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*Title:* INCREASING THE FRACTURE TOUGHNESS OF  
SILICON BY ION IMPLANTATION

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## INCREASING THE FRACTURE TOUGHNESS OF SILICON BY ION IMPLANTATION

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This study was motivated by some earlier indications that the fracture toughness of silicon could be increased by ion implantation. The location of fracture in hydrogen implanted silicon was found to change depending on the dose of implanted ions. For relatively low doses, fracture occurred at the center of the damage region created by implantation. However, for larger doses, the fracture location switched to the deeper edge of the implanted zone. This implied that the center of the implanted region experienced toughening due to ion implantation at the higher dose level. In addition, an initial increase in fracture toughness with radiation dose has been observed experimentally in some ceramics. After the initial increase, the fracture toughness reaches a peak and then decreases with further irradiation. The toughness increases found thus far are modest (25-100%). In attempts to explain the experimental results, several toughening mechanisms (such as deflection of the crack by the irradiated damage) have been proposed. However, the proposed mechanisms predict only a 40-80% increase in fracture toughness, which does not account for the highest levels of toughness observed.

Our recent molecular dynamics (MD) calculations have found a previously unknown toughening mechanism acting in silicon, which can also explain the earlier experimental observations of toughening induced by irradiation. In our MD simulations, ion implantation produced clusters of disordered atoms. The presence of these clusters allowed silicon to deform plastically as a crack approached, blunting the crack tip and arresting crack growth. The MD calculations show a factor of 3 increase in fracture toughness. We have conducted experiments with silicon implanted with a small dose ( $10^{14}$  ions/cm<sup>2</sup>) of alpha particles uniformly distributed to a depth of 25  $\mu$ m. A 20% increase in fracture toughness is observed. Additional experiments with higher implantation doses are planned for the immediate future.

Number of the related conference topics: 3

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# **Increasing the Fracture Toughness of Silicon by Ion Irradiation**

