

**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

JUNE 2025

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

by

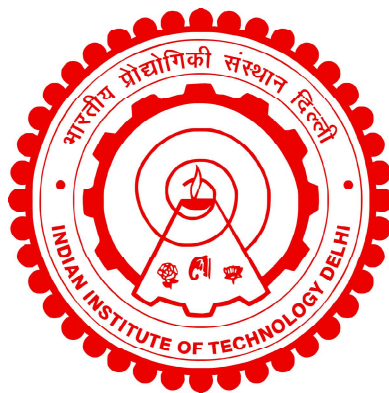
ASHISH SINGH

Department of Applied Mechanics

Submitted

in fulfillment of the requirements of the degree of Doctor of Philosophy

to the



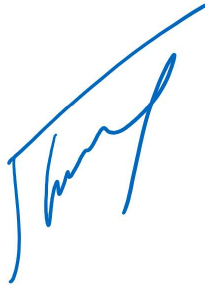
INDIAN INSTITUTE OF TECHNOLOGY DELHI

JUNE 2025

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.



09/07/2025

Dr. Gaurav Singh

Associate Professor

Department of Applied Mechanics

Indian Institute of Technology Delhi

Hauz Khas, New Delhi, India - 110016

Acknowledgements

I am grateful to everyone who supported me throughout my Ph.D. journey.

I am especially thankful to Prof. Gaurav Singh, my advisor, for his continuous support and guidance during my research. His expertise has been very helpful throughout this journey.

I also want to thank to my SRC members, Prof. BP Patel, Prof. Ajeet Kumar, and Prof. Naresh V. Datla. Their feedback has played an important role in refining this research work.

I am deeply thankful to my parents for everything they have done for me, especially their unwavering support over the past several years. I sincerely thank my wife for her constant support, love, and patience throughout this journey. I am also grateful to my sisters for their unwavering encouragement and belief in me.

Furthermore, I also want to thank my friends, and siblings for their continuous support throughout this journey.

I also acknowledge Prof. Subhas Ghosal (NIT Durgapur) for his initial support and the IIT Delhi HPC facility for providing essential computational resources

Finally, I am deeply grateful to the Almighty for his endless blessings and guidance.

Ashish Singh



09/07/2025

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 इंटेन्सिटी 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 इंटेन्सिटी 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 मिक्सड-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 इंटेन्सिटी 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।

Contents

Certificate	i
Acknowledgements	ii
Abstract	iii
Contents	v
List of Figures	ix
List of Tables	xiii
Abbreviations	xv
Symbols	xvii
1 Introduction	1
1.1 Motivation	1
1.1.1 Applications across length scales	3
1.2 Fracture mechanics	4
1.2.1 Phenomena of Fracture	4
1.2.2 Mechanics of Fracture	4
1.2.3 Experiments and Simulations in Fracture Mechanics	6
1.2.3.1 Experiments	6
1.2.3.2 Simulations	12
1.3 Atomistic simulation	14
1.3.1 Preparation of silicon and silica	15
1.3.2 Mechanical properties	15
1.3.2.1 Inter-atomic potentials	15
1.3.2.2 Quenching rate	16
1.3.2.3 Testing temperature	17

1.3.2.4	Strain rate	17
1.3.2.5	Ensemble	17
1.3.2.6	Simulation box	18
1.3.3	Atomistic stress calculation	21
1.3.4	Fracture mechanics through atomistic simulations	26
1.3.4.1	Mode I test	27
1.3.4.2	Mixed-mode test	41
1.3.5	Plasticity	46
1.4	Research gap	52
1.5	Objectives	53
1.6	Thesis structure	54
1.7	Softwares used	54
1.7.1	LAMMPS	54
1.7.2	OVITO	55
1.7.3	Python	55
1.7.4	Atomsk	55
2	Critical SIF for crystalline silicon	57
2.1	Structure, orientation, geometry and loading	57
2.2	Global (remote boundary) method	60
2.3	Local (near tip) method	60
2.3.1	Virial	60
2.3.2	Analytical	61
2.4	Local analytical method	67
2.4.1	Elasticity tensor components calculation	67
2.4.2	Choice of suitable inter-atomic potential	68
2.5	Mechanical response of uncracked sample	72
2.6	Mechanical response of cracked sample	73
2.6.1	Critical state identification	74
2.6.2	Stress calculation	75
2.7	Critical SIF	82
2.7.1	Continuum	83
2.7.2	Analytical	85
3	Critical SIF for amorphous silica	89
3.1	Preparation of sample	89
3.2	Structure, geometry, and loading	90
3.3	Global method	93
3.4	Local method	94
3.4.1	Virial	94
3.4.2	Analytical	94
3.5	Local analytical method	95
3.5.1	Elasticity tensor components calculation	95
3.6	Mechanical response of uncracked sample	97

