

Crystal plasticity analysis of scale dependent mechanical properties of ferrite/cementite fine lamellar structure in pearlite steel

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Pearlite steel is one of the most important metallic materials in industry due to strong yet ductile property. The microstructure has lamellae configuration in which fine layers of ferrite and cementite are piled up alternately in a sub-micron intervals. The major factors for excellent property of pearlite are considered that strengthening of ductile ferrite lamellae by size effect [1] and plastic deformation of brittle cementite lamellae [2]. Recently, we studied these mechanisms and showed that plastic deformation of cementite lamellae was stabilized when yield stress and strain hardening rate of ferrite lamellae were increased [3]. In this conference, we will show the change of mechanical properties of ferrite lamella in pearlite quantitatively by a strain gradient crystal plasticity analysis.

As a simplified pearlite model, we employ three-laminated structures where a ferrite lamella is sandwiched by cementite lamellae. The properties of tensile deformations and shear deformation of the model are studied. Thickness of each lamella is from 100 to 500 nm. Crystal orientations of the ferrite and cementite are defined based on Bagaryatsky model [4]. A crystal plasticity finite element method for body-centered cubic crystal structures is used. We assume the Schmid's law for slip activation and the slip systems of ferrite lamellae are $\{110\}\langle 111\rangle$ and $\{112\}\langle 111\rangle$ while plastic deformation of the cementite lamellae is not considered. The critical resolved shear stress of a slip system is given by the lattice friction, contribution from the accumulated dislocations and lamellar wall. Density increment of the statistically stored dislocations is evaluated by Kocks model and density of the geometrically necessary dislocations is evaluated by spatial gradients of plastic shear strain. The mean free path of moving dislocations is given by a function of the accumulated dislocation as well as the layer thickness. Obtained results of macroscopic stress-strain relation of the ferrite phase show increases of yield stress and work hardening rate with the reduction of interlamellar spacing.

This research was supported by Japan Science and Technology Agency (JST) under Collaborative Research Based on Industrial Demand "Heterogeneous Structure Control: Towards Innovative Development of Metallic Structural Materials".

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Grain Growth in Porous Oxides: Diffuse Interface Modeling and Experiments

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We present a 3D phase field model for investigating the grain growth process in ceramics. The grain growth process in ceramics is complicated by the interaction between the pores and the grain boundaries. As such, in addition to grain boundary migration, the model takes into consideration pore migration via surface diffusion and hence pore coalescence. Therefore, the model is able to fully capture the microstructure evolution in porous ceramics. All model parameters are obtained from material properties.

Application of the model to uranium dioxide shows that the grain growth in this material is sensitive to the level of porosity. The effects of porosity, temperature, mobilities, and initial microstructure on the grain growth process were investigated. Furthermore, the model captures the pore breakaway phenomenon which takes place due to the difference between the pore mobility and the grain boundary mobility as observed experimentally. The model results agree well with grain growth experiments. This research was performed as a part of the Energy Frontier Research Center, Center for Materials Science of Nuclear Fuel funded by the U.S. Department of Energy, Office of Basic Energy Sciences.

Through-process Modeling for Alloy Design and Process Optimization for Cold Spray Processing

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Military aircraft that require high maneuverability, durability, ballistic protection, reparability, and energy efficiency need structural alloys with low density, high toughness, and high strength. The cold spray process, a dynamic powder consolidation technique, produces materials that meet these needs. The primary focus of this effort is to develop a through-process model to be utilized as a predictive tool to design optimum materials and processing parameters for the cold spray process. The four stages in the through-process model are powder production, powder preparation, cold spray processing, and post-processing. Extensive computational thermodynamic and kinetic models are employed for the first two stages to aid in novel material design. Finite element analyses using Johnson-Cook method are used in modeling the third stage. Model predictions are compared with experimental microstructure, microchemistry, and mechanical properties.

