FIGURE 1: Sliding and delamination of Li_xSi thin film electrodes from the Cu current collector. (A) Atomic structure of the interdiffused Li-Si-Cu interphase between a Li_xSi electrode and a Cu-current collector. (B) Interface sliding facilitated by the formation of well-delineated and weakly bonded Si-Cu and Li-Cu crystalline atomic layers within this interphase structure. (C) Shear stress versus shear strain response demonstrating distinct regions of stress build-up and release leading to interface sliding, and stress accumulation leading to interface delamination.

volume changes during repeated lithiation and delithiation charge cycles lead to colossal cracking of the Si electrode. Recent studies have shown that Si electrodes of small feature sizes, such as nanowires, nanoparticles, porous structures, and thin films, display significantly higher reversible charge capacities and longer cycle life. In fact, a critical feature size of these nanostructured Si electrodes exists, below which fracture would be completely mitigated. It is believed that the improved fracture resistance originates from the ability of the nanoscale structure to accommodate the lithiation-induced strain by plastic deformation, resulting in lower stresses present during volume changes. However, the delamination of crack-free nanostructured Si electrodes from current collectors after a critical number of charge cycles has been widely reported, resulting in the loss of electrical contact and consequent capacity fade. Even though the cracking of Li_xSi thin films can be mitigated through patterning individual Si islands, the uncracked electrode still delaminates from the current collector after a critical number of charge cycles. To date, much is still unknown about the interface bonding the Si electrode and a metal current collector, such as Cu. Studies have suggested that sliding readily occurs along the Si-Cu interface to accommodate the massive volume changes in lithiated-Si during charge cycling. However, understanding the mechanisms of interface sliding and delamination is complicated by significant intermixing of Cu, Si, and Li atoms at the interface between a lithiated-Si film and the Cu substrate.

METHODS & RESULTS

Using first-principle calculations, we recreate model structures of the interdiffused Li-Si-Cu interphase (Fig. 1A) and show that the interdiffusion among Li, Si, and Cu atoms leads to the formation of well-delineated, crystalline Si–Cu and Li–Cu atomic layers at intermediate Li concentrations (Fig. 1B). These atomic layers are weakly bonded in shear, and readily slide to relieve the interfacial stresses during lithiation processes. Ideally, interface sliding between the Si electrode and the Cu current collector will help limit film stresses introduced by the lithiation process. However, sliding between the Si–Cu and Li–Cu atomic layers cannot occur indefinitely. The formation of pinning defects in the form of $LiSi_3$ compounds along the interface can eventually inhibit sliding (Fig. 1C). The consequential buildup of interfacial stresses leads to delamination failure of the Si electrode from the Cu-current collector. Understanding the atomic-scale mechanisms that promote or impede sliding provides the critical first steps toward designing Si-Cu interface structures to mitigate electrode failure.

WHY BLUE WATERS

To our knowledge, detailed analyses of the sliding and delamination processes of lithiated-Si electrodes from the current collector are virtually non-existent due to the computational complexity of such systems. Firstly, the lithiated-Si structures are amorphous. Recreating these structures requires substantial intermixing between Li and Si atoms through a heating and quenching process in *ab initio* molecular dynamics (MD) simulations and density functional theory (DFT) calculations which are computationally expensive. The computational complexity, coupled with a large number of computational runs to elucidate the interface mechanics as a function of lithium concentration, makes this a process that requires the capacity of Blue Waters. The proposed DFT and *ab initio* MD calculations were performed on Vienna *Ab initio* Simulation Package (VASP).

NEXT GENERATION WORK

Our next focus will be on elucidating the deformation and fracture mechanics of the Solid Electrolyte Interphase, which is critical to the performance of high-capacity lithium ion battery electrodes.

PUBLICATIONS AND DATA SETS

Wang, H., and H.B. Chew, Molecular dynamics simulations of plasticity and cracking in lithiated silicon electrodes. *Extreme Mech. Lett.*, (2016), p. 503–513.

Harpale, A., M. Panesi, and H.B. Chew, Plasma-graphene interaction and its effects on nanoscale patterning. *Phys. Rev. B*, 93 (2016), p. 035416.

