Atomistic Exploration of Impurity Effects on the Intrinsic Brittleness of Silicon Carbide

Derek Warner and Kelvin Leung, School of Civil & Environmental Engineering
Cornell University, Ithaca NY 14853
AFOSR Grant #FA9550-11-1-0273

Overview

Primary Objective: Utilize advanced atomistic modeling techniques to investigate the role of impurity elements and nonstoichiometry on high temperature SiC crack tip behavior

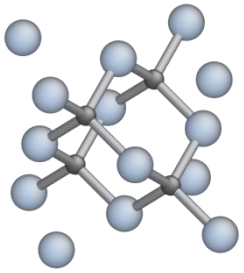
Timeline: 3 year project
Initiated September 15, 2011

Potential Outcomes:

1. Improve understanding of fracture mechanisms in SiC
2. Identify impurity elements that are influential to crack growth in SiC
3. Provide guidance in choosing crack tip constitutive relations
4. Develop a foundation for future atomic-scale investigations of fracture in chemically complex materials

Technical Challenges: Four longstanding challenges exist for performing meaningful atomistic simulations of deformation and fracture processes

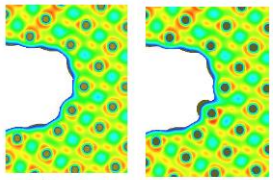
1. Spatial scaling
2. Temporal scaling
3. Interatomic interactions
4. Vast configuration space



Approach

1. Identify key crack tip mechanisms and important regions in configuration space:
   - Large 3D atomistic simulations
   - Penny shaped cracks with empirical potentials
   - Investigate effects of crystallography, crack tip geometry, loading type, & temperature
2. Examine key mechanisms and configurations more carefully with regard to spatial scale, time scale, interatomic potentials
   - Concurrently coupled atomistic - discrete dislocation framework
   - *Specific mechanisms*: Variational Transition State Theory via Finite Temperature String Method
   - *Specific configurations:* Parallel replica + hyperdynamics
3. Examine the effect of impurities and nonstoichiometry on the key mechanisms and configurations
   - QM-based continuum models

The images to the right show the difference in electron density at an aluminum crack tip when a single hydrogen element is present



Building on our experience with metallic systems

Highlights

- Publication on Hydrogen Embrittlement was highlighted by Physics, on the cover page of Physical Review B, and as an "Editors' Selection", Summer 2012
- Our publication on extended timescale atomistic modeling of crack tip behavior was listed as the second most read paper in the journal Modeling and Simulation in Materials Science and Engineering during the period July 15th through August 15th of 2012.

Publications

- I. Szlufarska, K.T. Ramesh, and D.H. Warner. "Simulating Mechanical Behavior of Ceramics under Extreme Conditions." Annual Review of Materials Research (2013)
- R. J. Zamora, A.K. Nair, R.G. Hennig, D.H. Warner. "Ab initio Prediction of Environmental Embrittlement at a Crack Tip in Aluminum." Physical Review B Rapid Communication 86(2012), 060101(R),
- K.L. Baker and D.H. Warner. "Extended Timescale Atomistic Modeling of Crack Tip Behavior in Aluminum." Modeling and Simulation in Material Science and Engineering, 20 (2012), 065005
- N.A. Erwin, E.I. Wang, A. Osysko, and D.H. Warner, "A Continuously Growing Web-Based Interface Structure Databank." Modeling and Simulation in Material Science and Engineering, 20 (2012), 055002

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Derek Warner, Kelvin Leung, and Zhiliang Pan
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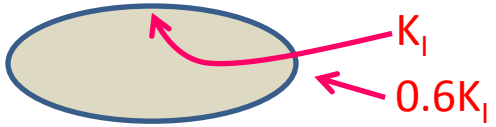
Questions

1. What are the important crack tip configurations to study?
2. What are the important crack tip mechanisms to study?
3. How can we accurately and efficiently model these?

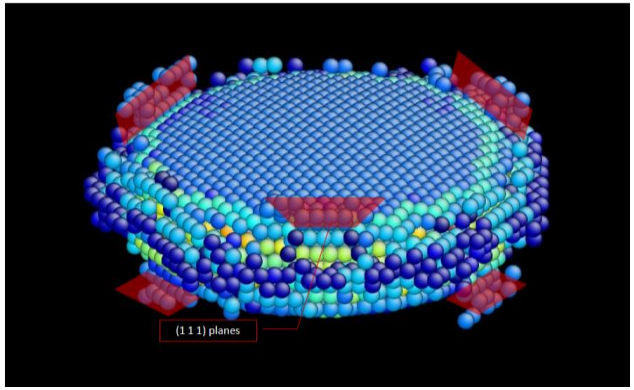
Governing Configurations

- Crack Planes:
  - **Griffith's Theory:** Fracture occurs on planes of lowest surface energy, i.e. 111 planes of SiC
  - **Experiment:** Fracture of polycrystalline SiC shows many {111} surfaces
- Crack Growth Directions:
  - **Continuum Fracture Mechanics**: growth of penny crack in most ductile directions controls



