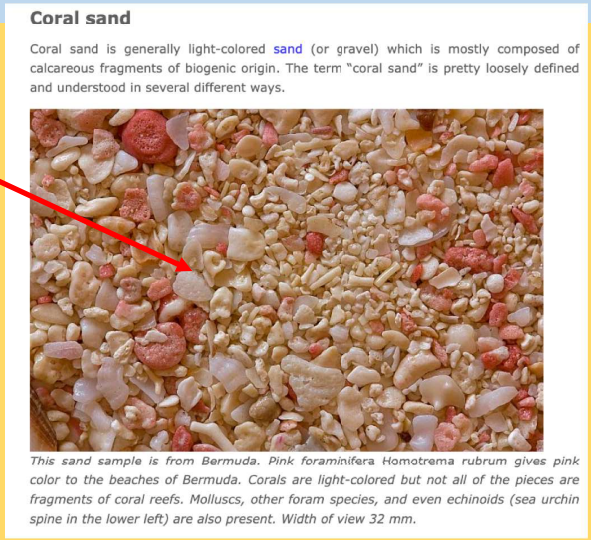
Discussion Related to Questions from Lecture 1

Can fracture mechanics be used to study materials at the nanometer and smaller scales?

The answer is yes, but it may require abandoning the use of continuum theories of fracture in favor of models and simulation tools including molecular dynamics and others. There have been many advances in such paradigms over t he past few decades.

Can fracture mechanics be used to study coral sand? Erosion process or fracture of a single grain?

Yes



What differences are there between the mechanics of a crack in a single material and an interface crack?

There has been a large volume of work done in the past decades on linear and nonlinear interfacial fracture mechanics. This topic is beyond the scope of this short course, but I may say something about it at the end of the third lecture.

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Coupled quantum mechanical/molecular mechanical modeling of the fracture of defective carbon nanotubes and graphene sheets

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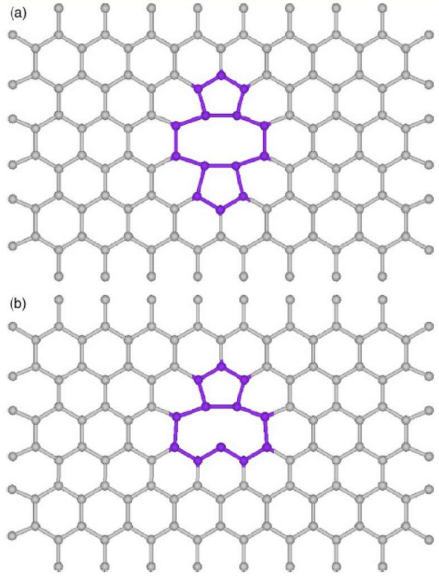

FIG. 1. (Color online) (a) Two-atom and (b) one-atom vacancy defects shown on a graphene sheet.

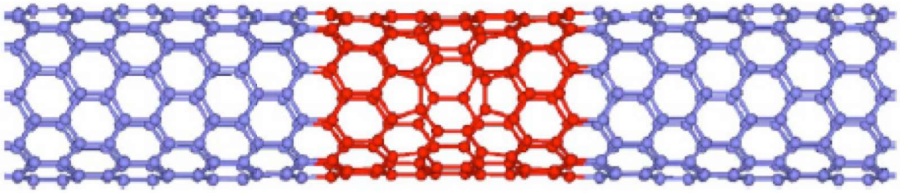

FIG. 2. (Color online) Coupled QM/MM model: the central region constitutes the QM fragment (QM atoms, dark red dots; MM atoms, light blue dots).