**J. G. Swadener**

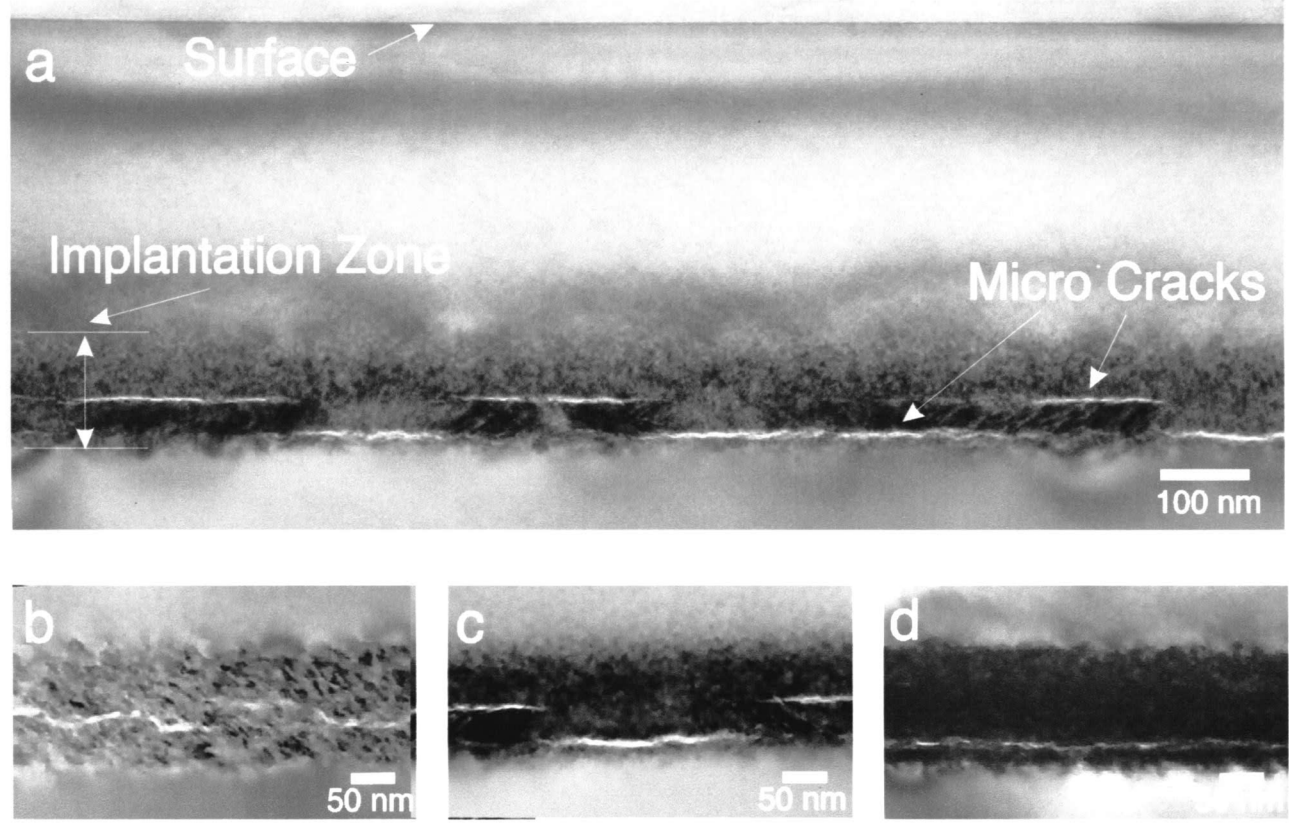
**Michael I. Baskes**

**Michael Nastasi**

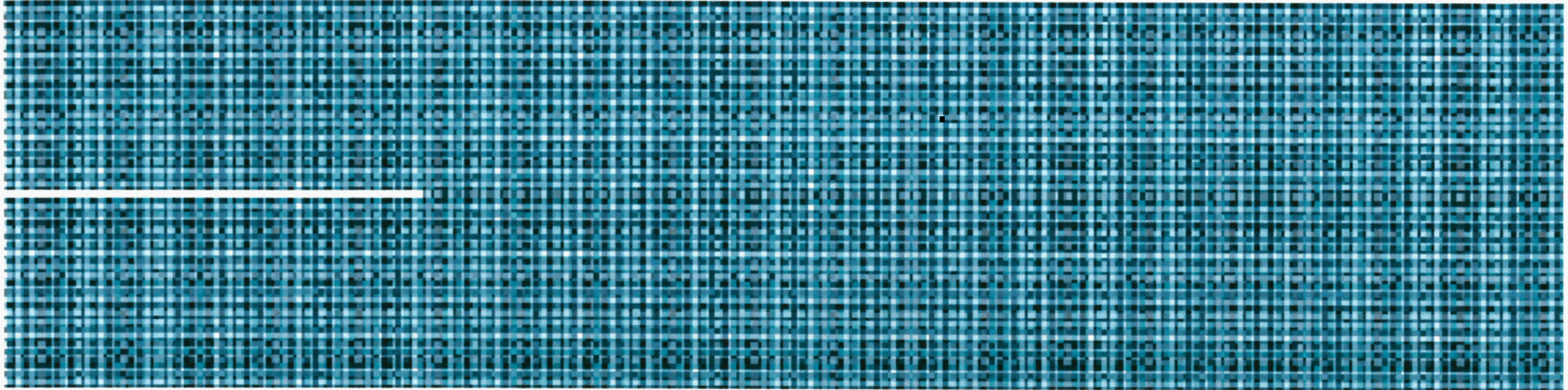
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# Crack Location Depends on Ion Dose