  - **Atomistic Vantage:** <112> is most ductile direction on {111} crack plane due to co-planner partial dislocation nucleation

We will consider
a straight {111} <112> crack

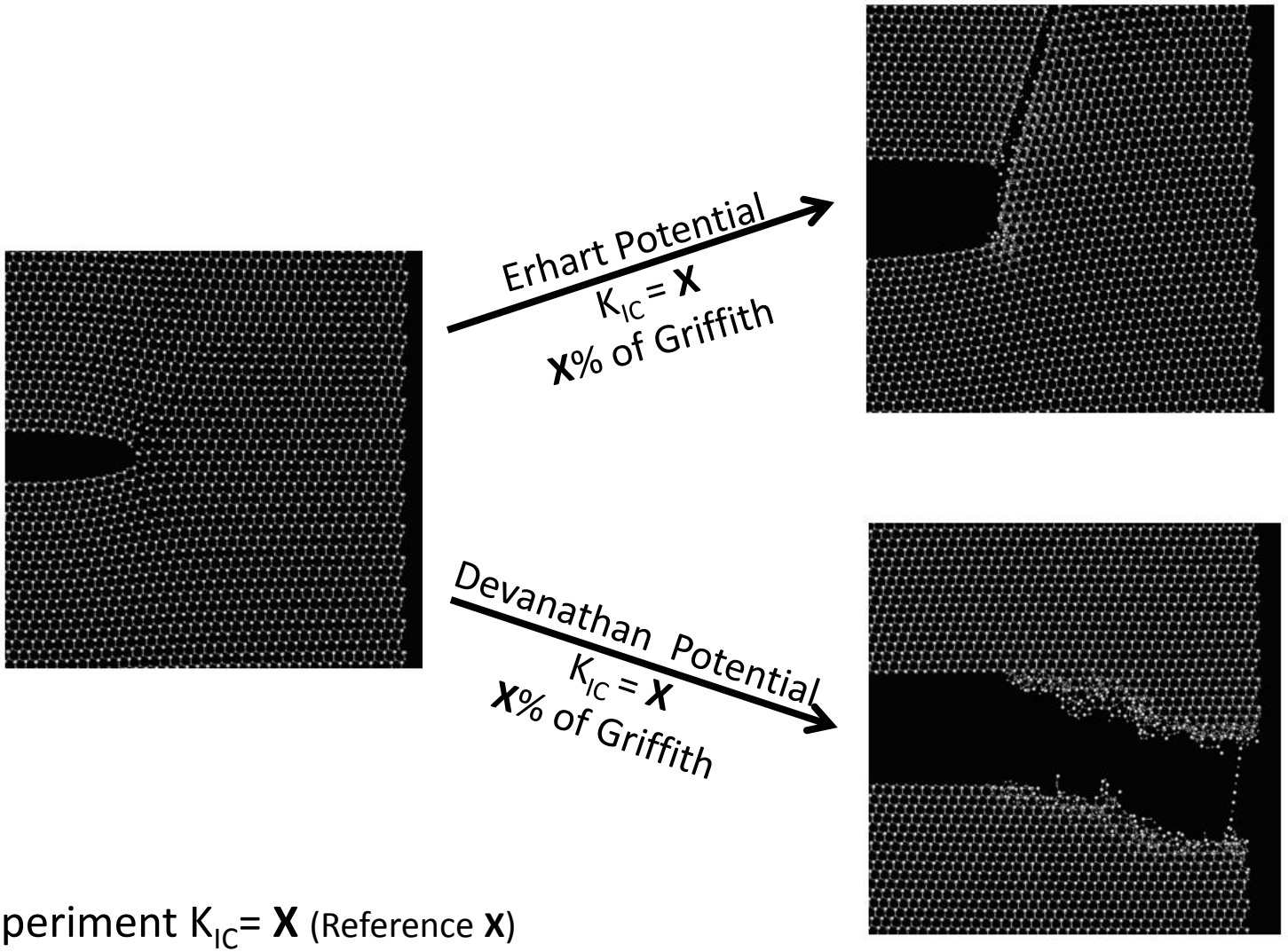


Molecular Dynamics Simulation Setup

- Through crack under mode I loading
- 200A x 200A x 20A with a 60A through crack
- Traction & plane stress boundary conditions
- Potentials:
  - Devanathan et. al (1998) potential
    - Modified Tersoff potential with improved repulsive part
  - Erhart & Albe (2005) potential
    - Tersoff potential with emphasis on generality
- Temperature: 0 K to 800 K with 200 K increment
  - (Melting Temperatures)
- Strain rate: 10^7/s to 10^9/s

