Multiscale Modeling of Ultra High T Ceramics

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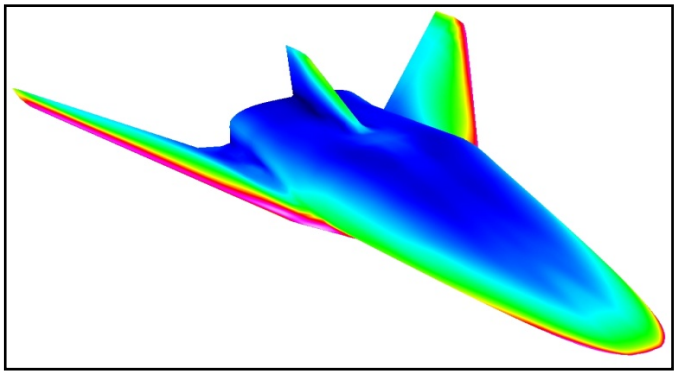
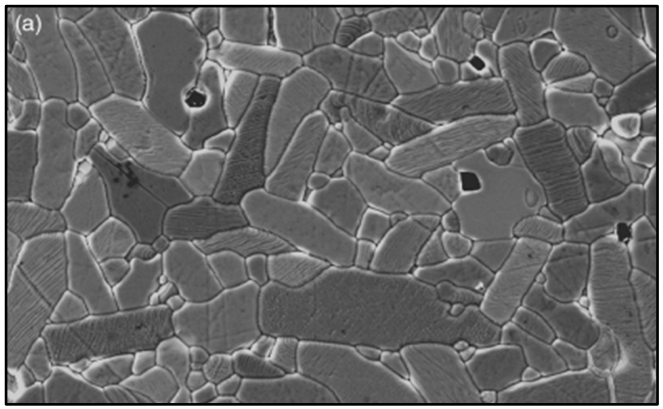
Background

- **NASA** requires high performance materials
- **Material modeling** will:
  - Discover fundamental mechanisms
  - Enable design of new materials
  - Accelerate development cycle
- **Example material**: high T Ceramics ZrB_2
  - Hypersonic leading edges, etc
  - Polycrystalline material
- **Modeling problem**: thermal conductivity
  - Dependence on grains and interfaces
  - Important for thermal management
- **Future work**
  - Design new microstructures
  - Apply methodology to other materials



