MECHANICS OF CRACK PROPAGATION INITIATION IN CRYSTALLINE SILICON AND AMORPHOUS SILICA AT ATOMISTIC SCALE

ASHISH SINGH

Department of Applied Mechanics

INDIAN INSTITUTE OF TECHNOLOGY DELHI

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by

ASHISH SINGH

Department of Applied Mechanics

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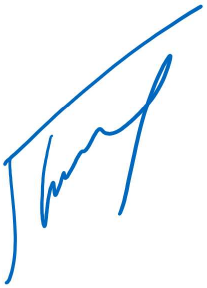
Certificate

This is to certify that the thesis titled **Mechanics of crack propagation initiation in crystalline silicon and amorphous silica at atomistic scale**, submitted by **Mr. Ashish Singh**, to the Indian Institute of Technology, Delhi, for the award of the degree of **Doctor of Philosophy**, is a bonafide record of the research work done by him under our supervision and guidance. The thesis works meet the requisite standards, and the candidate is worthy of consideration for the Degree of Philosophy by the institute's regulations.

The results in this thesis have not been submitted in part or in whole to any other institute or university for the award of any degree or diploma.



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Dr. Gaurav Singh
Associate Professor
Department of Applied Mechanics
Indian Institute of Technology Delhi
Hauz Khas, New Delhi, India - 110016

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Abstract

This thesis work utilizes the local near-tip stress field at the critical state, just before crack propagation initiation, to measure critical stress intensity factor in crystalline silicon and amorphous silica using atomistic simulations. Compared to the already utilized methods, which employ global overall/remote stress to find critical energy release rate and then relate it to critical SIF, the method used in the present work is more direct as it makes measurements in the near-tip region where crack propagation will indeed initiate.

Furthermore, the local near-tip stress field method is the only way to study crack propagation initiation under mixed-mode conditions in amorphous solids since any global measurement (like remote/overall stress) will be agnostic to individual mode contributions. A crack propagation initiation criteria has thus been derived in the present work by utilizing the near-tip measured stress intensity factors at the critical state. A rigorous validation has been conducted at all stages of this work.

Since the continuum concept of deformation gradient has been used, the methodology developed in the present work can be applied to any other kind of crystalline or amorphous solid. An atom has been considered as a continuum point, and hence, the method does not distinguish between the number or type of elements involved or their atomic structure as a solid.

सार

यह शोध कार्य क्रैक के बढ़ने की प्रारंभिक स्थिति से ठीक पहले की स्थिति में उपलब्ध क्रैक टिप के पास रहने वाली स्ट्रेस फील्ड का उपयोग करता है, ताकि क्रिस्टलाइन सिलिकॉन और अमॉर्फस सिलिका में एटॉमिस्टिक सिमुलेशन्स के माध्यम से क्रिटिकल स्ट्रेस इंटेंसिटी फैक्टर को मापा जा सके। पहले से प्रयुक्त विधियों की तुलना में, जो क्रिटिकल एनर्जी रिलीज़ रेट प्राप्त करने के लिए ग्लोबल (ओवरऑल/रिमोट स्ट्रेस) का उपयोग करती हैं और फिर उसे क्रिटिकल स्ट्रेस इंटेंसिटी फैक्टर (क्रिटिकल SIF) से सम्बद्ध करती हैं, वर्तमान कार्य में प्रयुक्त विधि अधिक प्रत्यक्ष है, क्योंकि इसमें मापन क्रैक टिप के पास में किया जाता है जहाँ वास्तव में क्रैक की वृद्धि आरंभ होती है।

इसके अतिरिक्त, क्रैक टिप के पास रहने वाली फील्ड विधि ही एकमात्र ऐसी विधि है जिसके माध्यम से अमॉर्फस पदार्थों में मिक्स्ड-मोड स्थिति के अंतर्गत क्रैक की वृद्धि की शुरुआत का अध्ययन किया जा सकता है, क्योंकि कोई भी ग्लोबल मापन (जैसे रिमोट/ओवरऑल स्ट्रेस) व्यक्तिगत मोड योगदानों के प्रति संवेदनशील नहीं होता। वर्तमान शोध में, क्रिटिकल स्थिति पर क्रैक टिप के पास क्षेत्र में मापे गए स्ट्रेस इंटेंसिटी फैक्टर्स ($SIFs$) का उपयोग करके क्रैक वृद्धि की शुरुआत हेतु एक मानदण्ड प्राप्त किया गया है। इस कार्य के प्रत्येक चरण पर कठोर मान्यकरण किया गया है।

चूंकि इस अध्ययन में डिफॉर्मेशन ग्रेडिएंट की कंटिन्युअम अवधारणा का उपयोग किया गया है, इसलिए यह विकसित मेथडोलॉजी किसी भी क्रिस्टलाइन या अमॉर्फस पदार्थ पर लागू की जा सकती है। प्रत्येक एटम को एक कंटिन्युअम पॉइंट के रूप में माना गया है, अतः यह विधि किसी भी तरह की एटॉमिक स्ट्रक्चर या तत्वों की संख्या व प्रकार में भेद नहीं करती है।