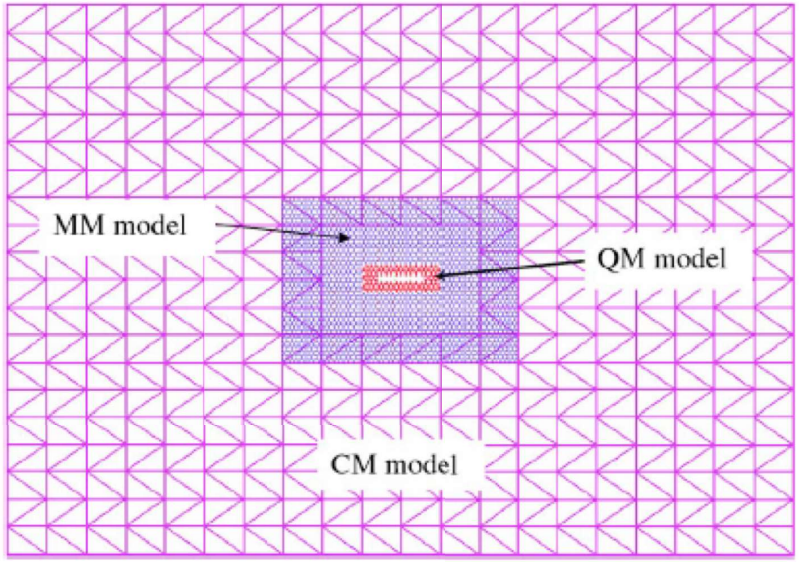

FIG. 11. (Color online) A coupled QM/MM/CM model.

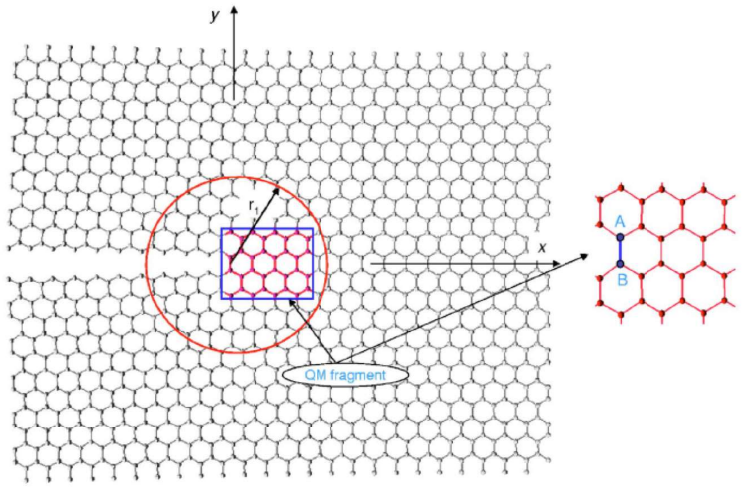

FIG. 13. (Color online) A graphene sheet containing a crack. The quantum fragment is shown in the inset. The bond A–B forms the crack tip. Note that r_1 is large enough to enclose the quantum fragment.

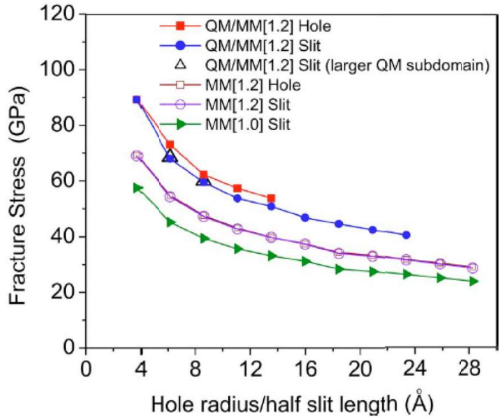

FIG. 7. (Color online) Dependence of the fracture stress of a [50,0] CNT on the defect size for holes and slits. PM3 was used for all the QM/MM calculations. The scaling factor used for the MM potential is given in the square brackets. The MM[1.2] Hole and MM[1.2] Slit results are so close as to be nearly indistinguishable.

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Dimensionality effects in crystal plasticity, from 3D silicon to 2D silicene

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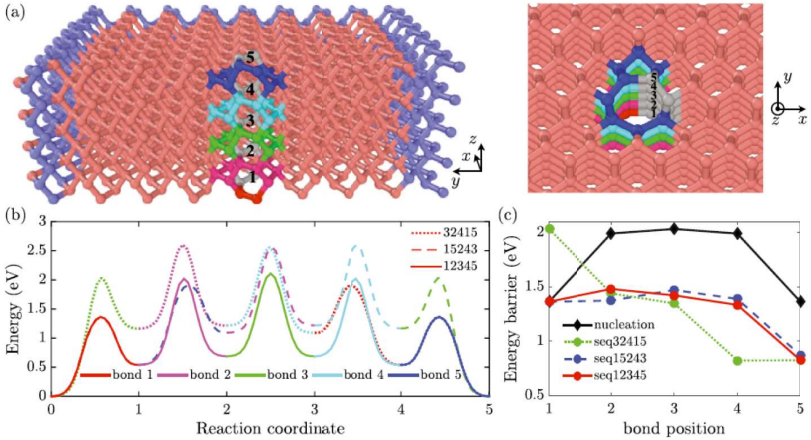