Molecular Dynamics Simulations

Brittle crack growth is observed with both potentials **at 0°K**



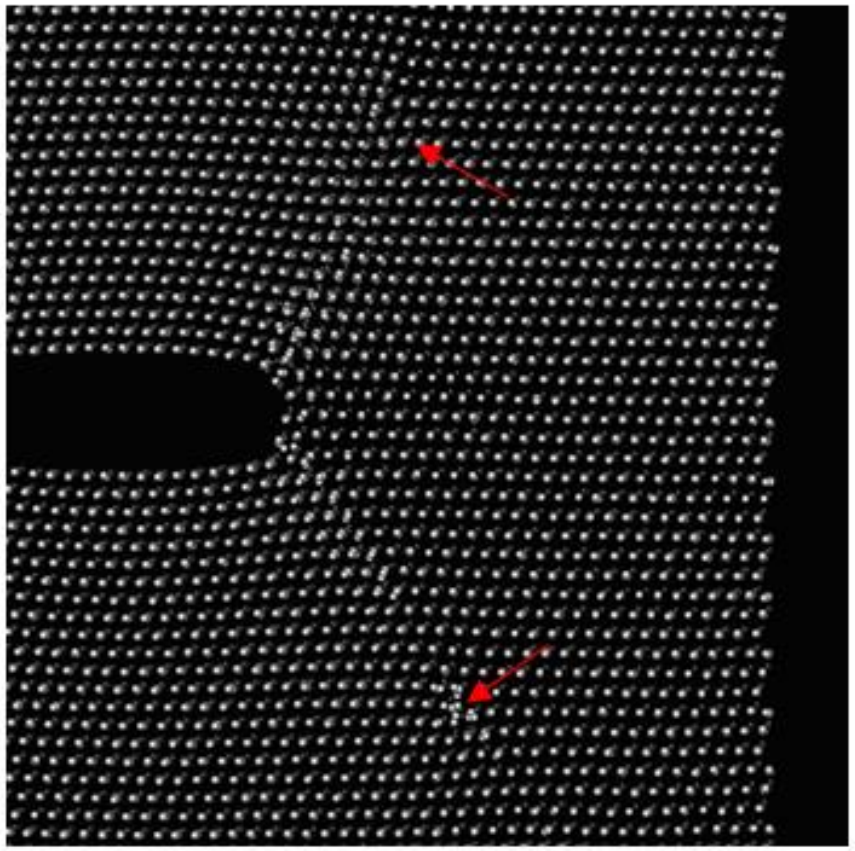
Experiment K_{IC}= **X** (Reference **X**)

Molecular Dynamics Simulations at Intermediate Temperatures

- **200°K Erhart** potential nucleates full dislocations from crack tip on {111}
- **400°K+ Erhart** potential nucleates full dislocations on both {111} and {100}
- **Devanathan** potential continues to exhibit brittle response at both temperatures

