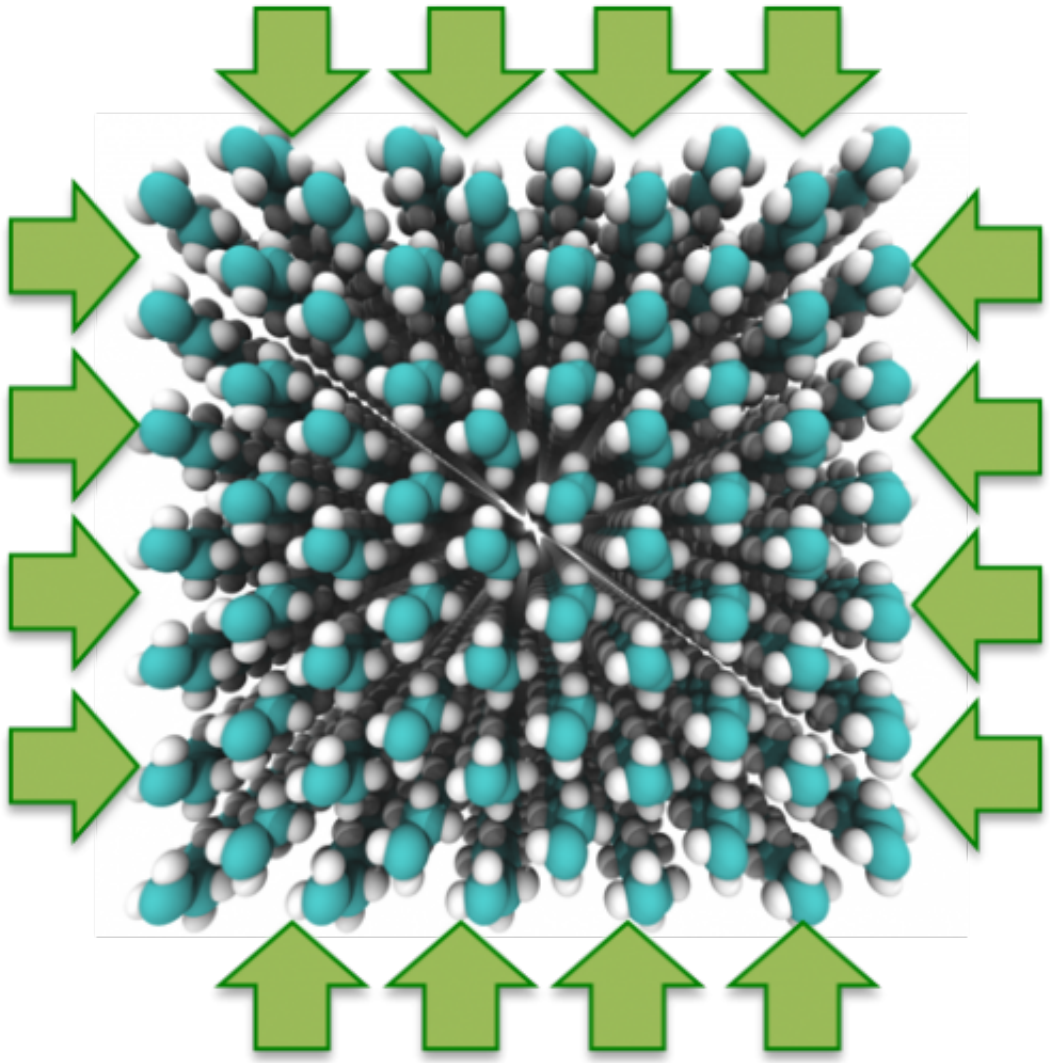
Polymers designed for protection

March 11 2015, by Dr. John H. Beatty



The new AIREBO-M Potentials validated against a pressure-volume isotherm at T=533K for polyethylene crystals. Note the AIREBO-M potentials show nearly perfect agreement with REAXFF calculations and experimental data. However the AIREBO-M potentials are much more computationally efficient than REAXFF calculations, and will allow upscaling of calculations to perform much

larger simulations (Reference 2). Credit: U.S. Army

Today's Soldiers rely on polymers as part of their protective systems. Polymers are molecular chains that can vary from a few linked monomers to millions of chemical units. With highly tunable properties and versatile processing they have become ubiquitous in use. In the defense community polymer fibers are particularly well known, especially polyamide fibers such as Kevlar and Nomex and polyethylene fibers such as Dyneema and Spectra. By combining good ballistic protection with a minimal weight penalty these materials have become commonplace in Soldier protection systems.

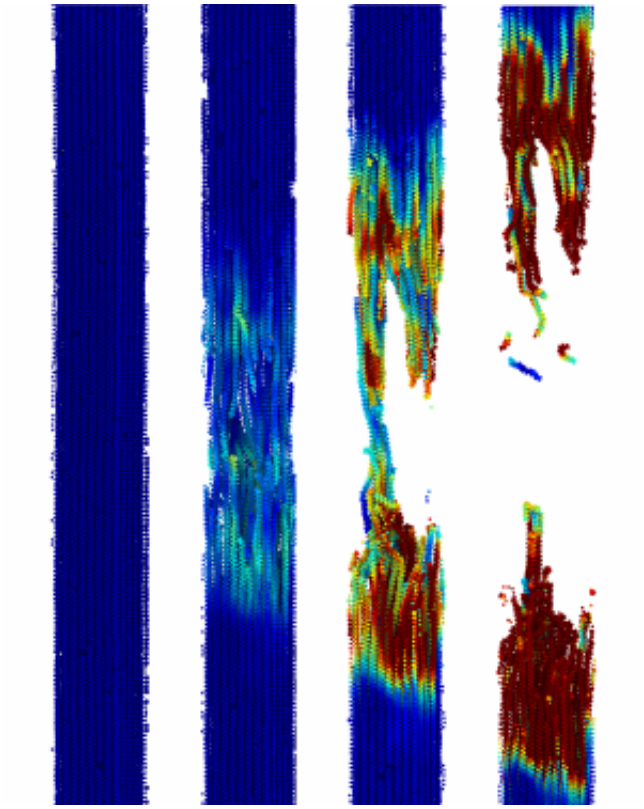
But 20 to 30 years from now, our Soldiers will need protective systems that can stand up against tougher threats that are certain to be developed. Right now, even the most sophisticated material combinations involving polymers cannot match up against the kinds of threats our national intelligence suggests Army Soldiers will face in future conflicts.