Experimental Verification of Through-Process Modeling of Cold Spray Al Alloys

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The cold spray process is a cost effective process for repairing damaged parts or creating structural bulk materials for military aircraft that require high maneuverability, durability, ballistic protection, and energy efficiency. A high strength, high toughness, light weight alloy is needed for this application. Conventional aluminum powders are currently being used in this process. However, there is a need for a tailored alloy that would optimize the properties of the deposited materials. A through-process model that includes powder production, powder pre-processing, the cold spray process, and post-processing would benefit the current trial and error cold spray process immensely and would aid in the search for an optimal cold sprayable alloy. Thermodynamic and kinetic models are utilized to create the powder production and pre-processing stages. These models can identify the optimum microstructure and microchemistry of the material and any pre-processing steps required. The particle impact model predicts the deformation of powder particles during impact. Current work focuses on the characterization of the microstructural evolution to verify and enhance the powder production and pre-processing models as well as the particle impact model. Particle, grain size and microstructural morphology for powders and corresponding cold sprayed materials are determined through optical and scanning electron microscopy. X-ray diffraction along with scanning and transmission electron microscopy are used to identify the phases present and precipitate morphology. Finally, mechanical property testing will be correlated to the amount of deformation predicted by the particle impact model.

Experimental investigation of the plastic behavior of halite single-crystals at room temperature and 400°C: In-situ approach

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Halite deforms plastically or creeps by several mechanisms: intragranular dislocation glide, grain boundary sliding, pressure solution, ... Among those, the first one, also called crystal plasticity (CP), is a key mechanism at low or moderate strain rates and at room temperature up to high temperatures. Natural rock salt is a crystalline material, consisting of almost pure NaCl which is a ionic crystal, with cubic symmetries. Dislocation glide has been observed to take place on three families of slip planes, respectively dodecahedral $\{011\}$, octahedral $\{111\}$ and cubic $\{001\}$, along the same family of glide directions, $\langle 011 \rangle$. The activation of a given system depends on how at a given stage, its critical shear stress compares with the resolved shear stress which may be estimated, given the crystal orientation and the loading mode. The critical shear stress is temperature, history and strain rate dependent. Despite numerous experimental studies, the conditions for the activation of slip systems, i.e. the critical shear stresses and their evolutions (strain hardening) are not well known which has motivated our study of the crystal plasticity of NaCl single crystals deformed in uniaxial compression at different temperatures and strain rates, using several initial crystal orientations. The originality of our approach is to use the Digital Image Correlation (DIC) technique and to observe two faces of our samples which are high purity halite single crystals which are oriented and cut. The DIC method allows to compute the strain field and to evaluate quantitatively the heterogeneity of the local deformation which can be related to local mechanisms such as intracrystalline slip. Compression experiments are performed using both a uniaxial press installed inside a SEM for microscopic tests and a standard uniaxial press equipped with a 10 kN load cell for macroscopic tests. Parallelepiped samples with axes oriented parallel to $[001]$ (sample M00), 45° to $[001]$ in (010) (sample M45) and 30° to $[001]$ in (011) (sample M30) have been prepared. Tests have been performed at room temperature and at 400°C, the strain rate, deduced from the machine constant displacement velocity ranges between $2.4 \times 10^{-6} \text{ s}^{-1}$ and $2.4 \times 10^{-5} \text{ s}^{-1}$, the and strains of about 5% are reached. At room temperature, the rheological behavior is characterized by an elastic deformation followed by plastic flow with strain hardening. The DIC technique indicates that, for crystals M00 and M45, plasticity is happening by slip on two conjugate dodecahedral systems, whereas for crystals M30 slip occurs on one cubic slip system. The computed critical resolved shear stresses τ_c are $\sim 7.5 \text{ MPa}$ and 24 MPa for dodecahedral and cubic systems, respectively. The plastic flow is directly dependent on the number of active systems. The strain hardening is linear for the dodecahedral systems and follows a power law for the cubic system. At high temperature a plastic flow takes place with very little hardening. The DIC technique indicates that slip occurs on the systems which present the highest Schmid factor, i.e. dodecahedral, octahedral and cubic systems for crystals M00, M45 and M30, respectively. The critical resolved shear stresses of these 3 different systems have almost the same value.