Erhart Potential
K_{IN}= **X** at 200°K
K_{IN}= **X** at 400°K

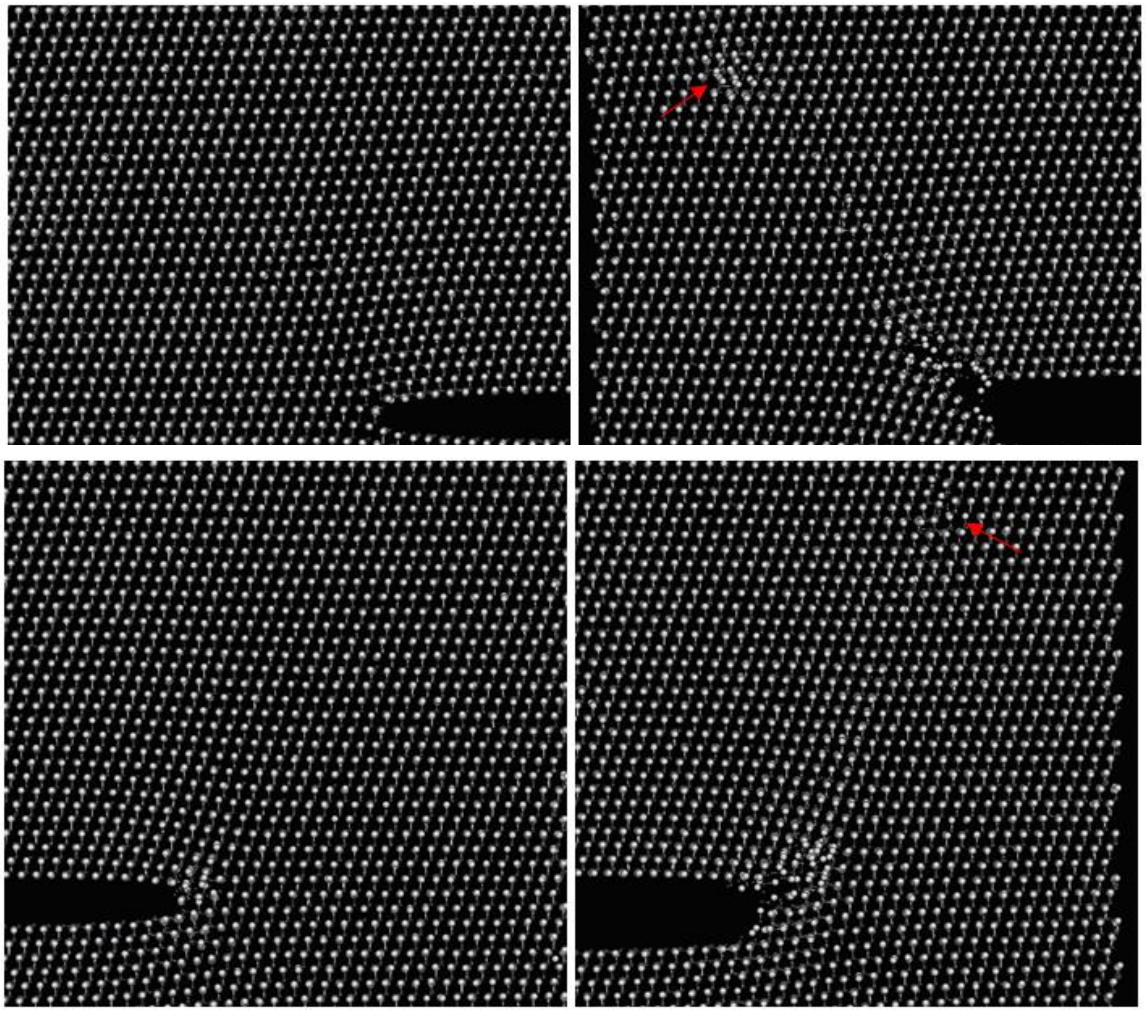
Devanathan Potential
K_{IC}= **X** at 200°K
K_{IC}= **X** at 400°K