Wang, H., X. Wang, S. Xia, and H.B. Chew, Brittle-to-ductile transition of lithiated silicon electrodes: Crazing to stable nanopore growth. *Jour. Chem. Phys.*, 143 (2015), p. 104703.

Li, R., and H.B. Chew, Closed and open-ended stacking fault tetrahedra formation along the interfaces of Cu-Al nanolayered metals. *Philos. Mag.*, 95 (2015), p. 2747-2763.

Wang, H., et al., Atomic-scale mechanisms of sliding along an interdiffused Li-Si-Cu interface. *Nano Lett.*, 15 (2015), 1716-1721.

Harpale, A., M. Panesi, and H.B. Chew, Communication: Surface-to-bulk diffusion of isolated versus interacting C atoms in Ni(111) and Cu(111) substrates: A first principle investigation. *Jour. Chem. Phys.*, 142 (2015), p. 061101.

Li, R., and H.B. Chew, Planar-to-wavy transition of Cu/Ag nanolayered metals: A precursor mechanism to twinning. *Philos. Mag.*,95 (2015), p. 1029-1048.

LATTICE QCD ON BLUE WATERS

PI: Robert Sugar[1]
Collaborators: Alexei Bazavov[2], Kate Clark[3], Carleton DeTar[4] Daping Du[5], Robert Edwards[6], Steven Gottlieb[2], Balling Joo[6], Kostas Orginos[7], Thomas Primer[8], David Richards[6], Doug Toussaint[8], and Frank Winter[6]

[1]University of California Santa Barbara
[2]Indiana University
[3]NVIDIA
[4]University of Utah
[5]Syracuse University
[6]Thomas Jefferson National Accelerator Facility
[7]College of William and Mary
[8]University of Arizona

EXECUTIVE SUMMARY

The goal of this project is to develop highly optimized code for the study of quantum chromodynamics (QCD) on Blue Waters to carry out calculations that will have a major impact on high-energy and nuclear physics. We have optimized and used the Chroma code for the simulation of Clover quarks and the MILC code for the simulation of HISQ quarks. Our long-term objectives with highly improved staggered quark (HISQ) are to generate gauge configurations with physical-mass up, down, strange and charm quarks, to use these configurations to calculate fundamental parameters of the standard model of high energy physics, and to perform precise tests of the standard model. The objective of our Clover quark program is to determine the excited mass spectrum of strongly interacting particles (hadrons) within QCD.

INTRODUCTION

The standard model of high energy physics encompasses our current knowledge of the fundamental interactions of nature. The model has successfully explained a wealth of data from accelerator and cosmic ray experiments over the last 40 years. However, it has been difficult to extract many of the most interesting predictions of quantum chromodynamics (QCD), the component of the standard model that describes the strong interactions. The only way to do so, from first principles and with controlled errors, is through large-scale numerical simulations. These simulations are needed to obtain a quantitative understanding of the physical phenomena controlled by the strong interactions, to determine some of the fundamental parameters of the standard model, and to test them. Despite the successes of the standard model, high-

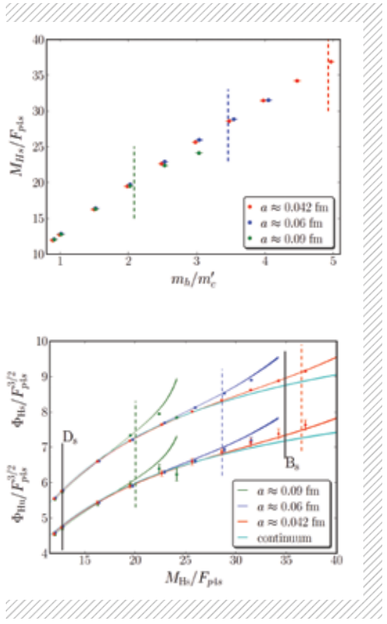

FIGURE 1: Heavy-quark discretization effects in the calculation of the leptonic decay of the B and Bs mesons. The upper panel shows the heavy-strange meson mass M_Hs in units of the quantity Fp4s, as a function of the ratio of the heavy-quark mass, m_h, to the simulation charm-quark mass, m_h/m_c. The lower panel shows the decay constants of a heavy meson made up of a heavy-quark and an up quark, and of a heavy quark and a strange quark, Phi_Hu and Phi_Hs, as a function of M_Hs. We are interested in the extrapolation of M_Hs to M_Bs.

energy and nuclear physicists believe that a more general theory will be required to understand physics at the shortest distances. Thus, QCD simulations play an important role in efforts to obtain a deeper understanding of the fundamental laws of physics.

