Stochastic Modeling of Microstructures

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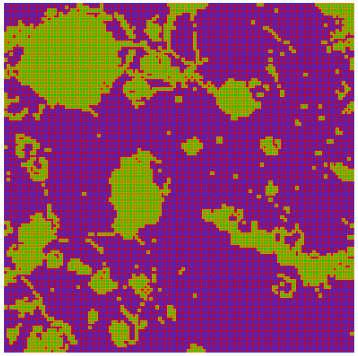
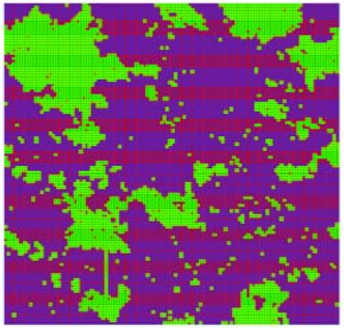
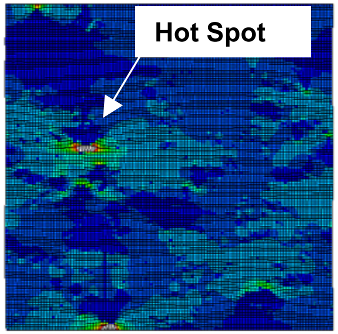
Engineering materials have inherently complex microstructures. To model their mechanical response accurately requires the numerical generation and computational simulation of multiple realization of the microstructures. Within our MRSEC, we have developed stochastic methods based on Torquato's "microstructure reconstruction" approach to generate two-phase microstructures and simulate their response to stress. We start with an experimental microstructure, extract key correlation functions describing this structure, and numerically generate a family of new, structures that are statistically equivalent to the experimental structure. The digital microstructures are mapped onto a finite element mesh for calculation of the spectrum of deformations in this family of microstructures. The results show what level of microstructural detail is needed to predict macroscopic behavior and what features, usually associated with "failure" or localization phenomena around local "hot spots", are particular to each specific microstructure within the family. The method then allows for systematic exploration of the microstructure of the "hot spots" so as to identify characteristic features detrimental to performance in this family of microstructures. Changes to the experimental microstructure, either actual or hypothetical, can be examined numerically to predict deformation and drive optimization of the microstructure. The figures below show an experimental structure, a statistically-identical family member, the deformation (strains) of that member just at the onset of, and after, shear-band localization at a "hot spot". The red and gray regions denote high strain.



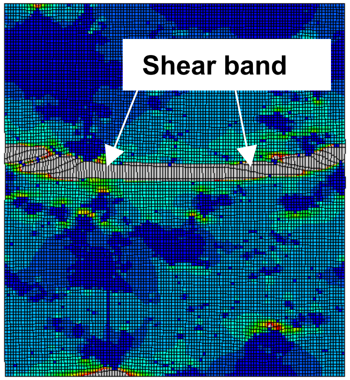
Experimental Structure



Statistically-identical Structure



Deformation at Localization



Localization

Strain-Induced Quantum Rings in Nanostructures

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When quantum dots are etched from strained-layer heterostructures, lateral sidewall expansion leads to a spatially inhomogeneous strain field within the layers and thus a lateral strain-induced confining potential. In the case of cylindrical vertical quantum dots, a ring-like strain-induced potential will exist near the perimeter of the dots (Fig. 1, left). We have employed magnetotunneling spectroscopy to probe the strain relaxation and subsequent strain-induced ring-like confinement in $D \sim 100$ nm Si/SiGe quantum dots. Quantum ring hole states confined by the strain-induced potential have been unambiguously observed: the state energy is periodic in the number of magnetic flux quanta enclosed by the ring orbit when a weak magnetic field is applied perpendicular to the ring plane – the fundamental signature of a quantum ring. In the smallest dots, Coulomb charging of quantum ring states has also been studied. Our approach enables the fabrication of nanostructures with states confined to the perimeter, making unique systems like coupled quantum rings or ellipses accessible to tunneling spectroscopy.

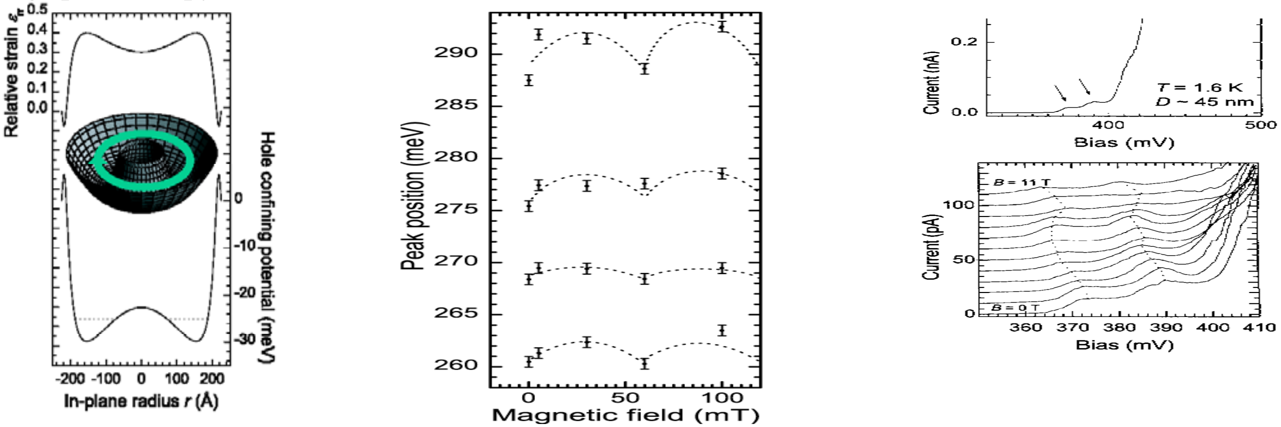

FIG. 1: (a) Inhomogeneous-strain-induced confining potential (left); conductance peak positions reflecting the periodic energy spectra of the strain-induced quantum ring hole states in a weak perpendicular magnetic field (middle); current steps near the tunneling threshold, corresponding to Coulomb charging of a quantum ring (right).

1. Jun Liu, A. Zaslavsky, and L. B. Freund, "Strain-induced quantum ring hole states in a vertically gated quantum dot", *Phys. Rev. Lett*. **89**, 096804 (2002).

2. Jun Liu, A. Zaslavsky, and L. B. Freund, "Single hole tunneling to strain-induced quantum ring hole states", *Phys. Rev. B (Rapid Comm.)* **66**, 161304 (2002).