Results are interpreted and analyzed with the help of CP-FEM simulations.

Solute segregation and dislocation mobility in binary alloys from dynamical variational Gaussian calculations

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Segregation and precipitation of solute atoms at defects and interfaces are common phenomena in alloys, but are difficult to model atomistically as they occur on timescales that far exceed those accessible with standard molecular dynamics. We present a dynamical version of the variational Gaussian method [1] for binary alloys based on the recently proposed Diffusive Molecular Dynamics approach developed to simulate kinetics of vacancy diffusion in crystalline structures at the atomic level [2]. In this approach, a phonon-free description of solids is coupled with statistical averaging over various configurations, from which free energies can be efficiently computed.

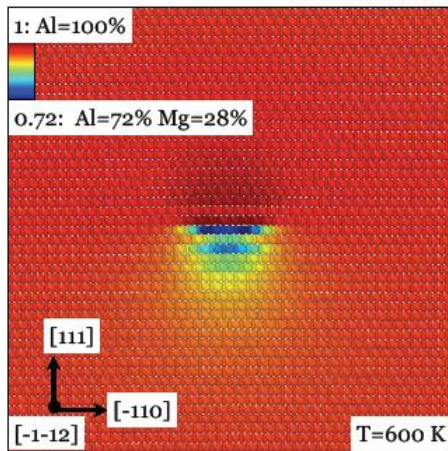


Figure 1: Occupation probability field of Al-Mg crystal (5% Mg) with split partial dislocations.

Atomic positions are represented by Gaussian density fields, whose amplitude is interpreted as an occupation probability that indicates the relative local concentration of each atomic species. Interactions arise from a “thermalized” embedded atom (EAM) potential, and the free energy of the alloy is minimized by optimizing atomic positions and vibrational amplitudes coupled with relaxational dynamics of the concentration fields.

Using this technique, we compute the concentration profile of solute atoms near vacancies, dislocations, and stacking faults for a wide range of solute concentrations and temperatures. Figure 1 shows an example of solute magnesium atoms segregation around a

split edge dislocation in fcc aluminum, where the concentration of magnesium is enhanced in the region under tensile stress. At lower temperatures, ordered intermetallic phases appear, whose symmetry is sensitive to the details of the chosen EAM potential. We then “reverse coarse grain” and construct atomistic realizations of the solute atmosphere around edge dislocations, from which we predict the depinning stress for dislocation glide with molecular statics.

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Stability of a quadruple node in the interfacial network in 3D

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In his 1951 paper Herring presented a concise equation for the mechanical equilibrium of a triple junction (TJ) line formed by three intersecting interfaces [1]. Whereas Herring's original treatment of TJ was confined to two dimensions, here we examine mechanical equilibrium of a quadruple node (QN) in a general three-dimensional interfacial network. The QN is a fundamental unit element of the grain boundary (GB) network in which four grains intersect (see figure). Although topology of a QN is simple, its geometry in a grain boundary network formed by crystal grains is rather complex: even discounting the microscopic variables, it takes 17 macroscopic (geometric) degrees of freedom to uniquely characterize grain mis-orientations and interface plane inclinations associated with a single 4-node [2].

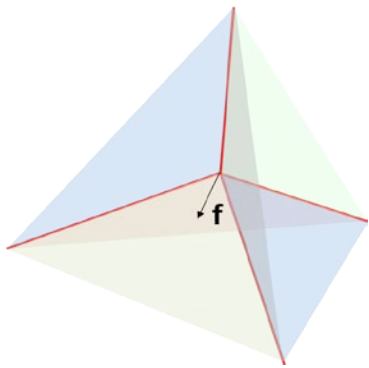


Figure: 4-node is a junction of four grains, six grain boundary interfaces and four triple lines.