Höchbauer et al. (2002) J. Appl. Phys., v92, 2335



# Molecular Dynamics Simulation of Fracture in Silicon



MEAM potential used to describe directional bonding in silicon

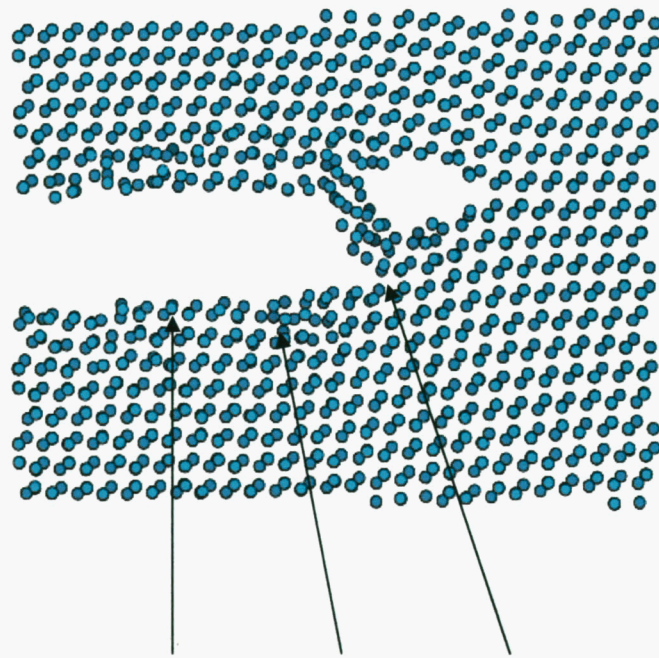
Constant temperature: 300 K

55,000 atoms, free in in-plane directions, periodic out-of-plane

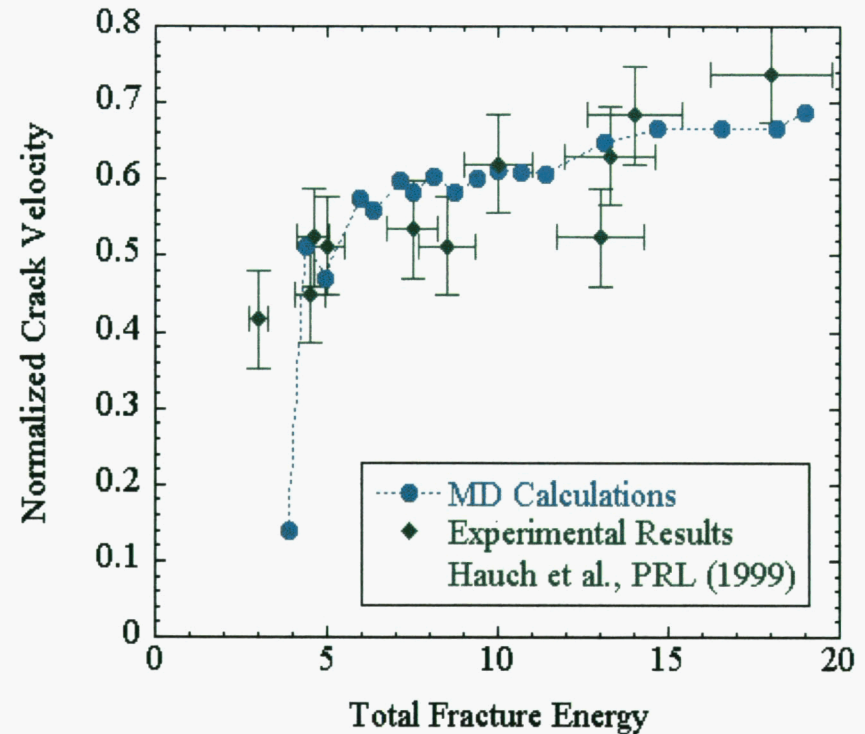
Cracks propagated at constant energy release rate

# Atomistic Study of Fracture in Silicon

Energy consumed during fracture determines crack speed



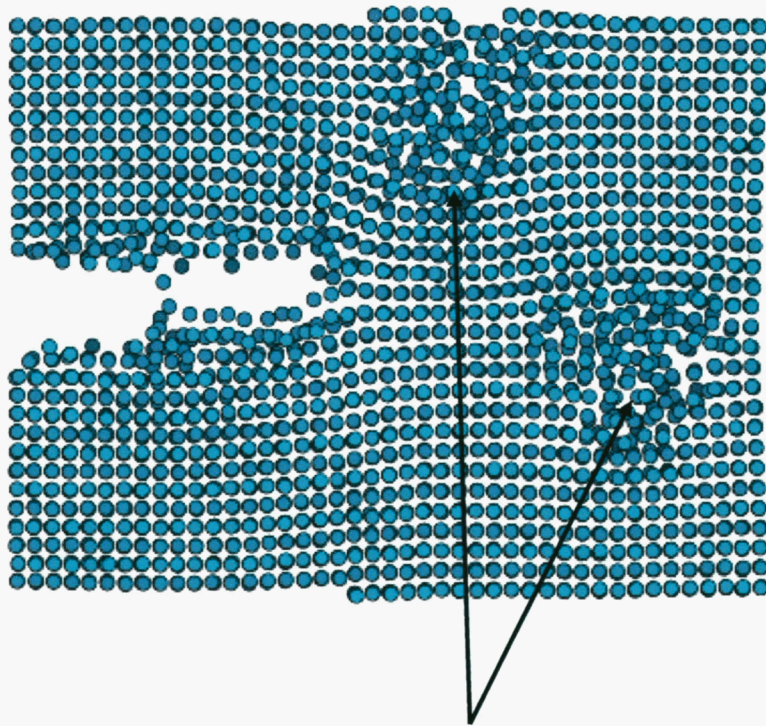
Surface cleavage, defects, uneven surfaces and phonons contribute to the energy consumed during dynamic fracture