Fig. 6. Atomic structure of $n_z = 4.5$ Si film (left) cut in the middle of the simulation domain along x-axis to display dislocation core, (right) top view on the core structure, where different colors correspond to different layers along z-axis, while bonds that undergo rotation during glide are shown in gray color and numbered according to z coordinate. NEB calculated (b) MEP for one complete glide step via different sequences of bond rotations and (c) corresponding energy barriers as functions of rotated bond position and sequence. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

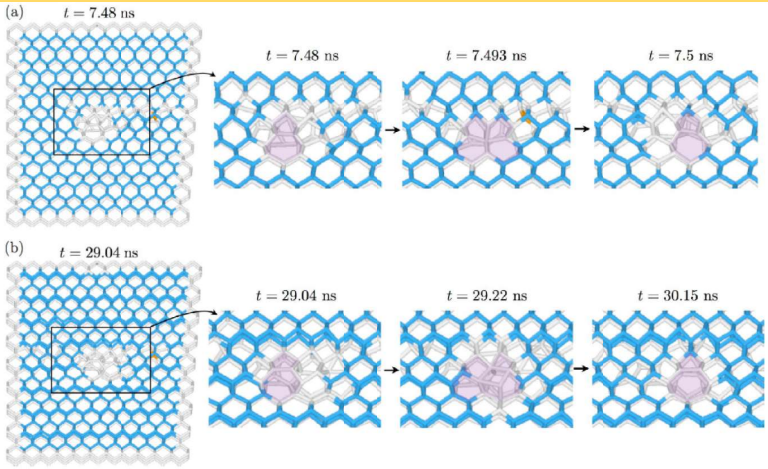

Fig. 10. MD simulation snapshots of 4.5-layers Si film with an edge dislocation at $T = 610$ K under applied shear strain $\gamma = 4\%$ sliced along $z-$direction at (a) 2nd and (b) 4th layers. Here blue color corresponds to bonds between atoms having cubic diamond environment, while gray represent other atomic coordination reflecting dislocation core and free surface atoms. The whole simulation domain (left), as well as zoomed images near the dislocation core are included. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

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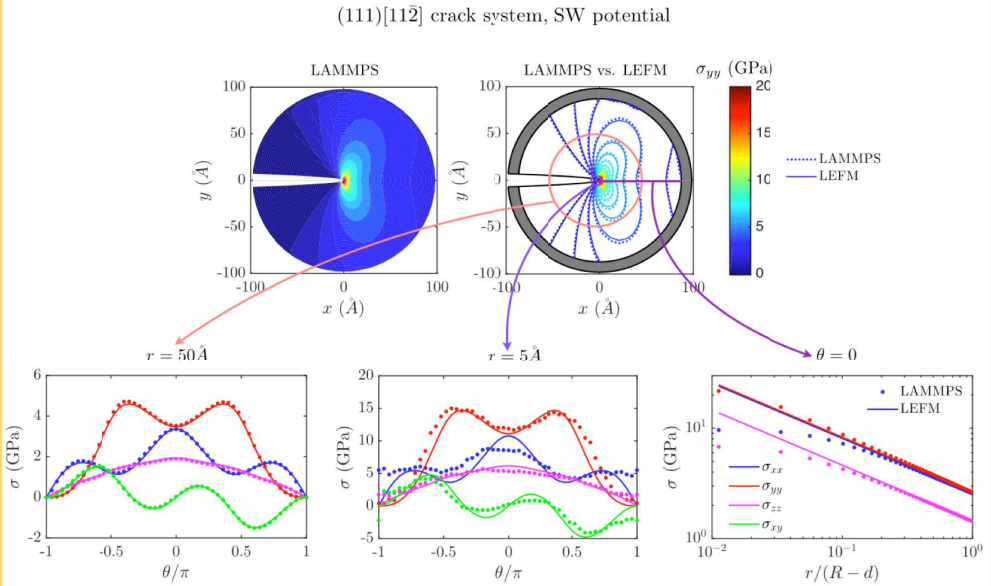
ORIGINAL PAPER