High dimensionality of the phase space can give rise to complex anisotropies associated with the QNs. Here we examine the thermodynamic driving force acting on a QN and derive equations defining its mechanical equilibrium in an arbitrary interfacial network. We discuss how the newly derived equilibrium conditions differ from the two-dimensional TJ equilibrium conditions of Herring. Using a selected set of QN geometries as test cases, we demonstrate how interface energy anisotropy can drive GB network evolution to instances where some of the QN become partially or completely locked in space.

Implications of such locking for statistical properties and stability of GB networks and methods for computational modeling of such effects will be discussed.

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Phase transitions in metallic grain boundaries

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Recent experimental measurements of Ag impurity diffusion in the S5(310) grain boundary (GB) in Cu revealed an unusual non-Arrhenius behavior suggestive of a possible structural transformation Divinski et al., [Phys. Rev. B 85, 144104 (2012)]. On the other hand, atomistic computer simulations have recently discovered phase transformations in high-angle GBs in metals Frolov et al., [Nat. Commun. 4, 1899 (2013)]. We present atomistic simulations of Ag diffusion and segregation in two different structural phases of the Cu S5(210) GB which transform to each other with temperature. The obtained excellent agreement with the experimental data validates the hypothesis that the unusual diffusion behavior seen in the experiment was caused by a phase transformation. Together, the simulations and experiment provide the first convincing evidence for the existence of structural phase transformations in high-angle metallic GBs and demonstrate the possibility of their detection by GB diffusion measurements and atomistic simulations.

Molecular Origins of the Mechanical Behavior of Hybrid Molecular Materials

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Hybrid organosilicate molecular films processed from small organosilane precursors exhibit unique electro-optical properties while maintaining excellent thermal stability. They can be inexpensively processed using sol-gel or chemical vapor deposition and have application in emerging nanoscience and energy technologies. A fundamental challenge for their integration and application, however, remains their inherently mechanically fragile nature that derives from the oxide component of the hybrid glass network and the presence of terminal hydroxyl and organic groups that reduce network connectivity.

We use molecular dynamics (MD) based simulated annealing to create highly accurate molecular models of hybrid glasses [1,2]. We can create large, distortion-free models with well-controlled network connectivity from any number of existing and potential molecular precursors. Accurate nanoporous models can be generated by employing a strategy that mimics the synthetic porogen burnout approach. Elastic properties are simulated through MD and fracture energy can be accurately simulated using our new minimum-cut fracture model that accurately predicts the 3-D cohesive fracture path at the atomic scale (**Fig. 1**).

A complementary method that we are developing to characterize and model hyper-connectivity is based on a mean-field approach. Characterizing the network connectivity of hybrid glasses is typically very complex because of the absence of long-range order in the glass network and the highly complicated molecular structure consisting of both homo-nuclear (i.e., Si-Si and C-C) and hetero-nuclear bonds (i.e., Si-C, Si-O), and monovalent bonds (i.e., Si-H and C-H). The mean field approach we have been implementing enables us to characterize hyper-connectivity by simply counting the average number of network bonds, $\langle r \rangle$, in the molecular structure without relying fully on a complex analysis. We have already demonstrated that $\langle r \rangle$ is correlated very well with both the elastic modulus and cohesive fracture properties of hydrogenated

amorphous SiC hybrid films with stoichiometric compositions (Si/C~1) (**Fig. 2**).

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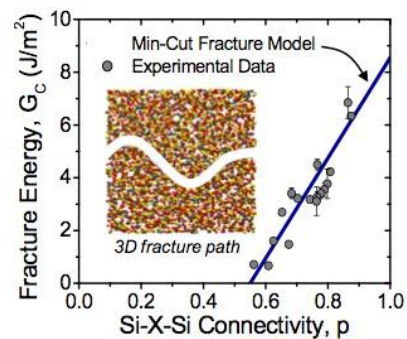


Figure 1: Predicted and experimental scaling of the fracture energy of hybrid organosilicate films as a function of with Si-X-Si network connectivity.

