN potentials.

Regarding its computational performance, it is about 20 to 170 times slower than traditional potentials, but much faster than DFT. It enables large-scale MD simulations with DFT accuracy, as shown, for instance, for crack nucleation on a grain boundary.

Conclusions:
- ML potential emerge as next-generation models, though they are severely limited by the lack of transferability due to the lack of physics.
- PINN is one example of physics guided ML models.
- The direction of the field goes into the integration of ML and physics.
- Work in process includes multicomponent PINN.

References:
[1] G.P. Purja Pun et al, "Physically informed artificial neural networks for atomistic modeling of materials" *Nature Communications*, 10 (2019) 2339.

Xin Yan. Time-scaling in atomistic and the rate-dependent mechanical behavior of nanostructures
(Joint work with Pradeep Sharma)

Overview and motivation:
Atomistic simulations provide a unique window to look at the microscopic behavior of materials. It has been extremely useful to study 2D materials, alloys, biomaterials or nanoindentation experiments for instance. However, the time scale accessible to molecular dynamic simulations is highly limited and often below the time scales of interest, which often leads to the use of unreasonably high strain rates. Processes such as creep, corrosion or protein folding are thus very hard to model. Many methods have been developed to overcome this difficulty, though the time scale problem is yet unsolved.

Approach and results:
The proposed approach combines four techniques: autonomous Basin Climbing (ABC), nudged elastic band (NEB), kinetic Monte Carlo (kMC) and transition state theory (TST), to study low strain rate phenomena. In particular, ABC is used to identify the energy minima and saddle points, NEB is used for the calculation of the energy barriers, and kMC and TST are used to select the transition pathway and advance time.

This technique is demonstrated over three materials and processes at high and low strain rates, to highlight the strong sensitivity of mechanical deformations to strain rates. The high strain rate simulations can be benchmarked against molecular dynamics simulations, while the approach described above will enable to perform the slow strain rate simulations.
- Nano-pillar compression of Ni. At high strain rates, the nanopillars deform to a barrel shape, as it may also be seen in molecular dynamic simulations. At low strain rates though, the behavior is very different: there is amorphization and surface reconstruction. This behavior is inaccessible to MD simulations, but similar experimental observations have been made.
- Plasticity in amorphous Li-Si nanostructures. This is an important material for energy storage applications and it exhibits large mechanical deformations during loading-unloading. Here, the stress-strain curve exhibits a strong strain rate sensitivity. At low strain rates, the onset of yield is lower, the curve displays more

fluctuations and the residual stresses are larger upon unloading. The underlying deformation mechanisms leading to this behavior can be understood using atomistic visualization. These indicate that when the material has more time to deform (low strain rates), the strain is distributed throughout the sample and many more atoms exhibit non-affine displacements (shear transformation zones).

- Void nucleation in Li-Si alloys for various concentrations of Li. Here again, the behavior is also strongly affected by the strain rate, and voids nucleate at lower strains for slower loading conditions.

Conclusions:
- Time-scale bottleneck in atomistic simulations is still far from completely solved.
- Methods such as those based on ABC can provide new insight for these problems.

References:
[1] X Yan et al, "Time scaling in atomistics and the rate-dependent mechanical behavior of nanostructures", Nano Letters 16 (2016): 3487-3492.
[2] X Yan et al, "Elucidating the atomistic mechanisms underpinning plasticity in Li-Si nanostructures", Physical. Review Materials 1 (2017) 055401.

Session 11: Scale Bridging II

Dan Mordehai. Calculating the activation parameters of thermally activated dislocation mechanisms
(Joint work with Stav Nisany, Tomer Gur-Apter)

Overview and motivation:
Plasticity in defect free materials are controlled by nucleation of dislocations, and this process is here examined using molecular dynamic simulations, with the caveat that the strain rates are always much larger than in experiments.

Approach and results:
Nucleation is a thermally activated process, where the energy barrier depends on temperature and the external force. The point where the energy barrier disappears can be denoted as spontaneous nucleation. The most common method to compute activation barrier for the nucleation event is the nudged elastic band (NEB), although it corresponds to zero temperature. Wei Cai proposed a strategy to compute the entropic contribution, but it is very tedious.

Experimentally, Chris Schuh proposed to extract the cumulative distribution function (cdf) of the strength from nanoindentation experiments, in order to estimate the energy barrier under some simplifying assumptions (due to the complicated stress field). This ideas were further exploited by Dan Gianola, who considered tensile deformation of nanowires, where the stress field is much more simple. Here, approximations were also made on the relation between the energetic and entropic part of the energy barrier. Mordehai brings this a bit further and noted that the activation volume can be extracted form the width of the distribution without assuming any specific form of the energy barrier.

