Atomistic Configurations and Energetics of Crack Extension in Silicon

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A fundamental question in understanding fracture at the atomic level is how a sharp crack advances by a sequence of bond breaking events. Such insights would elucidate a wide range of phenomena, such as slow crack growth and environmental effects. In this work we apply a reaction pathway analysis to determine the minimum energy path for bond breaking along 3D, atomically sharp crack fronts in Si. Treating this path as a reaction coordinate we investigate the atomic configurations as well as the energetics of the crack front during the advancement of the crack tip by one atomic spacing. We find the crack-front extension occurs through a kink mechanism, the nucleation of a double kink followed by the spreading of this kink pair across the front. This scenario is essentially the same as the mechanism for a dislocation to glide in the diamond cubic lattice of Si . We are able to extract activation barriers in terms of kink nucleation and migration energies. Our investigation also leads to manifestations of lattice trapping and directional cleavage anisotropy effects beyond those discussed in 2D simulations [1,2].

References

[1] T. Zhu, J. Li and S. Yip, "Atomistic configurations and energetics of crack extension in silicon," *Physical Review Letters*, **93**, 205504, 2004.
[2] T. Zhu, J. Li and S. Yip. "Atomistic characterization of 3D lattice trapping barriers to brittle fracture", *Proceedings of the Royal Society of London* A, in press (2006).

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