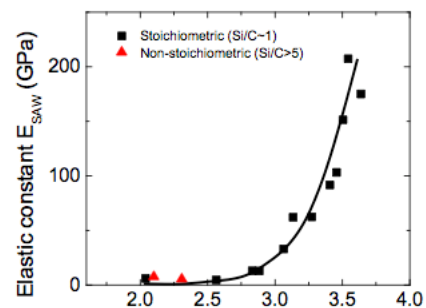


Figure 2: Hybrid elastic constant as a function of the average network bonds $\langle r \rangle$ calculated using mean field theory

Influence of Interfaces on the Intrinsic Growth Stresses in Nanoscale Metallic Thin Films

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Nanocrystalline thin films are structures with large surface area-to-volume ratios which enable interfacial and grain boundary energies to play a dominant role in the stability and properties of the thin films. Using a laser interferometer technique, the intrinsic growth stresses have been measured for both multilayered and alloy thin films. For the multilayers, which include Ti/Nb and Ti/W, changes in phase have been observed in individual layers for Ti/Nb but not equivalent layer thicknesses for Ti/W. These phase transformations have been correlated to the thermodynamic interfacial energy reduction and stress behavior of the film. For the alloy films, which include Ni-Cu and Fe-Pt, the stress states have been shown to be tunable with which solute element segregates to the grain boundaries, as measured by atom probe tomography. The phase and stress behavior of both classes of films have been rationalized through the use of a hybrid Molecular Dynamics and Monte Carlo simulation that captures the segregation and mixing behavior at the interfaces and/or grain boundaries which are compared to the experimental findings.

Microscale plastic strain distribution in slip dominated deformation of Mg alloys

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Though mean-field crystal plasticity models have played an important role in advancing our understanding of the plastic anisotropy of polycrystalline Mg alloys, these mean field predictions can never hope to adequately capture the significant inter- and intragranular plastic strain heterogeneity that has been reported in Mg alloys (see e.g. [1]). While such local strain heterogeneity may be a consequence of twinning, it can also be found in situations where plasticity is slip dominated. In this work the local plastic strain distribution has been evaluated via a micromechanical approach involving coupled EBSD and digital image correlation (DIC) measurements [1-2]. These experiments have been performed on a Mg-RE alloy deformed in tension parallel to the prior rolling direction under conditions favoring slip, rather than twinning. These experiments reveal that the local equivalent strain can be up to 5-6 times the macroscopic tensile strain. This strain localization is seen to not correlate in a simple way to crystallographic orientation. Instead, a strong correlation between strain amplitude and distance to nearest grain boundary is observed, this highlighting the importance of the mechanical interactions between adjacent grains having different orientations. In an attempt to better understand the origins of the observed plastic strain distribution full-field crystal plasticity simulations using a spectral based viscoplastic model have been performed. The simulated strain field exhibits similar features compared to the experimental ones when a sufficiently large anisotropy between the flow stress on basal and non-basal slip systems is adopted.