MD results agree with experiments for cracks traveling 2-3 km/s

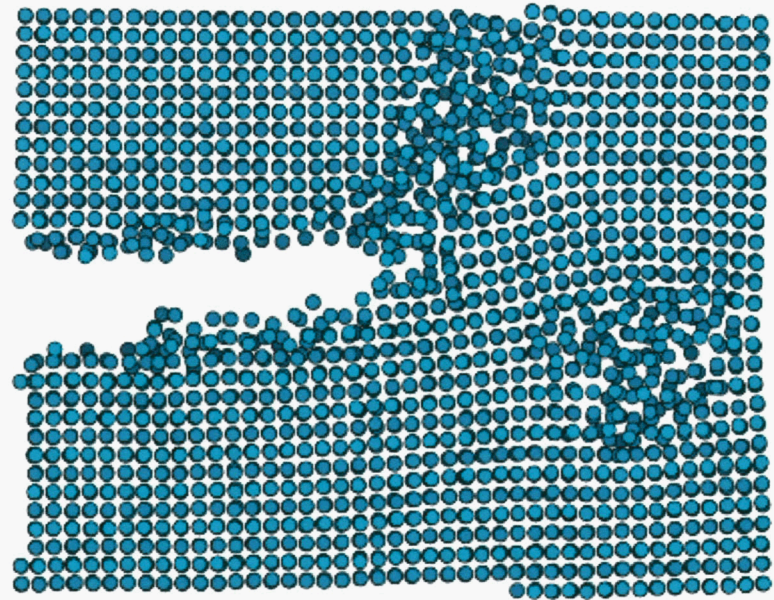
# Implantation damage causes crack arrest

Fracture propagating on (110) planes in virgin material



Damage cascades from 500 eV atoms

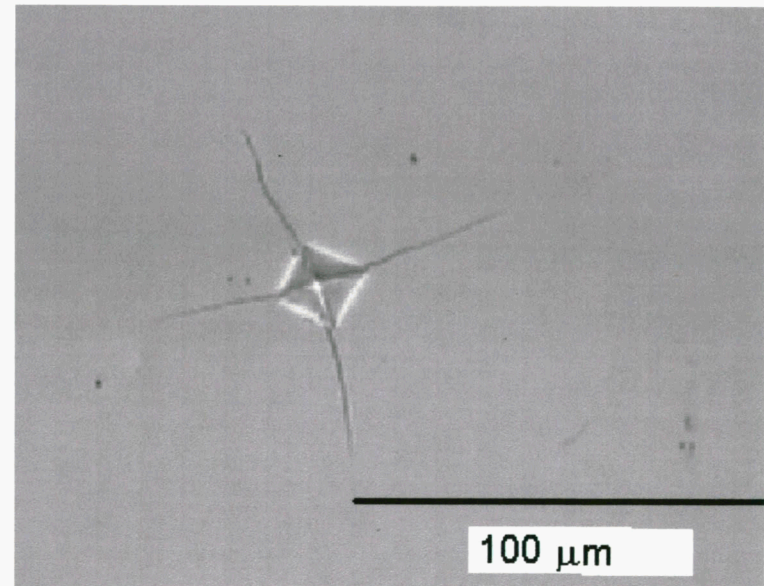
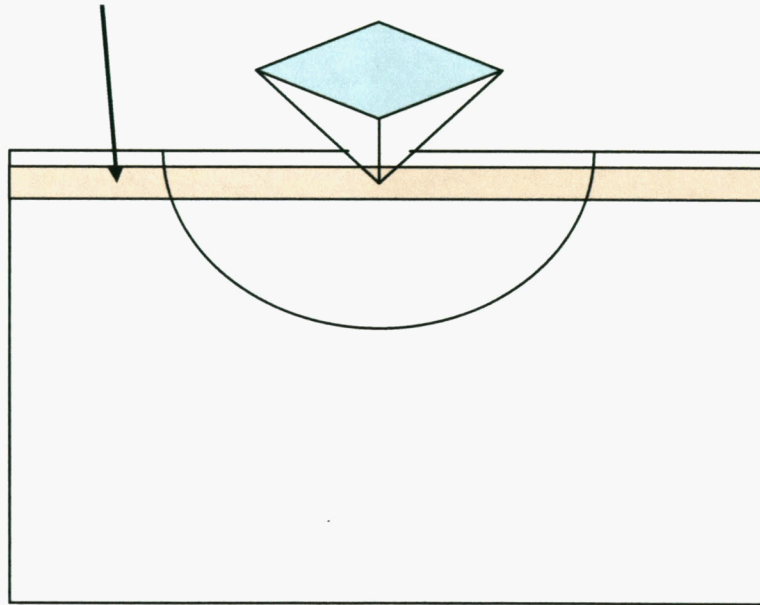
Fracture arrests at beginning of damage