This strategy was applied to MD simulations of faceted Mo nanoparticles. When neglecting the entropy barrier, it was obtained that the energy barrier follows a power law with exponent near 1.5, which appears in many thermally activated processes: STZ in glasses, stretched proteins, twin boundary motion. Entropic contributions were then considered, using the Meyer-Neldel compensation rule model, although the fit was not completely ideal.

This same strategy was also applied to MD simulations of tensile tests in nanowires along the [110] direction. Here nucleation does not always occur at the same point, as it also depends on temperature. Sometimes nucleation occurs at the acute angle of the cross section and others at the obtuse angle. Here, cdf are extracted for each, where higher order CDF approximations are used.

Conclusions:
- A method is proposed to directly extract activation volumes form cdf, coming from simulations or experiments.
- Applied to nucleation-controlled plasticity in nanostructures.
- Nucleation models for multiple sites are currently under development.

References:
[1] D. Chachamovitz and D. Mordehai," The Stress-Dependent Activation Parameters for Dislocation Nucleation in Molybdenum Nanoparticles", *Scientific Reports* 8, 3915 (2018)

Andrea Liu. What we learn from machine learning
(Joint work with S. S. Schoenholz, E. D. Cubuk, R. J. S. Ivancic, F. Landes, T. A. Sharp, D. J. Strickland, S. L. Thomas, G. Biroli, O. Dauchot, D. J. Durian, D. S. Gianola, E. Kaxiras, D. Reichman, J. Rottler, D. J. Srolovitz)

Overview and motivation:
In liquids any particle can rearrange at any time. In crystals, particles in defects like dislocations are far more likely to move than those in the crystalline environment. In glasses, are all particles the same, or are there some particles with a higher propensity to rearrange? This has been an open question for decades. Identifying such particles from the structures and whether the structure can actually tell something about the dynamics has been a 50-year-old standing problem. The complexity of this problem is evident from the fact that structure changes little while dynamics can change a lot. It turns out that this long-standing problem is extremely easy to solve with machine learning.

Approach and results:
The key is that machine learning uses many structural variables to find the linear combination that correlates best with particle rearrangements. This in contrast to traditional methods, which are often based on a single variable. Examples of these quantities are g(r) for various values of r. A hyperplane is then constructed that best separates the rearranging from non-rearranging particles. The distance to that hyperplane defines a variable called the softness. Softness encodes the relation between structure and dynamics. Interestingly, it only depends on particle positions (not the interactions), which is good for experiments. However, the hyperplane is not universal (different for each system), in contrast to dislocations.

A close look to the apparent paradox that in glassy dynamics structure barely changes while dynamics changes a lot (e.g. like WCA and LJ potentials), reveals that softness is different and captures the important structural signatures. Interestingly, relaxation times as a function of softness are almost identical for the two systems (can use same hyperplane).

This idea has been tested for many systems (e.g., atoms, polymers, colloids, grains) with different interactions (e.g. van der Waals, covalent, hard core repulsions), and with different sources of rearrangements (e.g., thermal, mechanical), spanning various orders of magnitude in particle size and stiffness and for all these systems this method to predict rearrangements works. Interestingly, these systems indicate that there is a universality of the yield stress in disordered solids as well as a universality in the response of softness with strain.

Furthermore, the rearrangement probability for a fixed softness is Arrhenius, which implies that there is an energy barrier to rearrange, which depends on softness. However, since there is a distribution of softness in the material, the overall dynamics is not Arrhenius. Interestingly, there is a temperature where the rearrangement probability is independent of softness. This temperature corresponds to the onset of glassy behavior. This seems to work very well for other systems as well.

Applying the above analysis to polycrystals allows visualizing the softness of the various grain boundaries and other defects such as vacancies. In this system as well, the probability of rearranging is also Arrhenius, which allows extracting free energy barriers. In contrast to glassy systems, the curves don't cross and so there is no onset temperature.

Conclusions:
- Softness is a hidden structure parameter that correlates strongly with glassy dynamics.
- The concept of softness works across all spectrums of order/disordered materials.
- There is a barrier height associated to each softness, which indicates a relation between structure (softness) and energy landscape.

References:
[1] E.D. Cubuk et al, "Structure-property relationships from universal signatures of plasticity in disordered solids" *Science*, 358 (2017) 1033.
[2] T.A. Sharp et al, "Machine learning determination of atomic dynamics at grain boundaries", *Proceedings of National Academy of Sciences* (115) 2018: 10943-10947.

Discussions and open challenges

The following challenges and opportunities have been identified based on the various presentations and ensuing discussions.