METHODS & RESULTS

Our objective is to perform calculations of QCD to the precision needed to support large experimental programs in high-energy and nuclear physics. We are using two formulations of lattice quarks. The HISQ formulation is being used to calculate parameters of the standard model, and to perform precise tests on it. In particular, the HISQ formulation is being used to calculate the masses of quarks, which are the fundamental building blocks of strongly interacting matter, and to determine elements of the Cabibo-Kobayashi-Maskawa (CKM) matrix, which are the weak interaction transition couplings between quarks.

Our primary objective with the Clover formulation of lattice quarks is to perform a calculation of the mass spectrum of strongly interacting particles (hadrons). The determination of the excited-state spectrum of hadrons within QCD is a major objective for experiments and is a focus of the $310 million upgrade of Thomas Jefferson National Accelerator Facility. In particular, the GlueX experiment at Jefferson Laboratory will search for "exotic" mesons. These particles are a signature for new states of matter, specifically the presence of gluonic degrees of freedom, predicted by QCD, but thus far not clearly observed. The spectroscopy effort is intended to determine whether the equations of QCD do, in fact, realize the existence of such exotic states of matter. These calculations will be performed before the experiments and, will therefore, provide crucial information about the decay signatures of such exotic states that **will inform and guide the experimental searches**.

Lattice QCD calculations have two steps: First, one generates and saves gauge configurations, which are representative samples of the QCD ground state. Second, the gauge configurations are used to measure a wide range of physical quantities. Generating gauge configurations is the rate-limiting step and requires the most capable computers available. The most computationally expensive component of the second step is to calculate the Green's functions for the propagation of quarks in the gauge configurations. The light quarks used in this calculation also require highly capable computers.

We have made major progress in our efforts to generate gauge configurations and quark propagators using Blue Waters, including the most challenging ensembles undertaken to date. The new HISQ configurations have been used to make the most precise determination to date of the decay properties of some mesons containing strange and charm quarks [1-4]. This work has led to the evaluation of several CKM matrix elements that are important for tests of the standard model; and produced the most precise ratios among up, down, strange, and charm quark masses. The HISQ configurations are also being used in a new, very promising calculation of the decay properties of B and Bs mesons [4]. Important advances have been made in the development of code for the generation of gauge configurations and quark propagators with the Clover formulation [5], and through new approaches for the determination of resonance parameters. **Ground-breaking** results have been obtained for the scattering of K, pi and eta mesons [6-9].

WHY BLUE WATERS

The precision possible with lattice QCD calculations in recent years has reached within a fraction of a percent. Such precision is needed to test the standard model and to obtain a detailed understanding of physical phenomena controlled by the strong interactions. The advent of petascale computers, like Blue Waters, are playing a critical role in these advances.

NEXT GENERATION WORK

The next generation Track-1 systems will allow us to account for the electromagnetic effects and isospin violations in the quark masses and to work at even smaller lattice spacings. These advances will enable us to determine a wide range of quantities at the sub-percent level, making lattice QCD calculations reliable tools in the support of the large experimental programs in high energy and nuclear physics.

PUBLICATIONS AND DATA SETS

Bazavov, A., et al., Determination of |V_{us}| from a lattice-QCD calculation of the K -> pi l nu semileptonic form factor with physical quark masses, *Phys. Rev. Lett.* 112 (2014), 112001 [arXiv:1312.1228].

Bazavov, A., et al., Charmed and light pseudoscalar meson decay constants from four-flavor lattice QCD with physical light quarks, *Phys. Rev.*, D90 (2014) 074509 [arXiv:1407.3772].

Bazavov, A., et al., Gradient Flow Analysis on MILC HISQ Ensembles, *Proceedings of Science (Lattice 2014)* 090 (2014) [arXiv:1411.0068].

