Wing Crack Dynamics in Silica Glass

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Outline

- Introduction
- MD simulation on silica glass
- Dynamic fracture simulations
- Discussion
- Summary
Compressive Loading on the Materials Causes Crack Growth from the Pre-Existing Cracks

Wing Crack Models Assuming Quasi-Static Loading

Wing crack emanate from pre-crack tip

\[ \theta = 70.5^\circ \]

Wing crack turns toward the maximum compression \( \sigma_1 \) direction

Nemat-Nasser and Horii, 1982

M. F. Ashby and C. G. Sammis, 1990
PAGEOPH 133, 489 (1990)

Florian Lehner and Mark Kachanov, 1996
Int. J. Frac. 77, R69 (1996)
Recent Experiments Regarding Cracking under Dynamic Compression

S. Lee, G. Ravichandran

M. Zhou, A. J. Rosakis and G. Ravichandran

D. Rittel

- Wing crack initiation and growth mechanism
- Local properties such as stress and temperature distribution
- Effects of confinements
- ...

Experimental and theoretical efforts have not been able to ascertain damage mechanisms underlying initiation, growth, and arrest of wing cracks at the level of material heterogeneity.
Molecular Dynamics Method

Equations of motion of atoms:

\[ \{ r_1(t), \ldots, r_N(t) \} \]

\[ m_i \frac{d^2 r_i(t)}{dt^2} = - \frac{\partial V}{\partial r_i} \]

Interatomic potential for Silica:

\[ V = \sum_{i,j} v_{ij}^{(2)}(r_{ij}) + \sum_{i,j,k} v_{ijk}^{(3)}(r_{ij}, r_{ik}) \]

Steric repulsion  Coulomb  Charge-dipole

Covalent bond bending & stretching
Validation of Silica Potential

- Neutron scattering experiment: Susman et al. ('91)
- MD simulations: Nakano et al. ('90)
Simulation Setup

Impactor

Impactor speeds: 150 m/s and 375 m/s

System Schematic
Wing crack dynamics at Impactor Speed
375 m/s

Shown here are pre-crack (light blue) and nanocavities (red, green, yellow, orange ... )
Wing crack dynamics at Impactor Speed
150 m/s
Wing Crack Initiation

Stress distribution

Nanocavities, crack nanocolumns grow in tensile stress region
Wing Crack Formation

Frictional sliding of precrack surfaces initiates cavities to form crack nanocolumns.

These nanocrack columns merge to form a wing crack.

The wing crack tip bends 70° towards maximum tension, as predicted theoretically and observed in experiments.
Temperature Change vs. Distance from the Crack Tip

![Diagram showing temperature change vs. distance from the crack tip](image-url)
Healing of Wing Crack and Nanocavities

The wing crack is arrested by confinement, similar to experiments

Wing crack dynamics pulse loading

The impacter is stopped after 20ps
Wing crack dynamics pulse loading
Wing crack & Damage Cavities at 0.5 and 1.0 nanosecond
MD simulations were performed to simulate the behavior of silica glass under dynamic compression.

The arrest and healing of wing crack is consistent with experiments.

Nanocavitation is shown to be the main growth mechanism for the wing crack.

Local properties such as stress and temperature helped us understand the behavior of wing crack.

Questions?
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