Fracture Toughness =  $9.3 \text{ J/m}^2$

# Indentation Fracture Experiments

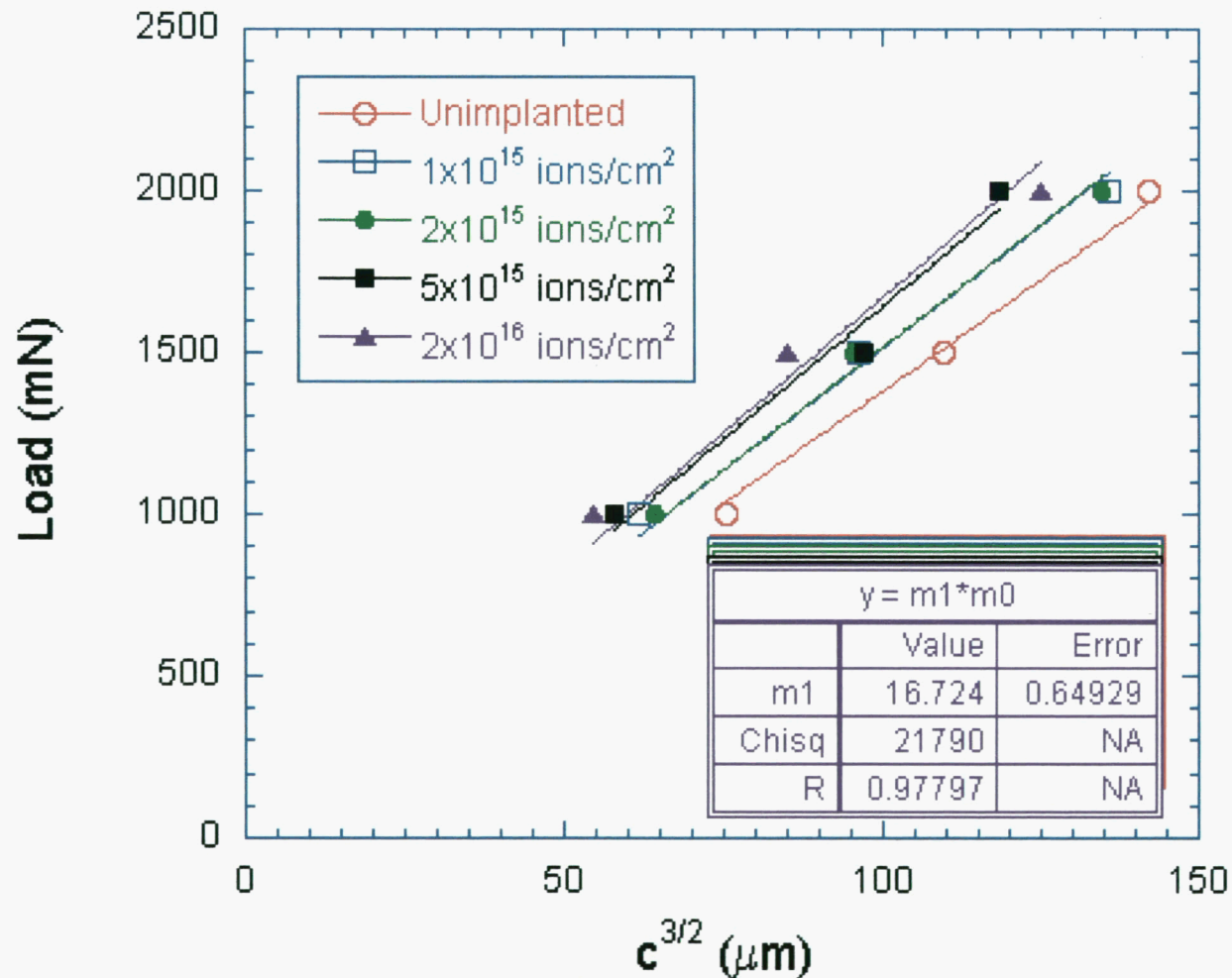
Implanted region