Calculation of the exchange-correlation energy functional in density functional theory.
The exchange-correlation potential accounts for all quantum mechanical interactions in DFT calculations. Although it is a universal function, i.e. material independent, it is presently unknown, and it therefore has to be modeled. This implies that strongly correlated systems cannot be modeled accurately. The calculation of this exchange-correlation energy

functional represents the Holy Grail in quantum mechanics. Important advances on this front haven been shown, for instance, by Vikram Gavini in his talk.

Non-Schmid effects and non-associated flow

As noted by Cottrell and emphasized in various talks during the workshop (see talks by John Bassani, David Rodney, Jaime Marian or Martin Diehl), associated flow has for too long been taken as the standard plasticity formulation, despite it being more of an exception rather than the rule. Fundamental advances in the microscopic understanding of non-associative flow rules have been achieved, for instance, by David Rodney, although many questions remain. Deviations of the dislocation pathway with respect to the glide plane are strongly material dependent, and it is still unclear what controls the magnitude of these deviations. In addition, most of the current understanding is based on screw dislocations, while fewer studies exist for mixed dislocations. At the macroscopic scale, two additional challenges have been identified. One relates the development of good homogenization methods for non self-adjoint problems, like the equations for non-associated flow; and the second one refers to numerical schemes that can actually resolve these effects and easily get convergence. Finally, it was also questioned whether non-normality flow rule could result as a consequence of the non-convex energy for grain boundaries and their associated mode switching.

The time scale challenge in multiscale material modeling

A recurrent theme in the workshop was the need to have modeling and simulation capabilities that simultaneously have atomistic spatial resolution and can reach diffusive time scales. Such a capability is important for the understanding of phenomena such as defect interaction, lithiation, corrosion or protein folding. Various strategies to deal with this challenge have been presented, including diffusive molecular dynamics (see Michael Ortiz's talk), concurrent atomistic-continuum method (see David McDowell's talk), phase field crystal (see Katsuyo Thornton) and methods based on autonomous basin climbing (see Xin Yan's talk). However, this challenge is far from being solved due to the lack of a comprehensive non-equilibrium statistical mechanics theory. Present approaches are currently problem specific and it is believed that a unified coarse-graining theory, although highly desired, is far from reach.

Symmetry and symmetry breaking

Many materials have underlying symmetries. The classical example is that of crystalline lattice, which is based on translational periodicity. However, a much more general description of material symmetries, which includes translations, rotations, and their combination was formalized with the theory of objective structures. Computational tools that can leverage these symmetries in their simulation (see Amartya Benerjee's talk) are opening the door to analyze and discover new material properties. Another interesting and related topic discussed during the workshop is that of symmetry breaking, which can lead to emergent flexoelectric and piezoelectric behavior (see Pradeep Sharma's talk).

Fluctuations at the nanoscale

Fluctuations are often neglected in the description of materials, as they tend to be insignificant at larger scales. However, they become extremely important at the nanoscale. For instance, thermal fluctuations can strongly impact the mechanical behavior (see Andrej's Kosmrlj talk), and they encode the signature of thermally activated processes (see Dan Mordehai's talk). Furthermore, fluctuations provide a computational microscope to get

insight into non-equilibrium phenomena such as interface motion (see Yashashree Kulkarni's talk).

Defect structure and evolution. An integrated theoretical-experimental approach
Multiple talks in this workshop have been devoted to the understanding of defect structure, interaction and evolution, via theoretical/computational techniques (e.g., Mauricio Ponga, David Rodney, David McDowell, Jaime Marian, Anter El-Azab, Yashashree Kulkarni, Nikhil Admal, Brandon Runnels, Garritt Tucker, Timothy Rupert, Katsuyo Thornton, Dan Mordehai) and experimental approaches (e.g., Jun Lou, Mitra Taheri). Many open questions still remain though, including, without being comprehensive, dislocation and point defect interaction, absorption at grain boundaries, grain boundary structure and evolution or dislocation defect drag. Presentations and discussions all converged to the need of integrated theoretical and experimental efforts to tackle these questions, to leverage the complexity/simplifications of real/numerical experiments and the spatial and temporal resolution of the various approaches.

Novel characterization tools in both experiments and simulations
Advances in high-resolution experimental techniques in space, time and energy, as well as increased computational resources are enabling a very detailed visualization of the materials' microstructure and evolution. Yet, extracting a mechanistic understanding from these massive amounts of data, either experimental or computational, require the development of characterization tools that can systematically identify the important degrees of freedom that correlate with a given behavior as well as quantify the various deformation mechanisms that may be simultaneously competing. Advances in this regard were discussed for instance by Garrit Tucker, who introduced shape moment descriptors to characterize the atomic environment in grain boundaries, or by Mitra Taheri, which utilizes machine learning to identify defects from very noisy data.