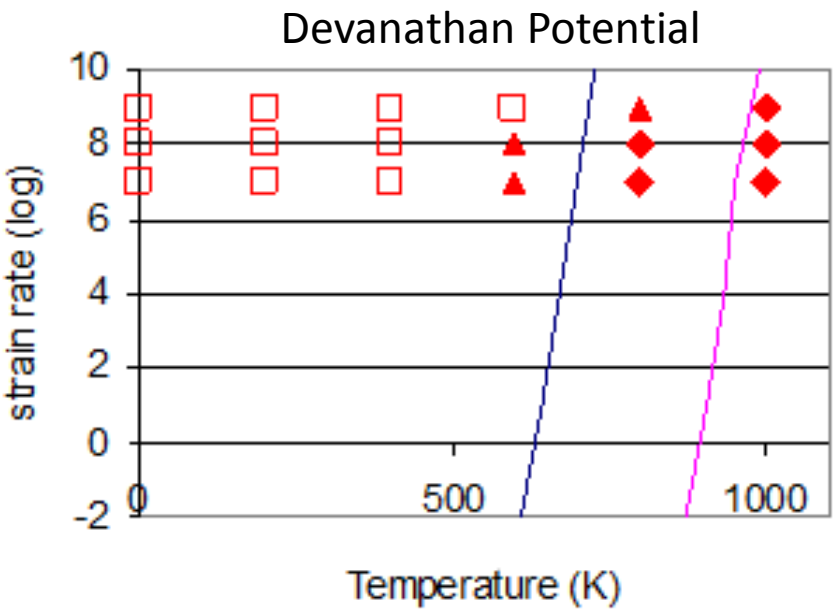
Erhart Potential at 400°K

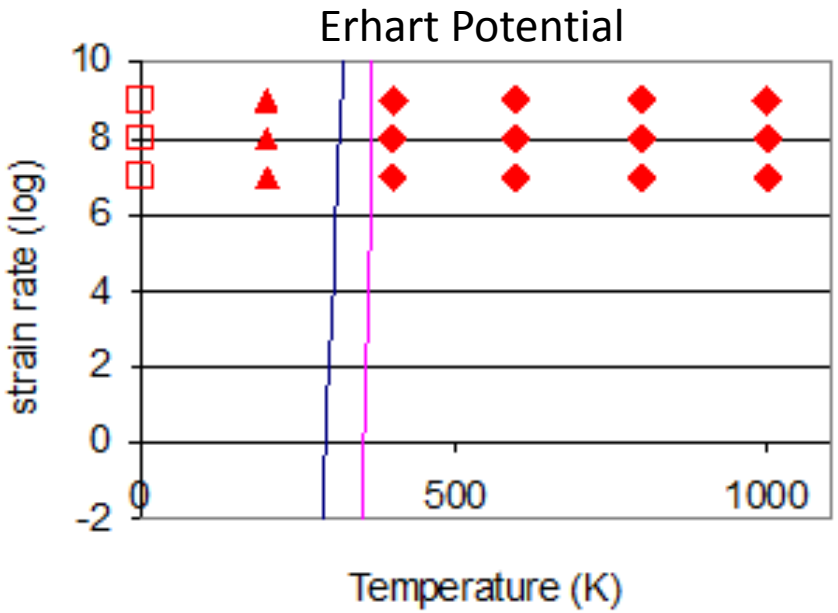
Molecular Dynamics Simulations at High Temperatures

- **1000K+ Devanathan** nucleates full dislocations on both {111} and {100}



Failure Mechanism Map





{111} dislocations

{111} & {100} dislocations

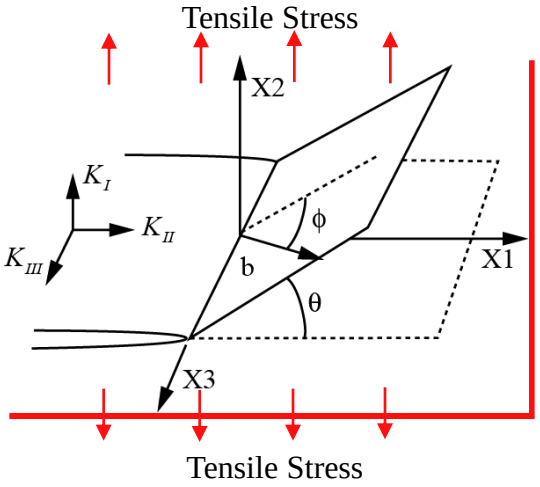
Brittle fracture

Transition from brittle to ductile crack tip response with increasing temperature

Continuum Analysis and Modeling

- Brittle Fracture
  - Governed by thermodynamics (Griffith)
  - Surface energy vs strain energy

$$K_{IC}^2 \frac{1-\upsilon^2}{E} = 2\gamma_s$$



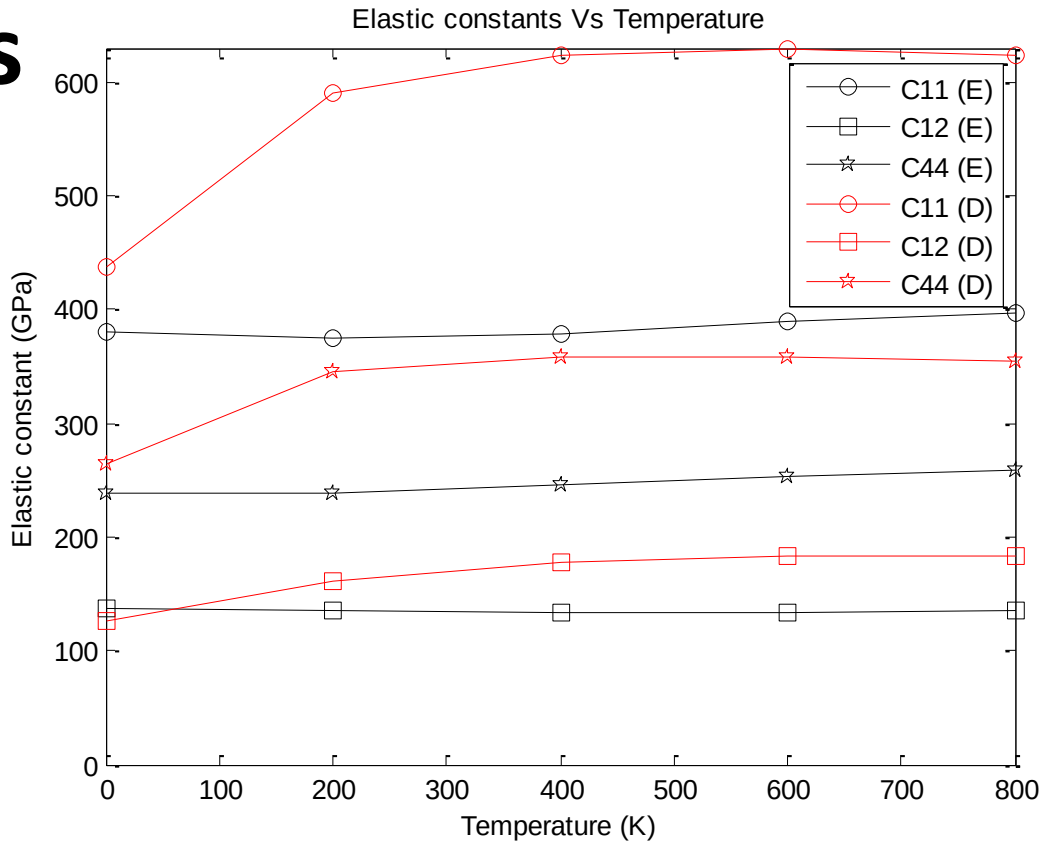
- Dislocation Nucleation
  - Governed by kinetics (Rice & Beltz)
  - Stacking fault & strain energies