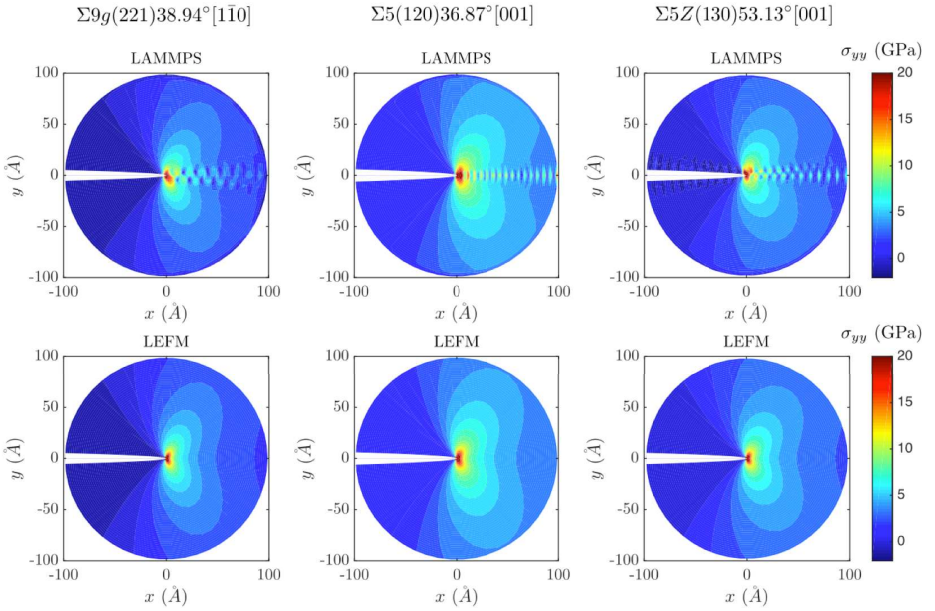
Atomistic modeling of the fracture toughness of silicon and silicon-silicon interfaces

Evgeniya Dontsova · **Roberto Ballarini**

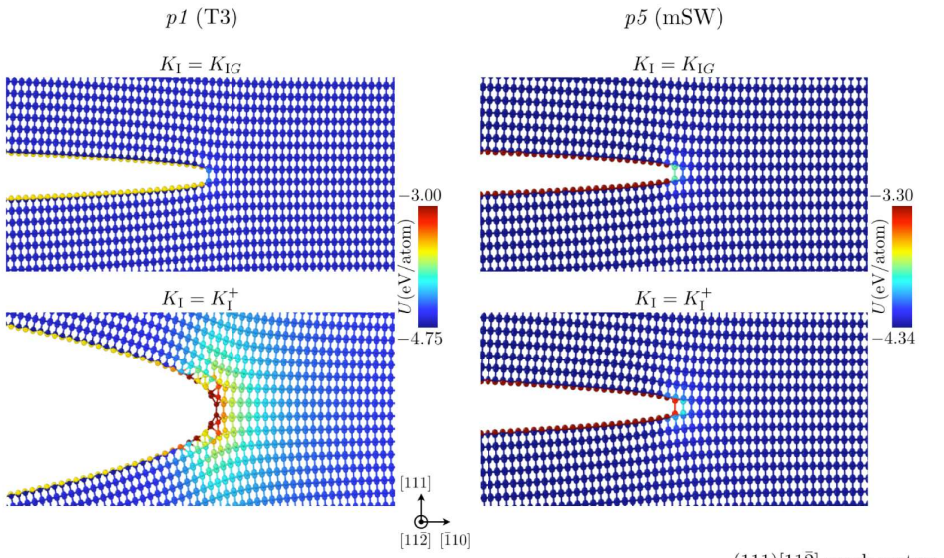
Stress field: atomistic versus continuum



Stress field at the interface: atomistic versus continuum

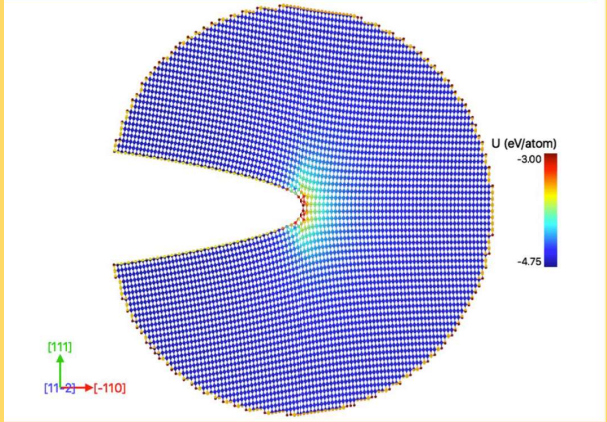


Ductile versus brittle crack propagation



(111)[11$\bar{2}$] crack system

Tersoff potential *p1* (T3): loading



Grain boundaries in Si crystal