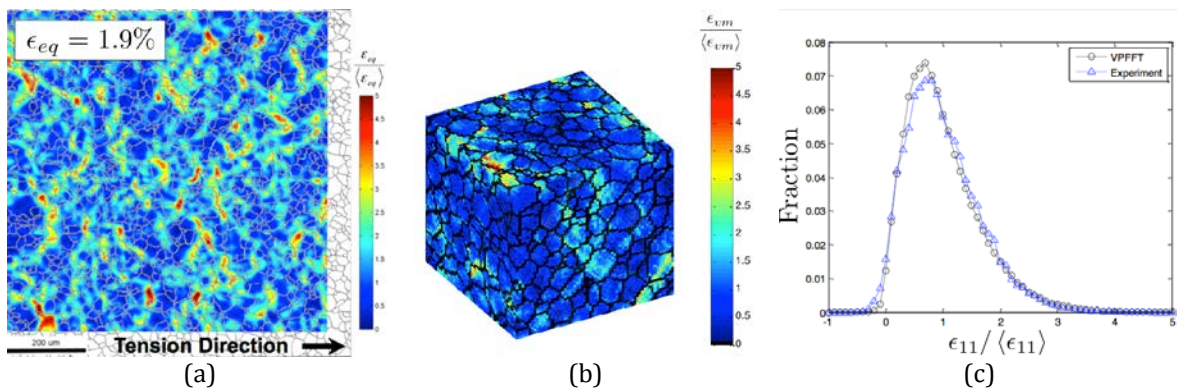


Figure 1: a) Experimental plastic strain distribution b) simulated plastic strain distribution using spectral method crystal plasticity model c) comparison of the histogram of plastic strains from experiment and simulation.

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Formation and structure of first water monolayer on TiO₂ rutile surface

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Mechanism of first water monolayer formation on TiO₂ (110) rutile surface has been described using a combination of ab initio and kinetic Monte Carlo (KMC) calculations in close collaboration with experiment. The ab initio calculations provided us with reliable information about the energetics of different molecular configurations, diffusion barriers and their dependence on coverage. This information was used in KMC to build a dynamic model of water layer formation. Water is found to partially dissociate on defect free TiO₂(110) at low coverage. Repulsive interaction between dissociated species and clustering of water around them, leading to a creation of hydrogen bonded net, are responsible for the observed dynamics and pattern formation during the layer formation. Interaction with experiment was crucial for this project as it proved theory with necessary knowledge about the composition of water layer at different coverages.

The Origin of Oxygen Strengthening Effect in α -Titanium

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Very small concentrations of O interstitials in hexagonal-close-packed (hcp) Ti can induce significant strengthening, but with the detrimental effect of lowering toughness. To provide new insights into this long-studied problem, we performed first-principles calculations to analyze the interactions between interstitial atoms and screw dislocation cores in hcp-Ti. Both indirect studies of generalized stacking fault energy and direct investigation of dislocation cores show that oxygen and other large interstitials are strongly repelled by the screw dislocation core. This repulsion forces these interstitials to move from their original interstitial site during dislocation slip. The origin of this repulsion is the structure of hcp lattice: in the hcp-Ti screw dislocation core, the interstitial volume is largely reduced. The results are shown to be in good agreement with recent experimental observations derived from in-situ small-scale mechanical tests of Ti samples with different oxygen concentrations and scanning transmission electron microscope (STEM) characterizations of their dislocation core structures.

WC-Co microstructure degradation study in rotary-percussive drilling

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Keywords: WC-Co, microstructure, wear, finite-elements, rotary-percussive drilling

This study investigates wear of WC-Co drill bit button during rotary-percussive drilling of hard rock at high pressure and high temperature conditions. Focus of the current study is on micro-mechanisms of WC-Co material degradation. In order to reproduce deformation and failure on such scale 2D finite-element models were generated based on a scanning electron microscopy (SEM) images of a real microstructures. The average size of generated models are 20x20 micro-meters, with 40 to 100 WC grains embedded in the Cobalt matrix (with volume fraction 5 to 20%). Plastic behavior were considered for both WC and Co. Two types of interfaces are modeled by means of cohesive zone elements: WC-WC and Co-WC. The loading is applied by indenter of different sharpness, which represents the rock contact surface micro-asperity.

Degradation mechanisms of a drill bit buttons from real drilling application and from button-rock impact tests have been studied by the use of scanning electron microscopy (SEM) and energy dispersive spectroscopy (EDS). Three main typical mechanisms are distinguished: (a) Co binder extrusion, (b) WC grains decohesion, (c) WC grains fracturing. Button-rock interaction conditions (contact morphology, contact temperature, ranges and types of interaction forces) were investigated using non-contact interferometry (rock and drill bit button surface roughnesses) and finite-element simulations (macroscopic button-rock impact, coupled thermo-mechanical microstructure behavior).