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Abbreviations

BCC	**B**ody **C**entered **C**ubic
CCI	**C**rack **C**losure **I**ntegrals
CNSR	**C**hevron-**N**otched **S**hort **R**od
CT	**C**ompact **T**ension
CTOD	**C**rack **T**ip **O**pening **D**isplacement
CZM	**C**ohesive **Z**one **M**odeling
DCB	**D**ouble **C**antilever **B**eam
EAM	**E**mbedded **A**tom **M**odel
ERR	**E**nergy **R**elease **R**ate
FEM	**F**inite **E**lement **M**ethod
FIB	**F**ocused **I**on **B**eam
FPZ	**F**racture **P**rocess **Z**one
HDNT	**H**igh-**D**ensity **N**anotwinned
LAMMPS	**L**arge-scale **A**tomic/**M**olecular **M**assively **P**arallel **S**imulator
LDNT	**L**ow-**D**ensity **N**anotwinned
LEFM	**L**inear **E**lastic **F**racture **M**echanics
MEMS/NEMS	**M**icro and **N**ano **E**lectro **M**echanical **S**ystems
MTS	**M**aximum **T**angential **S**tress
MVCCI	**M**odified **V**irtual **C**rack **C**losure **I**ntegral
OVITO	**O**pen **V**isualization **T**ool
PECVD	**P**lasma-**E**nhanced **C**hemical-**V**apor-**D**eposited
RVE	**R**epresentative **V**olume **E**lement
SED	**S**train **E**nergy **D**ensity
SERR	**S**train **E**nergy **R**elease **R**ates
SIF	**S**tress **I**ntensity **F**actor
STZ	**S**hear **T**ransformation **Z**one

SW	**S**tillinger–**W**eber **I**nteratomic **P**otential
TDCB	**T**apered **D**ouble **C**antilever **B**eam
TEM	**T**ransmission **E**lectron **M**icroscope
UEL	**U**ser **E**lement **S**ub-**R**outine
UFG	**U**ltrafine **G**rained
XFEM	**E**xtended **F**inite **E**lement **M**ethod

Symbols

ϕ	Potential energy
$\epsilon^o_{yy}, \epsilon^o_{xx}$	Remote strains in pulling direction
σ_o	Stress at critical state in crystalline silicon & amorphous silica
n	Homogenization atoms number
k	Averaging atom's number
E	Young's modulus
ν	Poisson's ratio
K_I	Stress intensity factor for Mode I
K_{II}	Stress intensity factor for Mode II
G_C	Critical energy release rate
J_C	Critical J-integral
K_{IC}	Critical stress intensity factor for Mode I
X_J and x_i	Initial and deformed atomic positions respectively
χ	Deformation mapping function
I	Identity matrix
Δx, Δy and Δz	Size of the sample
ϵ_{kl}	Strain tensor
ϵ_o	Remote strain
$c^{'}_{ijkl}$	Elasticity tensor components
c_{ijkl}	Transformed elasticity tensor components
E_{ij} and e_{ij}	Finite and infinitesimal strain tensors
E_{111}	Young's modulus in the plane strain condition
F_{iI}	Deformation gradient
K_{IC}	Critical stress intensity factor for Mode I
r_P	Region near crack-tip where linear elasticity is not valid
r_K	Region near crack-tip where linear elasticity is valid

R^2	Coefficient of determination
σ_{cr}	Remote boundary stress at the critical state
σ_n, σ_s	Far-field normal and shear stress at the instant of first bond rupture
$Y, Y_1, ...Y_n$	Geometrical parameters
$K_{I,i}$	Stress intensity factor
σ_{eq}	Equivalent stress
U, W	Strain energy and work done by external loads
A_{proj}	Crack surface area
K_{eff}	Effective stress intensity factor
S_{11}	Plane strain compliance
q	Dimensionless cubic parameter
γ	Surface energy density
Q	Correction factor
B, W	Specimen dimensions
δ	CTOD
σ_x	Hardy stress
σ_{ij}	Virial stress
p	Hydrostatic stress
K	Hardening parameter
G	Potential function
$\boldsymbol{\xi}$	Internal variables
$\mathrm{d}\lambda$	Plastic multiplier
α	Material parameter
σ_y	Yield stress
$\mathrm{d}\epsilon_{ij}, \mathrm{d}\epsilon^p_{ij}, \mathrm{d}\epsilon^e_{ij}$	Total, plastic, and elastic strain increments
F^a_y, F^b_y	Vertical components of the nodal forces at nodes a and b
u^c_y, u^d_y, u^e_y, u^f_y	Vertical displacements at the respective nodes
m_α	Mass of atom α in Ω
u^i_α	Velocity along the direction i of the atom α
u^j_α	Velocity along direction j of atom α
u^i	Local average velocity along the direction i of the atom α
u^j	Local average velocity along the direction j of the atom α
$f^\beta_{\alpha\beta}$	Force on atom α exerted by atom β
r_α	Atomic position of atom α
v^{rel}_α	Relative velocity of atom α

$f_{\alpha\beta}$	Force acting on atom α due to atom β
$r_{\alpha\beta}$	Vector connecting atoms α and β
$t(x, n; t)$	Tsai traction
u_c	Critical displacement
N	Number of atoms in the system
k_B	Boltzmann constant
m_i	Mass of the i-th atom
v_i	Velocity of the i-th atom
T	Temperature of the system
$A(s)$	Instantaneous value of property A at time s
S	Total observation time
$\langle A \rangle$	Ensemble average of property A
Γ	Phase space of the system
$\rho(\mathbf{x})$	Probability density function in phase space