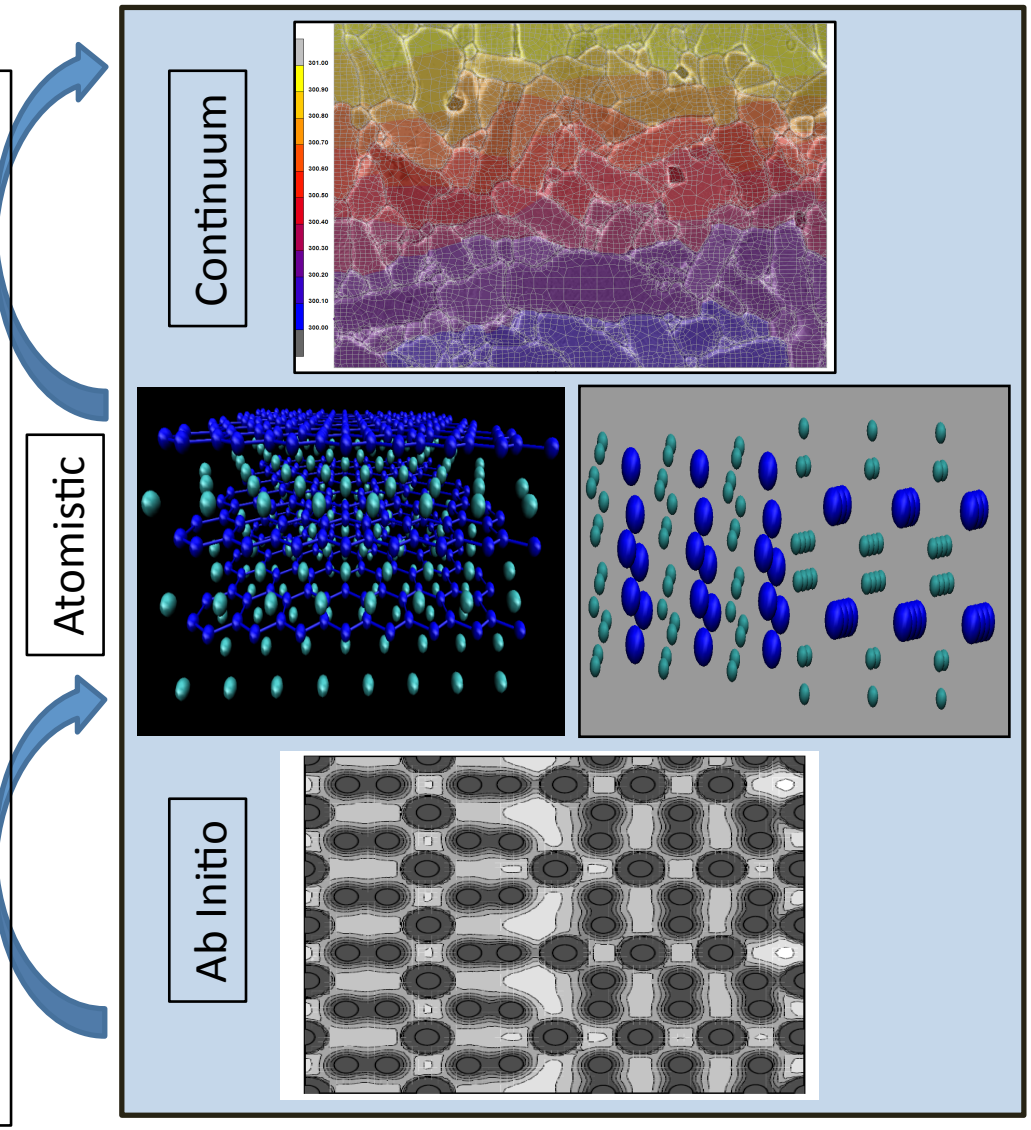
Leading edges of hypersonic vehicle



SEM image of UHTC microstructure

Approach

- **Project integrates 3 different methods**
  - *Ab Initio* - chemistry
  - *Atomistic* – atomic motion
  - *FEM* – macroscropics
- **Ab Initio is most fundamental method**
  - Determines chemical bonding
  - Validates atomistic results
  - Derives atomistic energy
- **Atomistic simulations**
  - Requires energy function
  - *Derived from ab initio data*
  - We derived for ZrB_2 in FY09
  - *First ZrB_2 atomistic simulations*
  - TC of crystals and interfaces
- **FEM methods**
  - Macroscopic continuum model
  - *Use parameters from atomistics*
  - FEM mesh built on SEM image



Part of the novelty of our approach is the integration of these distinct methods into one computational framework!

Results

1. **Ab initio interface computation**
   - Electronic bonding of interface
   - Validate atomistic results
2. **Crystal thermal conductivity (Fig 1)**
   - Green-Kubo method
   - *Convergence of TC with simulation time*
   - In-plane TC are equal (Kxx=Kyy)
   - Out-of-plane TC lower (Kzz<Kxx)
   - *Experimental agreement excellent*
3. **Grain boundary thermal resistance (Fig 2)**
   - Thermal gradient method
   - GB position at blue lines
   - Center "hot" region
   - Endpoints "cool" region
   - *Discontinuity gives interface resistance*
   - *Inaccessible to experiment*
4. **FEM thermal analysis (Fig 3)**
   - Fig 1,2 results used in Fig 3 model
   - Flux applied to top of image
   - Colors give temperature distribution
   - Non-uniform conduction

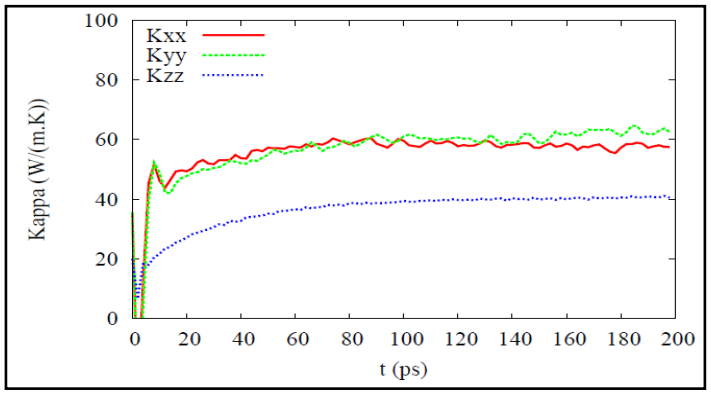


Fig 1: Single crystal thermal conductivity

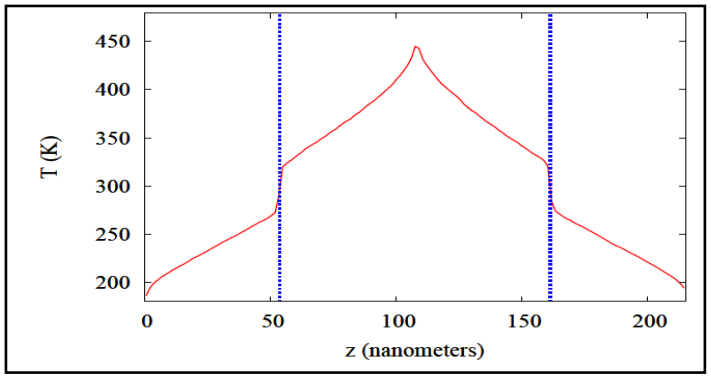


Fig 2: Grain boundary thermal resistance

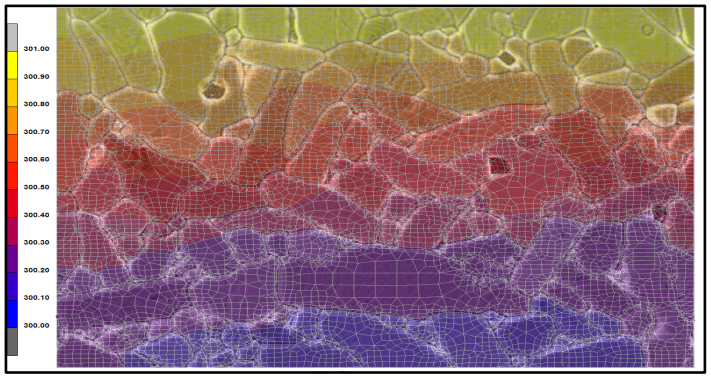


Fig 3: Imaged based FEM computation