Dominating degradation mechanisms at different sets of interaction conditions (mentioned above) accounting for the rock formation response, microstructure composition, grain size and morphology distributions were investigated through series of numerical computations.

Proposed approach could be used to: (a) suggest improvements for material manufacturing process, (b) provide engineers with a numerical tool capable of wear assessment at a macro-scale level, which can be used for optimizing drilling process and drill bit design.

Gas Adsorption in Microporous Materials: Ab Initio Based Grand Canonical Monte Carlo Simulations

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A multiscale approach based on ab initio and grand canonical Monte Carlo (GCMC) simulations is used to report the H₂, N₂, and CH₄ gas uptake behaviors of two microporous materials, i.e. zeolitic imidazolate frameworks (ZIF)-95 and -100, with exceptionally large and complex colossal cages. The force fields describing the weak interactions between the gas molecules and ZIFs in GCMC simulations are based on ab-initio MP2 level of theory aimed at accurately describing the London dispersions. We report the total and excess gas uptakes up to 100 bar at 77 and 300 K. Our results unravel the interplay between the uptake amount, pore volume, guest molecule size, temperature, chlorine functional group, and isosteric heat of adsorption in ZIFs. We found that while the uptake capacity of ZIF-100 outperforms ZIF-95 for small molecules (H₂), ZIF-95 offers a superior adsorption capacity for large molecules (CH₄). Moderately sized molecules (N₂) exhibit a more complex uptake behavior depending on the temperature. Furthermore, we show that the induced dipole interactions, such as those caused by –Cl functional groups, play a vital role on gas adsorption behaviors. This work provides the first report on the N₂ and CH₄ uptake of ZIF-95 and -100 using ab initio based GCMC simulations. Furthermore, it renders a valid path for a reliable computational-driven synthesis and discovery of numerous functionalized ZIFs - via introduction of ligand binding moieties in the pore spaces of ZIFs - to enhance gas adsorption and separation, and potentially enable size- and shape-selective catalysis.