$$\frac{Q_{3D}}{k_B T} = \ln\left(\frac{k_B T N \omega_0}{-\dot{K}_I \dfrac{dQ_{3D}}{dK_I}}\right)$$

$$Q_{3D} = 5{b_p}^3 0.287 \mu F \frac{(\cos^2\varphi + (1-\nu)\sin^2\varphi)}{(1-\nu)}\left(1 - \frac{K_{II}^{eff}}{K_{IIcrit}^{eff}}\right)^{\frac{3}{2}}$$

Finite Temperature Material Properties - Elastic Constants

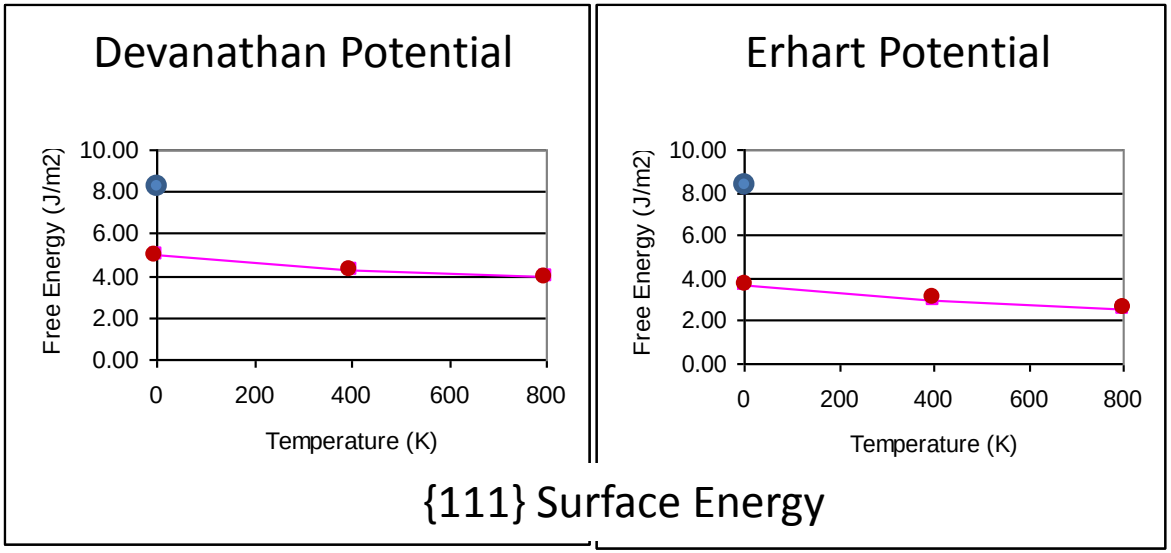
- Directly calculated with MD
- Reasonable 0K values, except Devanathan C11
- Devanathan showed anomalous increase with temperature
- Erhart showed relatively temperature independent response