3.7	Mechanical response of cracked sample	99
3.7.1	Critical state identification	100
3.7.2	Stress calculation	102
3.7.2.1	At each atomic site	103
3.7.2.2	Averaging	104
3.8	Critical SIF	111
3.8.1	Continuum	112
3.8.2	Analytical	113
4	Local SIFs in mixed-mode	117
4.1	Geometry and loading	117
4.2	Mechanical response of cracked sample	119
4.2.1	Critical state identification	119
4.2.2	Stress calculation	120
4.3	Local SIFs at critical state	125
4.3.1	Mode I	125
4.3.2	Mode II	130
4.4	Crack propagation initiation criteria	131
4.4.1	Linear	134
4.4.2	Quadratic	134
4.4.3	Parabolic	136
5	Conclusion	139
5.1	Conclusion	139
5.2	Future Work	141
	Bibliography	145
	List of Publications	177
	Brief Biodata	179

List of Figures

2.1	Cracked silicon sample consisting of 1,81,440 atoms subjected to a remote uniaxial strain loading along the x (pulling) direction	59
2.2	Atoms are in a definite pattern near a crack tip in silicon	61
2.3	Variation of normalized strain ϵ_{xx} along the crack line subjected to a remote loading along x (pulling) direction	66
2.4	Variation of normalized stress σ_{xx} in the mid-plane with different numbers of homogenization atoms in uncracked sample	67
2.5	Variation of normalized stress σ_{xx} in the crack-plane with different number of homogenization atoms in cracked sample	68
2.6	Variation of elasticity tensor components with atomistic system size of silicon with SW potential	69
2.7	Uncracked silicon sample consisting of 1,81,440 atoms subjected to a remote uniaxial strain along the x (pulling) direction	71
2.8	Overall mechanical response of silicon sample consisting of 1,81,440 atoms subjected to a remote uniaxial strain along x direction at 1 K under NPT ensemble	72
2.9	Linear region of mechanical response of uncracked and cracked silicon sample consisting of 1,81,440 atoms subjected to a remote uniaxial strain along the x (pulling) direction	74
2.10	Atoms around the crack tip at (a) 0.074 remote strain, (b) 0.075 remote strain (critical state), (c) 0.076 remote strain, (d) 0.077 remote strain	75
2.11	Cracked silicon sample subjected to a uniaxial strain loading along the x direction	76
2.12	Variation of normalized stress σ_{xx} in the crack plane with analytical FE methods	77
2.13	Meshing of an edge-cracked crystalline silicon specimen	78
2.14	Variation of normalized stress σ_{xx} along the crack plane calculated with SW potential for a cracked silicon specimen	83
2.15	Variation of stress σ_{xx} with inverse square-root distance from the crack tip at a remote strain of 0.075 for different number of atoms beyond first three atoms from crack tip	86
3.1	Methodology for the preparation of amorphous silica	91

3.2	Cracked amorphous silica sample subjected to remote uniaxial strain along the y direction	93
3.3	Random position of atoms in silica near crack tip	95
3.4	Uncracked amorphous silica sample subjected to a remote uniaxial strain along the y direction	98
3.5	Mechanical response of uncracked sample under different remote loading along the y direction	99
3.6	Cracked amorphous silica sample subjected to a different remote uniaxial strain loading along the y direction	100
3.7	Atoms around the crack tip at (a) 0.101 remote strain, (b) 0.102 remote strain, (c) 0.103 remote strain (critical state), (d) 0.104 remote strain, (e) 0.105 remote strain, (f) 0.106 remote strain	101
3.8	Variation of normalized strain ϵ_{yy} along the crack plane calculated over same homogenized atoms for a cracked sample at the critical remote strain of 0.103	102
3.9	Variation of normalized stress field along the crack plane calculated over different number of homogenization atoms at remote strain of 0.103. Averaging has been done over 10 neighbouring in-plane atoms	103
3.10	Variation of normalized stress field along the crack plane calculated over 40 homogenized atoms for a cracked sample at the critical remote strain of 0.103	105
3.11	Cracked silica sample subjected to a uniaxial strain loading along the y direction at a remote strain of 0.103 in FEM simulation (u_c is critical displacement obtained at a remote strain of 0.103)	106
3.12	Effect of number of FEM elements on normalized stress field in a cracked silica sample subjected to a remote loading of 0.103	107
3.13	Meshing of an edge-cracked amorphous silica specimen	107
3.14	Comparison of normalized analytical stress field ahead of the crack tip with FEM at remote critical strain 0.103 for a cracked silica sample in plane strain	108
3.15	Coarse mesh near the crack tip	109
3.16	Fine mesh near the crack tip	110
3.17	Dependence of normal stress near the crack tip with number of meshing elements	110
3.18	Log-log plot of the error with element size h	112
3.19	Variation of stress σ_{yy} with inverse square-root distance from the crack tip at a remote strain of 0.103 for different numbers of atomic sites beyond the first four from the crack tip	113
4.1	Cracked silica sample consisting of 2,01,600 atoms subjected to a remote uniaxial strain loading along the x direction and crack is inclined at 15°	118
4.2	Mechanical response of cracked sample inclined at various orientations	119