The Army Research Laboratory is investigating one possible solution to this problem: designing new polymers for superior protection capabilities by unraveling the complex relationship between polymer chemistry, microstructure and energy absorption.

As the nation's premier laboratory for land forces, ARL is currently undertaking a long-term effort to design new polymer fibers with the extreme ballistic environment in mind from the start. Designing the polymer's molecular chemistry and fiber microstructure to enhance its ballistic behavior is the aim. But it's a complicated process that involves the design and manipulation of these fibers across many length and timescales.

Central to this long-term goal is the need for ARL scientists to create validated models of these polymers at the molecular level and under high-rate loading conditions. Capabilities like this are the reason ARL established the Enterprise for Multiscale Research of Materials.

The ARL Enterprise for Multiscale Research of Materials has recently made breakthroughs that are allowing the team to more accurately model polymers at the molecular level at high strain rates, pressures and temperatures. The full suite of multi-scale modeling currently being developed will ultimately allow researchers to design ultra high molecular weight polyethylene - the core constituent for Dyneema and Spectra - for desired behavior at high strain rates.



The new AIREBO-Morse potentials (AIREBO-M) are used in a simulation to deform and break polyethylene fibrils. Large scale simulations like these will allow us to explore effects of defects and other important variables on the

properties of ultra-high molecular weight polyethylene (Reference 3), a material of great importance to ballistic protection. Credit: U.S. Army

Professor Mark Robbins, Johns Hopkins University, and ARL researchers Drs. Jan Andzelm and Tanya Chantawansri, along with graduate students, postdocs, and other ARL personnel, have collaborated to elucidate mechanisms associated with polyethylene using atomistic simulations and coarse-graining methods.[1-3] Key to modeling this system was the development of reactive potentials to be used in atomistic modeling of the Ultra-High Molecular Weight PolyEthylene (UHMWPE) system.

The team of researchers lead by Robbins, Andzelm and Chantawansri have successfully accomplished this by using accurate quantum mechanical data to parameterize an atomistic potential, referred to as the "AIREBO-M" potential, that has been verified to be both computationally fast and accurate - the sweet spot in computational materials science as shown in figure 1.

"This potential is unique, and it's development was made possible by combining the expertise in state of the art electronic calculations at ARL with the complementary experience at JHU on classical models of polymers," said Professor Robbins. In addition, this development has widespread impact for other ARL programs and missions. This advance will have broader importance to the Army as "these potentials are general enough to be applied to many materials and will help in the advancement of other materials too, such as graphene and other novel 2-D polymers," said Dr. Andzelm.

Methods to "coarse-grain" and "back map" to the atomistic level have also been developed under this collaboration. This will allow

computations to further bridge times and length scales that are currently excluded from atomistic level modeling. In turn, these methods will feed higher level micro-mechanical models, such as those being developed in another portion of the program by Dr. Thao (Vicky) Nguyen of Johns Hopkins University.

Ten years down the road, "it could be possible for all-atom simulations ... to reach time and length scales only accessible to meso-scale simulations today," said Dr. Chantawansri.

Critical to developing computational models is the ability to synthesize and characterize well-defined model systems. This data provides valuable input and validation to the computational models, but for complex systems like ballistic fibers the production of appropriate model systems can be quite challenging. ARL's new in-house Center for Advanced Polymer Processing, led by Dr. Joseph Lenhart, is a state-of-the art facility with fine control over processing conditions that can not only provide these model systems but also provide complex fibers with advanced performance based on computationally predicted relationships between chemistry, microstructure and performance.

Recently, the team has used the jointly developed computational methods to model polyethylene fibrils being pulled at high rates as show in figure 2. This work is providing great insight into how these systems behave at small length scales.

"It is exciting that with modern computational resources, we get to theoretically address some really fundamental questions about the mechanics of these materials for the first time," said Thomas O'Connor, a graduate student at Johns Hopkins who works with these models.

More specifically, preliminary simulation results study the role of defects which could be responsible for the observed decrease in strength

in experimental fibers compared to theoretical predictions. Once researchers truly understand these processes, it will give the team knowledge that should allow researchers to design even better polymer molecules and fiber microstructures for better ballistic performance. And the parents of Soldiers in 30 years time can be rest assured that ARL has provided the scientific foundation to protect them to the fullest extent before they find themselves in harm's way.

More information: Computational Modeling of Polyethylene at ARL, Tanya Chantawansri, In-Chul Yeh, Timothy Sirk, Joshua Moore, John Brennan, Jan Andzelm, Mach Conference, Annapolis MD, April 9-11, 2014.

Provided by U.S. Army Research Laboratory