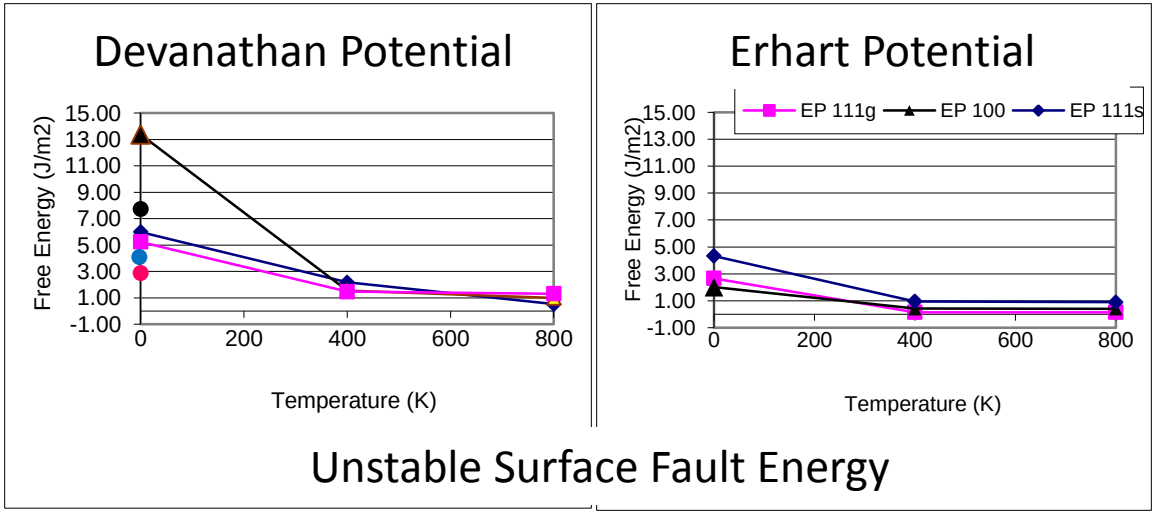


	Experiment [1]	Experiment [2]	This work DFT	This work Erhart	This work Devanathan
a0	4.36		4.33	4.36	4.28
C11	390	352	393	380	437
C12	142	140	156	138	126
C44	256	233	259	239	265

Experimentally, E decreases by about 10% from 0 to 1000K

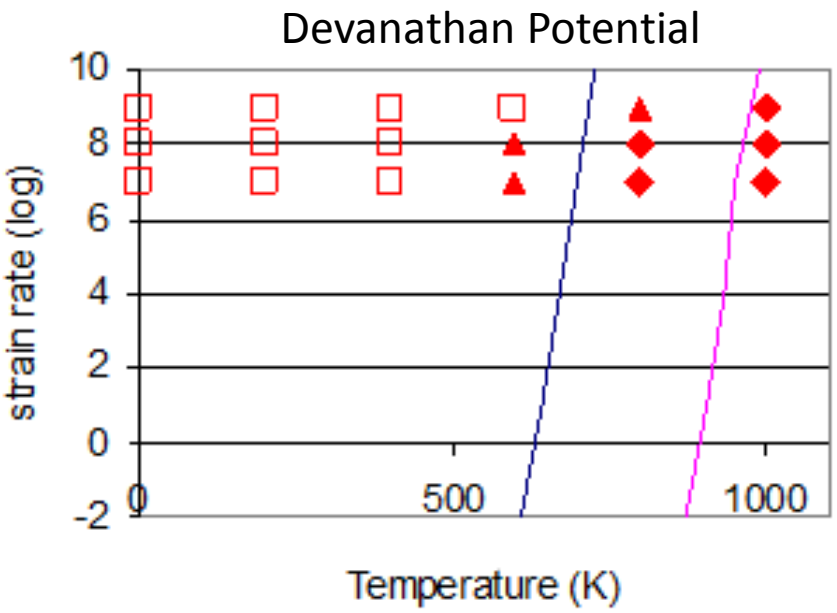
Finite Temperature Material Properties - Surface Energies

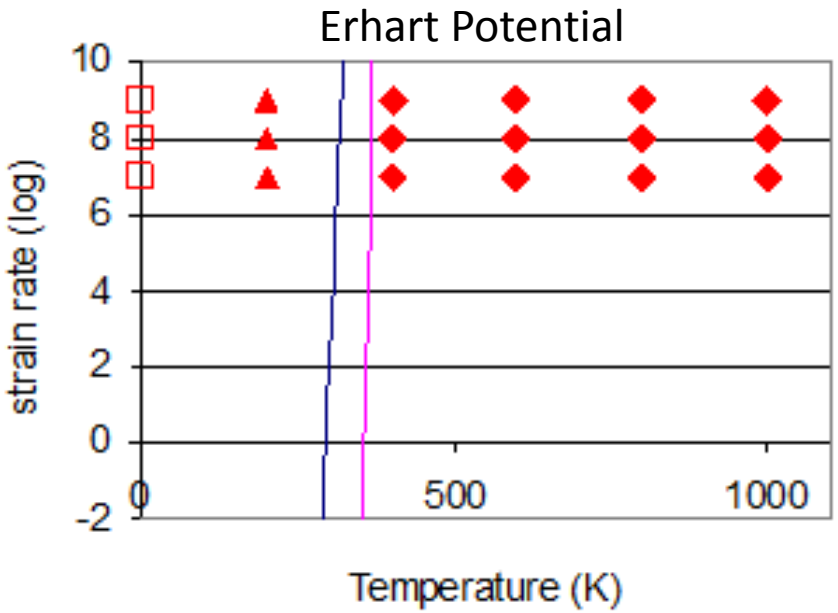




- All surface energies decrease with temperature
- Role of entropy is significant
- Complicated profiles