4.3	Atoms near the 0° inclined crack tip at (a) 0.091 remote strain (b) 0.092 remote strain (critical state) (c) 0.093 remote strain (d) 0.094 remote strain	120
4.4	Atoms near the 15° inclined crack tip at (a) 0.094 remote strain (b) 0.095 remote strain (critical state) (c) 0.096 remote strain (d) 0.097 remote strain	121
4.5	Atoms near the 30° inclined crack tip at (a) 0.097 remote strain (b) 0.098 remote strain (critical state) (c) 0.099 remote strain (d) 0.1 remote strain	121
4.6	Atoms near the 45° inclined crack tip at (a) 0.111 remote strain (b) 0.112 remote strain (critical state) (c) 0.113 remote strain (d) 0.114 remote strain	122
4.7	Coordinate transformation	122
4.8	Meshing of a central crack (0°) in an amorphous silica specimen . . .	123
4.9	Meshing of a 15° inclined crack in an amorphous silica specimen . . .	124
4.10	Meshing of a 30° inclined crack in an amorphous silica specimen . . .	124
4.11	Meshing of a 45° inclined crack in an amorphous silica specimen . . .	125
4.12	(a) Normalized stress field along the crack line in Mode I for 0° inclined crack (b) Normalized stress field along the crack line in Mode II for 0° inclined crack	126
4.13	(a) Normalized stress field along the crack line in Mode I for 15° inclined crack (b) Normalized stress field along the crack line in Mode II for 15° inclined crack	127
4.14	(a) Normalized stress field along the crack line in Mode I for 30° inclined crack (b) Normalized stress field along the crack line in Mode II for 30° inclined crack	128
4.15	(a) Normalized stress field along the crack line in Mode I for 45° inclined crack (b) Normalized stress field along the crack line in Mode II for 45° inclined crack	129
4.16	Linear form of crack propagation initiation criteria	135
4.17	Quadratic form of crack propagation initiation criterion	136

List of Tables

1.1	Potential parameters for MD simulations	16
2.1	Elastic constants of < 100 > silicon using various methods	69
2.2	Atomic sites considered for calculation of critical SIF	87
3.1	Variation of linear elasticity tensor components with system size in amorphous silica	96
3.2	Average value of elasticity tensor components variation with system size in amorphous silica	97
3.3	Mechanical properties of amorphous silica through various methods .	97
3.4	Atomic sites considered for calculation of critical SIF in amorphous silica	114
4.1	Local stress intensity factors at critical state for mixed-mode loading	130

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
$\epsilon_{yy}^o, \epsilon_{xx}^o$	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
$\Delta x, \Delta y$ 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_{il}	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, \dots, 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
ξ	Internal variables
$d\lambda$	Plastic multiplier
α	Material parameter
σ_y	Yield stress
$d\epsilon_{ij}, d\epsilon_{ij}^p, d\epsilon_{ij}^e$	Total, plastic, and elastic strain increments
F_y^a, F_y^b	Vertical components of the nodal forces at nodes a and b
$u_y^c, u_y^d, u_y^e, u_y^f$	Vertical displacements at the respective nodes
m_α	Mass of atom α in Ω
u_α^i	Velocity along the direction i of the atom α
u_α^j	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
$f_{\alpha\beta}^\beta$	Force on atom α exerted by atom β
r_α	Atomic position of atom α
v_α^{rel}	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