Optimized Phase-Field Fracture Models for Monocrystalline Silicon

Ralf Denzer[1,*] **and Praveenkumar Hiremath**[1]

[1]Division of Solid Mechanics, Lund University, Lund, Sweden
e-mail: ralf.denzer@solid.lth.se and praveenkumar.hiremath@solid.lth.se

KEYWORDS: *Phase-field Fracture, Molecular Simulations, Silicon.*

Reliable silicon devices require predictive fracture models that remain accurate at small length scales, where crystal orientation and surface effects play a dominant role. We present a optimization based calibration strategy for phase-field fracture models based on molecular statics and dynamics (MS/MD) simulations that explicitly resolve atomic-scale fracture mechanisms. Silicon specimens are subjected to controlled loading conditions to initiate and propagate cracks. Thereby, orientation-dependent fracture behavior is characterized through energy release rates, crack trajectories, and traction–separation relations. These atomistic observables are translated into continuum phase-field parameters, including the critical energy release rate $\mathcal{G}_c$, the internal length scale l_0, the choice of degradation function as well as the crack surface density function, yielding a brittle fracture formulation in single-crystal silicon.

The calibrated phase-field model reproduces some key fracture characteristics across selected crystal orientations, capturing both crack path selection and energy dissipation in good agreement with MS/MD results. Parametric studies highlight the influence of l_0, $\mathcal{G}_c$, the degradation and surface density functions on crack regularization and dissipation, while crystallographic effects are incorporated through the calibrated constitutive response. Overall, the proposed framework establishes a link between atomistic fracture physics and continuum-scale modeling, providing fracture simulations in silicon-based materials.

[1] J.A. Hauch, D. Holland, M.P. Marder, and H.L. Swinney. Dynamic Fracture in Single Crystal Silicon, *Physical Review Letters* 82 (1999), 3823-3826.

[2] B.-J. Lee. A modified embedded atom method interatomic potential for silicon, *Calphad* 31 (2007) 95–104.

[3] J.-Y. Wu. A unified phase-field theory for the mechanics of damage and quasi-brittle failure, *Journal of the Mechanics and Physics of Solids* 103 (2017) 72–99.

[4] B. Bourdin, G.A. Francfort, J.-J. Marigo, The Variational Approach to Fracture, *Journal of Elasticity* 91 (2008) 5–148.