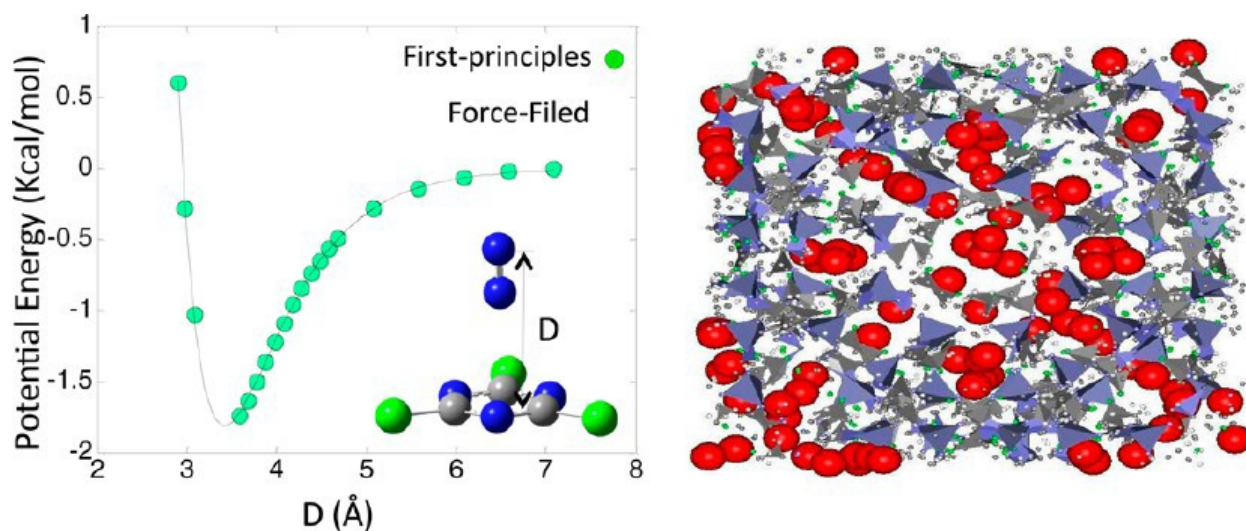


Figure 1. Interaction of N₂ molecules with the ZIF linker (left). A schematic of the porous ZIF structures with adsorbed N₂ molecules in red (right)

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Ultrahigh strength of nanotwinned Ag-Cu dilute alloys by atomistic simulations

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Nanotwinned (nt) materials with a high density of coherent twin boundaries (CTB) often display a high thermal stability, high yield strength, high ductility, and are more resistant to coarsening than their fine-grained counterparts. However, nt-materials are also known to exhibit a maximum in Hall-Petch strengthening behavior, dictated by dislocation nucleation mechanisms. Continuous strengthening beyond this maximum value has remained impossible experimentally. In this work we perform a systematic atomistic study of nt Ag-1%at Cu bicrystals containing CTB in various densities. First, we perform a thermodynamic relaxation at finite temperature using a variance constrained semi grand canonical Monte Carlo algorithm to place Cu atoms in thermodynamically favorable locations, followed by loading uniaxially along several orientations using molecular dynamics simulations. We study the effect on the overall yield strength of CTB spacing, Cu concentration, and temperature, and point to the causes for such marked yield strength increases observed in the experimental tests.

Comparison of dislocation-based model of recovery and cross-correlation based EBSD measurements in single crystals

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Subgrain growth during recovery has been investigated using simulations of two-dimensional discrete dislocation dynamics on a hexagonal lattice having three symmetric slip planes [1]. To account for elevated temperature (i) dislocation climb was allowed and (ii) a Langevin type thermal noise was added to the force acting on the dislocations. The growth exponent and the subgrain structure were examined.

Cross-correlation based analysis of electron backscatter diffraction (EBSD) patterns is often carried out to map plastic strain variations in deformed polycrystalline samples [2]. Firstly, the effects of sample surface preparation methods were investigated including Ar ion polishing and traditional electropolishing treatments. Then the distortion maps of the specimen are computed with the cross-correlation technique. This method is capable of detecting changes of the crystal orientation to higher accuracy, than the commercial software provided for standard EBSD devices that analyze each EBSD pattern individually.

In this work the simulation and experimental results were compared to characterize the evolution of dislocation structures and corresponding distortion fields in highly deformed Cu single crystals during low temperature annealing.

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Prediction of Microstructural Evolution during Sintering Process using Meso-scale Simulation and FIB/SEM Tomography

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Sintering is one of the critical processes deeply related with a degradation phenomenon in solid oxide fuel cells. However, because of the inherent complexities linking with multiple mechanisms, its quantitative understanding is still lacking. In this study, pure Ni, NiO, 8YSZ, NiO-8YSZ composite were sintered at a wide range of heating rates, and their densification behavior was analyzed by applying a master sintering curve concept. Besides, the microstructural details like porosity, grain size, pore size distributions and curvetures of sintered samples were quantitatively measured utilizing three dimensional reconstruction based on FIB-SEM technique. We also present three-dimensional kinetic Monte Carlo simulations based on Q-state Potts model in order to numerically predict the microstructural evolution of the composite system. To simulate a solid-state sintering process, we have incorporated three kinetic mechanisms into the model: Curvature-driven grain growth, pore migration by surface diffusion and densification mediated by vacancy action. The frequencies of each kinetics are determined to represent our experimental results. We show that our computational tool can successfully track the valid sintering pathway and would be used as a useful tool for designing an anode microstructure in solid oxide fuel cell systems.