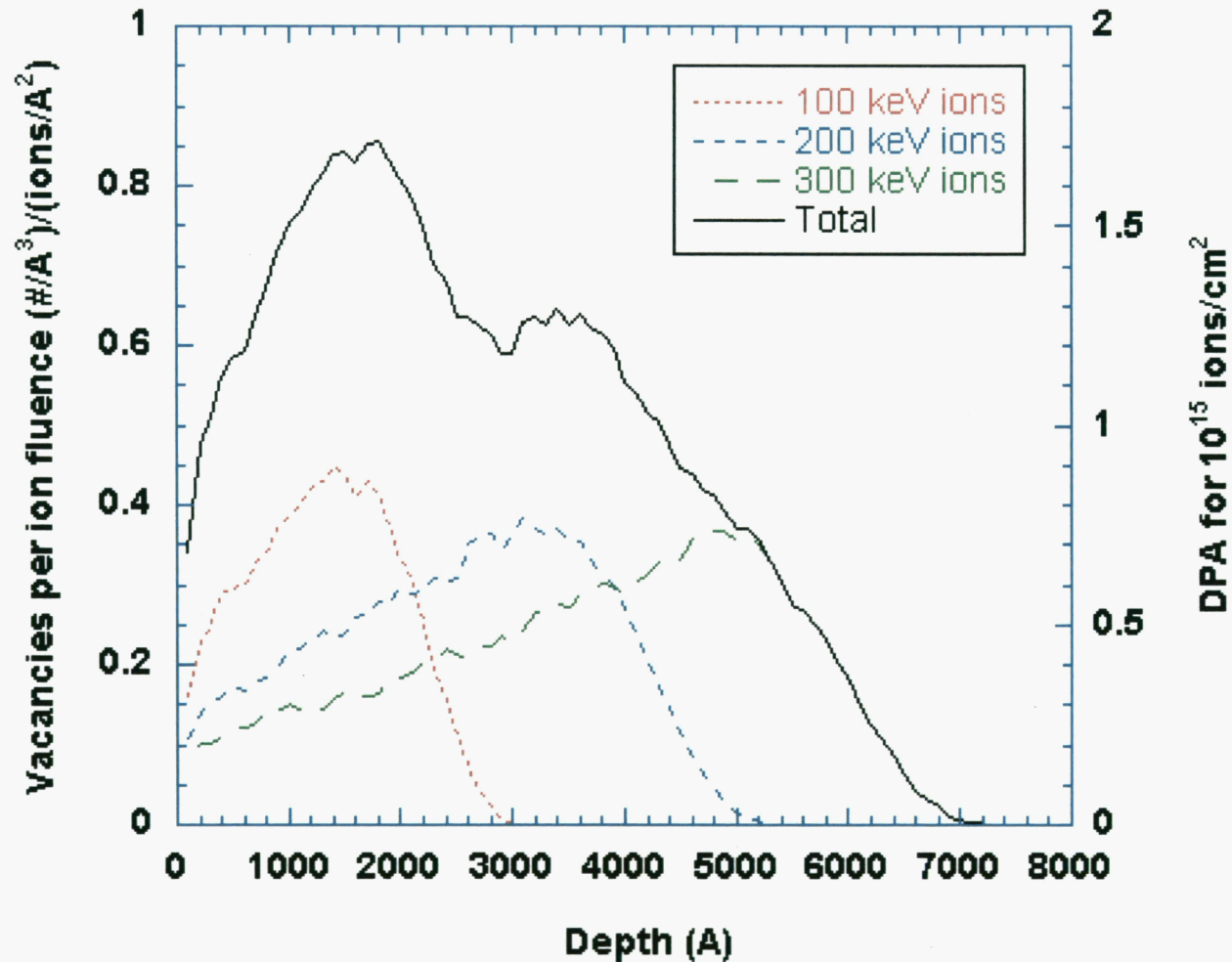


# Measurement of fracture toughness

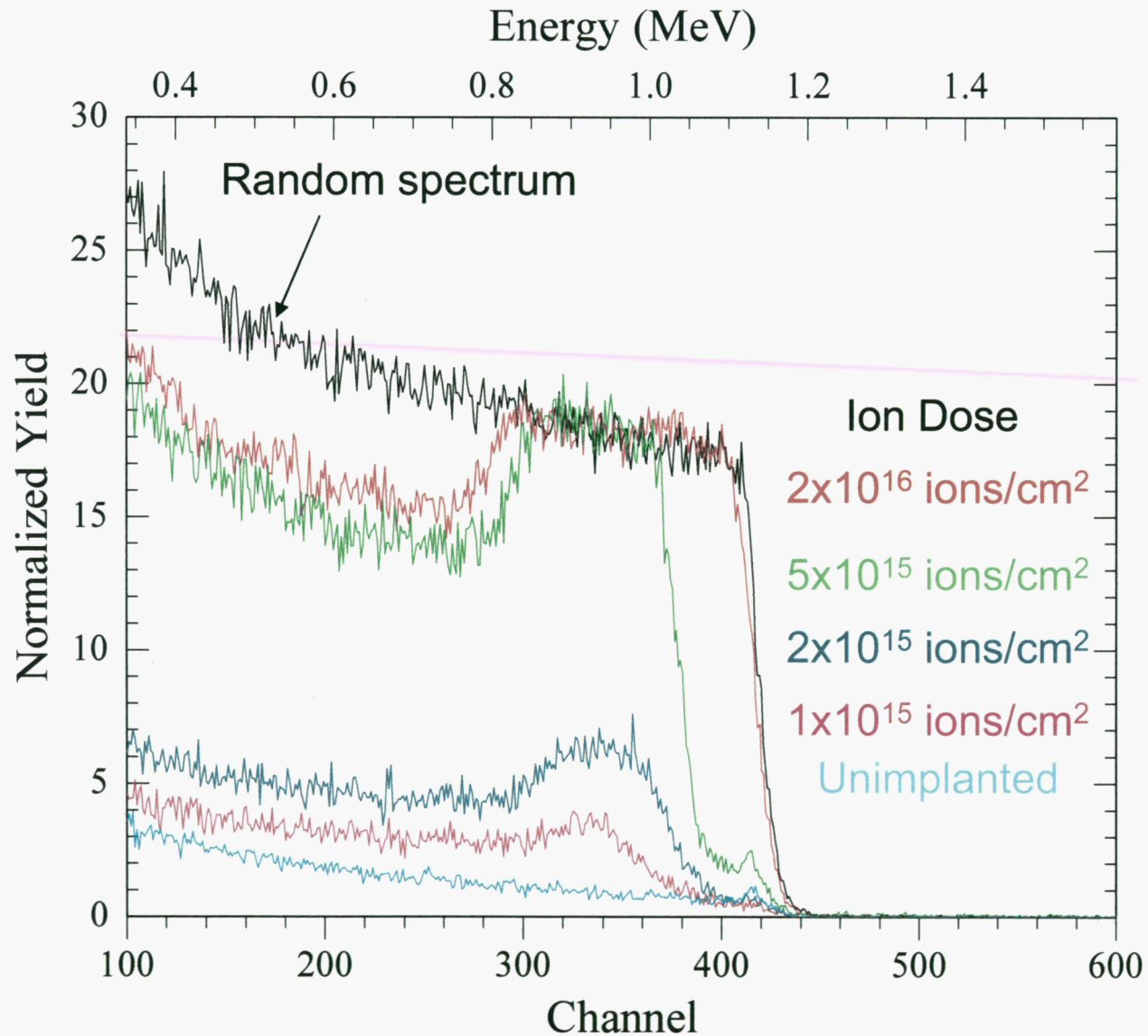