Bazavov, A., et al., Charmed and light pseudoscalar meson decay constants from HISQ simulations, *Proceedings of Science (Lattice 2014)* 382 (2014) [arXiv:1411.2667].

Bazavov, A., et al., Symanzik flow on HISQ ensembles, *Proceedings of Science (Lattice 2013)* 269 (2013) [arXiv:1311.1474].

Bazavov, A., et al., Leptonic decay-constant ratio fK/fpi from lattice QCD with physical light quarks. *Phys. Rev. Lett.* 110 (2013),172003 [arXiv:1301.5855].

Bolton, D.R., R. A. Briceno, and D. J. Wilson, Connecting physical resonant amplitudes and lattice QCD, *Phys. Lett. B* 757 (2016), pp. 50-56. [arXiv:1507.07928 [hep-ph]].

Briceno, R.A., et al., The resonant pi gamma -> pi pi amplitude from Quantum Chromodynamics, *Phys. Rev. Lett.* 115 (2015), 24200, [arXiv:1507.06622 [hep-ph]].

Clark, M.A., R.G. Edwards and B. Joo, IPDS '14, Proceedings of the A Framework for Lattice QCD Calculations on GPUs, F.T. Winter, *2014 IEEE 28th International Parallel and Distributed Processing.*

DeTar, C., et al., Charmonium mass splittings at the physical point, *Proceedings of Science (Lattice 2012)* 257 (2012) [arXiv:1211.2253].

Dudek, J.J., R.G. Edwards, C.E. Thomas, and D.J. Wilson. Resonances in coupled pi K - eta K scattering from quantum chromodynamics. *Phys. Rev. Lett.* 113 (2014), 182001, [arXiv:1406.4158 [hep-ph]].

Gamiz, E. et al., K semileptonic form factor with HISQ fermions at the physical point, *Proceedings of Science (Lattice 2013)* 395 (2013) [arXiv:1311.7264].

Gamiz, E. et al., Charmed and strange pseudoscalar meson decay constants from HISQ simulations, *Proceedings of Science (Lattice 2013)* 382 (2013), [arXiv:1312.0149].

Mohler, D., et al., Low lying charmonium states at the physical point, *Proceedings of Science (Lattice 2014)* 085 (2014) [arXiv:1412.1057].

Primer, T., et al., Kaon and D meson semileptonic form factors from lattice QCD, *Proceedings of Science (Lattice 2014)* 374 (2014) [arXiv:1411.1651].

Wilson, D.J., J. J. Dudek, R.G. Edwards, and C.E. Thomas. Resonances in coupled pi K, eta K scattering from lattice QCD, *Phys. Rev.* D91 (2015) 054008, [arXiv:1411.2004 [hep-ph]].

Wilson, D.J., et al., Coupled pi-pi, K K scattering in P-wave and the rho resonance from lattice QCD, *Phys. Rev.* D92 (2015), 094502, [arXiv:1507.02599 [hep-ph]].

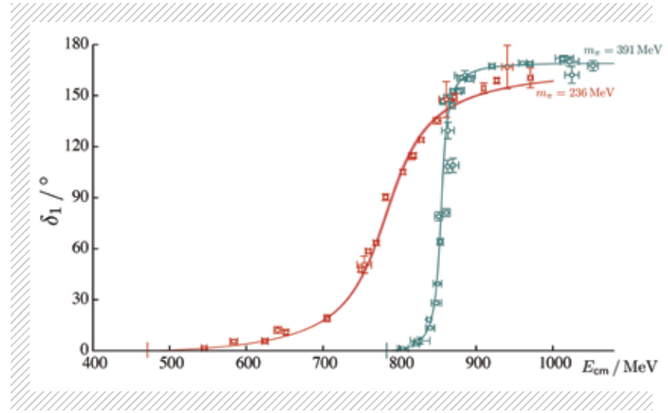

FIGURE 2: Isospin=1, P-wave phase-shift in the pi-pi elastic scattering region (below the Kbar-K threshold). Phase-shift points mapped from finite-volume energies in several volumes and moving frames using the Luscher formalism. Curve shows a Breit-Wigner fit to the energy dependence which shows a clear resonant line-shape. The mass and width of the resonance are in line with expectations for a calculation with m_pi = 391 MeV and m_pi = 236 MeV.