Overview
Predictive design of polymer matrices filled with inorganic energetic particles (e.g., Ni & Al), capable of exothermic reactions and energy dissipation upon extreme thermal and mechanical insults

Complex Chemomechanics
- Energetics of metal-oxide-polymeric interfaces under extreme thermal and mechanical environments poorly understood
- Challenging to quantify multiscale mechanical behavior of complex interfaces within composites, accompanied by chemical reactions

Research in Multiscale Models
- Implemented atomistic-level, computation-based predictive models of mechanical impact induced/assisted reactions in Ni and Al nanoparticles
- Demonstrated continuum-level, analytical models to predict static elastic properties of particle-interphase reinforced nanocomposites and validated the models with experimental results

Controlled Reactions
- Non-equilibrium molecular dynamics shows critical condition for Ni-Al reaction initiation, and dynamic reaction properties are affected by radius and surface roughness of the nanoparticles

Controlled Mechanical Properties
- Effective medium theory shows elastic modulus of nanocomposite is controlled by volume fractions of the nanoparticles and mechanical properties of the nanoscale particle-matrix interphase

MAIN ACHIEVEMENTS:
1. Atomistic simulations show self-sustained alloying reaction propagates, accompanied with melting and coalescence processes in Ni and Al nanoparticles of various radii induced via high strain rate mechanical impact in ns timescale
2. Extent and rate of the heat release during Ni-Al mixing are controlled by interfacial geometry and radii of nanoparticles

Fig. 1. High speed impact induced alloying propagations in Ni and Al nanoparticle

Fig. 2. Schematic method to estimate elastic properties of a composite comprising particles surrounded by interphase

1. Analytical model constructs particle-interphase region via an effective particle of identical size and shape (Figs. 2a-c), and equivalent elastic properties.
2. Nanocomposite comprising the effective particles is represented by a homogeneous effective medium (Fig. 2d).

HOW IT WORKS:
- Atomistic computational models using parallelized large scale, non-equilibrium molecular dynamics
- Continuum mechanical models using effective medium theory for static effective elastic properties

ASSUMPTIONS and LIMITATIONS:
- Uses semi-reactive interatomic potentials for Ni and Al
- Assumes non-oxidized nanoparticles in vacuum
- Limited to static elastic behaviors of the nanocomposites

Current Impact
- Design criteria for maximum dissipation established

Fig. 3. Final adiabatic temperature of Ni-Al collisions is higher and attained faster for 3 nm-radius nanoparticles (blue).

Fig. 4. Comparison of measured and model-based Young’s modulus for Ni-Al-epoxy nanocomposites (AFOSR data) requires interphase.

Planned Impact
- Identify critical loading conditions for Ni/Al oxide nanoparticles to collide in polymer matrices
- Investigate energetics of oxidized Ni/Al nanoparticles within polymeric matrices under impact using fully reactive molecular dynamics

Research Goals
- Provide multiscale design principles for reactive metal-oxide-polymer nanocomposites under mechanical stimuli to maximize energy transfer & dissipation.