At the nexus between physics and machine learning
Machine learning has emerged as a very powerful and highly accurate tool for data interpolation, with applications to multiscale modeling (see Jaroslaw Knap and Yuri Mishin's talk) and classification (see Mitra Taheri and Andrea Liu's talk). Although it is often seen as "magic" black box, it actually still requires a great amount of intuition (which data to use for training and validation set, which properties correlate with each other, etc.), but the outcome tends to be much better than with traditional approaches. However, machine learning tends to perform extremely poorly under extrapolation due to the absence of physics in its formulation. Strategies for integrating physics and machine learning are an important challenge. A great example of such integration can be found in the talk of Yuri Mishin, but many opportunities remain at this intersection.

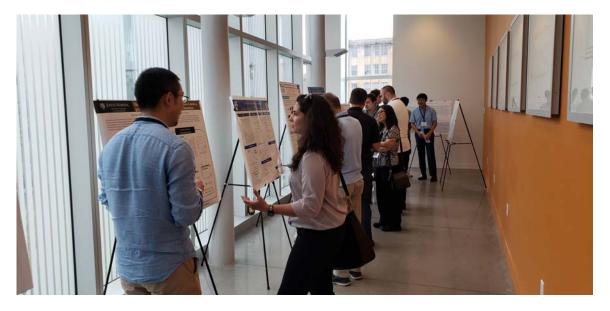*Plasticity in crystalline and amorphous media*
The understanding of plastic behavior in amorphous media has been proven to be highly challenging. In contrast to crystalline materials, where dislocations can be clearly identified as carriers of the plastic behavior, the identification of structural signatures in amorphous materials that correlate with the dynamics has been a 50-year-old challenge. Only recently (see talk by Andrea Liu), softness was identified thanks to machine learning as the sought after structural measure. It has also led to the identification of various universal relations greatly advancing the understanding of amorphous media. Interestingly, the concept of softness applies to a very wide range of materials, including also ordered media. A natural

question therefore rises as whether this could provide a new way of looking at plasticity in crystals and grain boundary phenomena.

Poster presentations

In addition to the oral presentations previously reviewed, a total of 20 posters were presented during the workshop. The authors, affiliations and poster titles are listed below in alphabetical order.

- Lu An, Villanova University
  Characterization of free-standing films and its applications

- Mohamed El Hedi Bahri, Princeton University
  Influence of thermal fluctuations on the elastic moduli of 2D materials

- Bryan Chem, University of Pennsylvania
  Ultra-broadband resonant metamaterial for enhanced wave attenuation

- Shuvrangsu Das, University of Pennsylvania
  Effects of brine inclusions and crystallographic anisotropy on the rheological response of sea ice

- Kshiteej Deshmukh, Carnegie Mellon University
  Bond energies of molecules using strictly-correlated-electron (SCE) limit of Density-Functional-Theory

- Martin Diehl, Max-Plank Institute for Iron Research
  Beyond crystal plasticity-multiphysics tools for integrated computational materials engineering

- Ahmed Ghareeb, University of Illinois at Urbana-Champaign
  An adaptive quasi-continuum approach for modeling fracture in nonlinear networks: Application to polymeric materials

- Yejun Gu, Johns Hopkings University
  The effect of hydrogen on the plastic deformation of metals as predicted from discrete dislocation dynamic simulations

- James Hickman, NIST
  Development of physically informed neural network (PINN) potentials with applications to silicon and germanium systems

- Shenglin Huang, University of Pennsylvania
  Discovery of size-dependent continuum diffusive models via fluctuation-dissipation relations

- Aakash Kumar, University of Pennsylvania
  Diffusion at the Ni/alpha-Al_2O_3 interfaces using reactive molecular dynamics

- Sergio Lucarini, IMDEA Materials
  Efficient algorithms for grain microstructure evolution

- Siddhartha Sarkar, Princeton University
  Buckling of thermalized cylindrical shells.

- Jaspreet Singh, University of Pennsylvania
  Cnoidal wave propagation in an elastic metamaterial
  Allosteric interactions in a birod model of DNA

- Shoham Sen, Carnegie Mellon University
  Recursive Projection Method as a means to improve convergence in Density Functional Calculations

- Chuanpeng Sun, University of Pennsylvania
  Stick-slip kinetics in a bistable bar immersed in a heat bath

- Erik Tamsen, Technische Universitat Dresden
  A fully consistent micro-macro transition approach for dynamics at finite strains

- Haoran Wang, Duke University
  Achieving high-fidelity molecular dynamics simulations by stochastic reduced order modeling

- Ting Wang, Army Research Laboratory
  Accelerated scale bridging with sparsely approximated Gaussian learning

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