$$K_{IC} = 0.16(E/H)^{1/2}(P/c^{3/2})$$



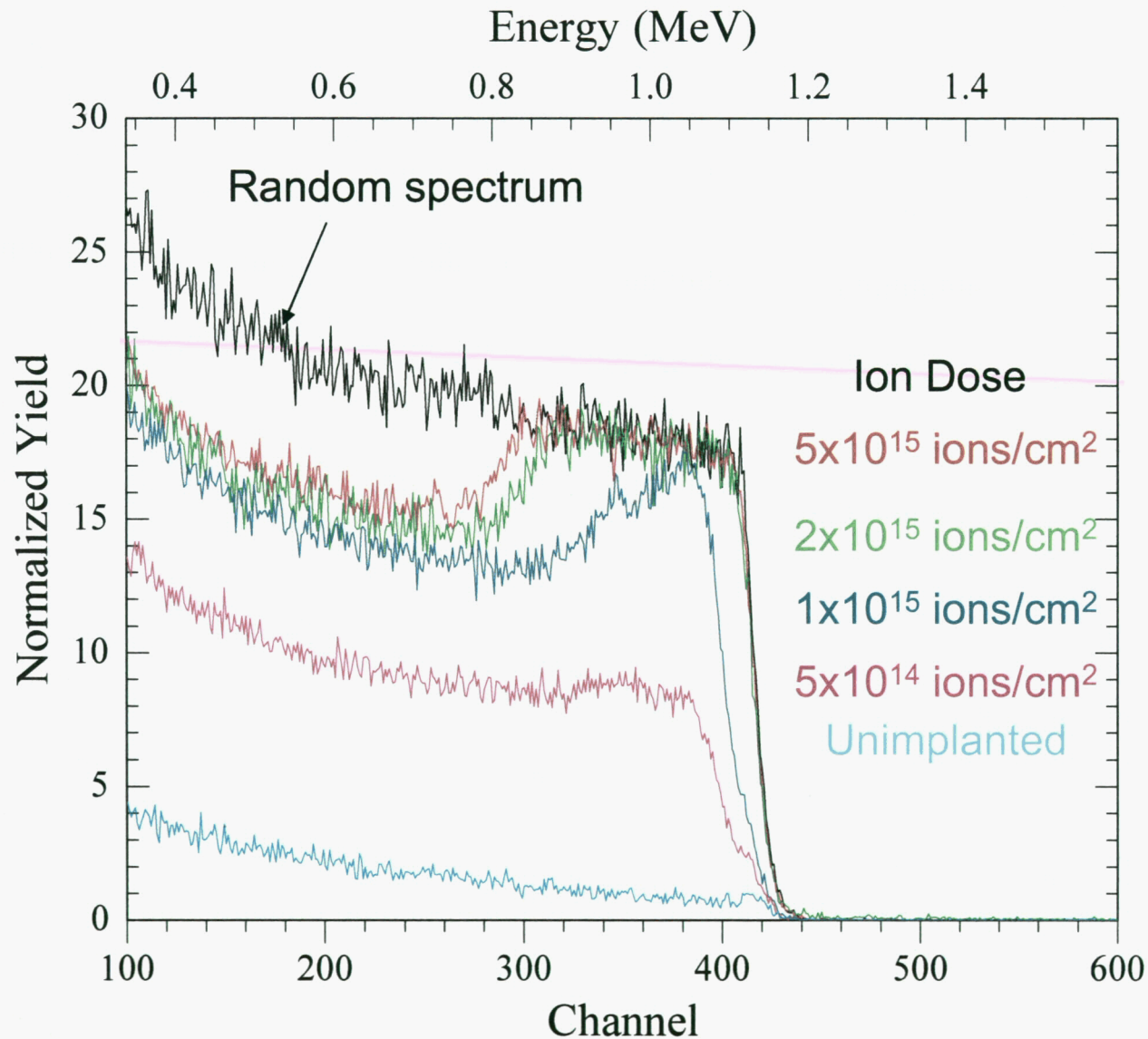
# SRIM calculations of damage in Si



# Channeling data for 300 keV Ne implanted in Si



# Channeling data for 100, 200 & 300 keV Ne ions



# Ion implantation increases fracture toughness