Failure Mechanism Map





{111} dislocations

{111} & {100} dislocations

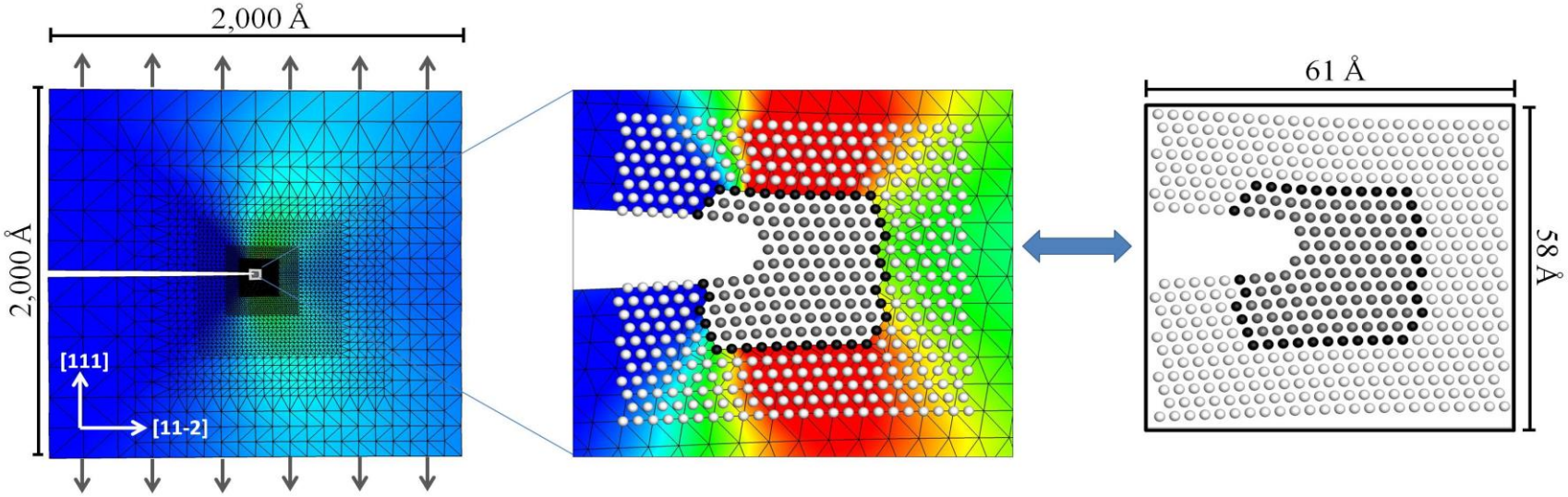
Brittle fracture

1. Continuum predictions are qualitatively consistent with MD simulations
2. Finite temperature material properties are important

Summary

1. Crack tip: observed a transition from cleavage to {111} and {100} dislocations emission with increasing thermal activation
2. Predicted similar behavior with continuum models
3. Uncertainty due to large variability and unphysical characteristics of popular SiC interatomic potentials
4. Importance of crack tip processes in crack growth

On Going Effort:
Direct QM Crack Tip Predictions



Approach: concurrent multiscale modeling – QM-CADD (Nair et al. JMPS 2011)

- Simple force balanced coupling between atomistic and continuum regions
- No ghost forces at interface + quantifiable & controllable coupling errors

Simulation Setup:

- Pad thickness
  - Long range surface forces require high smearing parameter
- Atomistic domain size
  - Using empirical potentials to quantify domain size effects

Pad Size Studies

	sigma=1.5	sigma=0.1
lattice constant (A)	4.33	4.33
C_{11} (Gpa)	393	393
C_{12} (Gpa)	126	126
C_{44} (Gpa)	259	259
100 surface energy 2γs (J/m^2)	9.20	11.40
111 glide plane surface energy 2γs (J/m^2)	13.63	15.70
111 shuffle plane surface energy 2γs (J/m^2)	6.25	9.28
111 glide plane unstable stacking fault energy γus (J/m^2)	3.34	3.438
111 shuffle plane unstable stacking fault energy γus (J/m^2)	3.61	3.96