15th International Conference on Fracture (ICF15)
June 11-16, 2023 Atlanta, GA USA

USING ANALYTICAL APPROACH FOR CALCULATING LOCALIZED STRESS FIELD NEAR CENTRAL SLIT CRACK IN AMORPHOUS MATERIAL AT ATOMISTIC SCALE

Ashish Singh*, Gaurav Singh

Department of Applied Mechanics, Indian Institute of Technology Delhi, Hauz Khas, New Delhi-110016, India
** Presenting Author email: ashish.singh@am.iitd.ac.in*

Abstract

The localized stress field helps in predicting the crack initiation and its growth in fracture mechanics. At an atomistic scale, a localized stress field has been calculated by virial theorem for anisotropic materials. However, there is still confusion regarding its validation and comparison, as its origin differs from continuum stress. Moreover, finding the localized stress field at the atomic site for amorphous materials are complicated and tedious by the virial approach due to the presence of different elements at disordered positions. Therefore, there is a need to develop a method which does not have there drawbacks. The present work has developed an analytical approach to calculate localized stress fields at an atomistic scale. First, the stress field calculated with this method has been validated in crystalline materials like silicon with virial and finite element (FEM) results. As this method validates linear elasticity near the crack tip. The same localized approach has been used in silica to validate stress field with FEM result. The proposed method in the present work can be used under mixed-mode conditions to study crack initiation and its growth in amorphous solids.

1. Introduction

The amorphous silica structure can be understood in terms of the ring and angle distributions, as it does not have long-range order like crystals. The rise in nanotechnology has led to an increase in the demand for amorphous silica as a substrate. Therefore, it is necessary to understand its fracture mechanics, as every material has some irregularities. These irregularities (like cracks and notches) amplify the stress field near the crack tip, which may lead to the fracture of materials. The amorphous silica has been prepared by step-wise quenching of a relaxed cristobalite sample. The sample consisting of 86400 atoms with dimensions 420.16 Å, 210.08 Å and 14.13 Å in x, y and z respectively have been modelled with BKS inter-atomic potential. The atomistic simulation has been performed under NPT conditions with a strain rate of 0.01/ps at 300 K. The lateral dimension has been free to deform, to allow Poisson's effect. The central slit crack of size 42 Å has been formed by breaking the bonds between mid-plane atoms without removing atoms. The analytical and FEM approaches have been used for further study. The analytical approach depends on the deformation gradient for strain calculation. The deformation gradient is calculated using atomic coordinates of deformed and undeformed states. Using Hooke's law, stress at a particular atomic site can be calculated.

2. Results

The localized stress field has been calculated at critical remote strain 0.130 as shown in Fig. 1(a). As shown in Fig. 1(b), crack growth is observed at remote strain 0.131, so critical state will be just before it (0.130). The summaries of this present work for amorphous silica for central slit crack are

a. The localized stress field calculated by analytical and FEM matches just before the crack tip, which validates linear elasticity, as shown in Fig. 2.
b. In FEM, linear quadrilateral elements of type CPE4 has been taken, as it clearly shown in Fig. 2, number of elements have negligible effect on localized stress field.

The identification of a critical state is crucial for predicting crack initiation. This critical state is used for calculation of critical stress intensity factor (SIF).

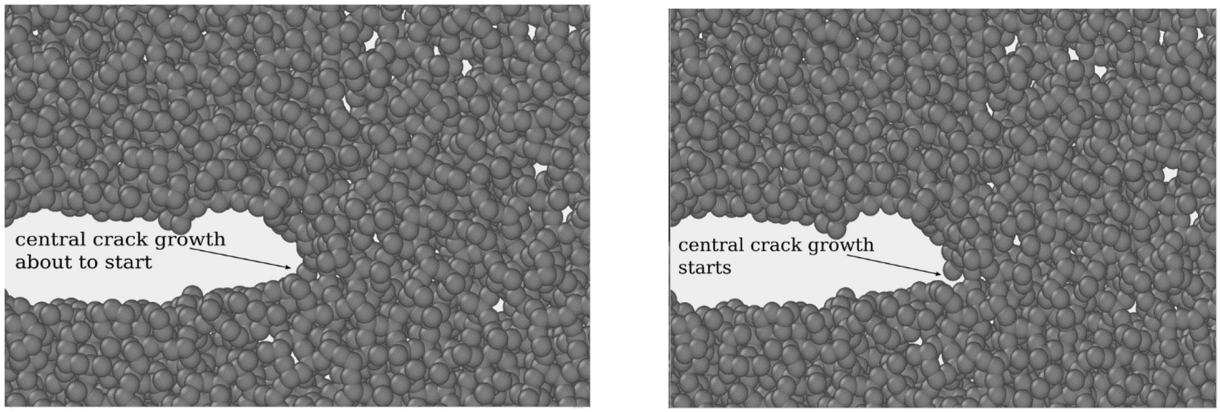

Fig.1 – (a) Crack condition at critical remote strain 0.130 (b) Crack condition at remote strain 0.131

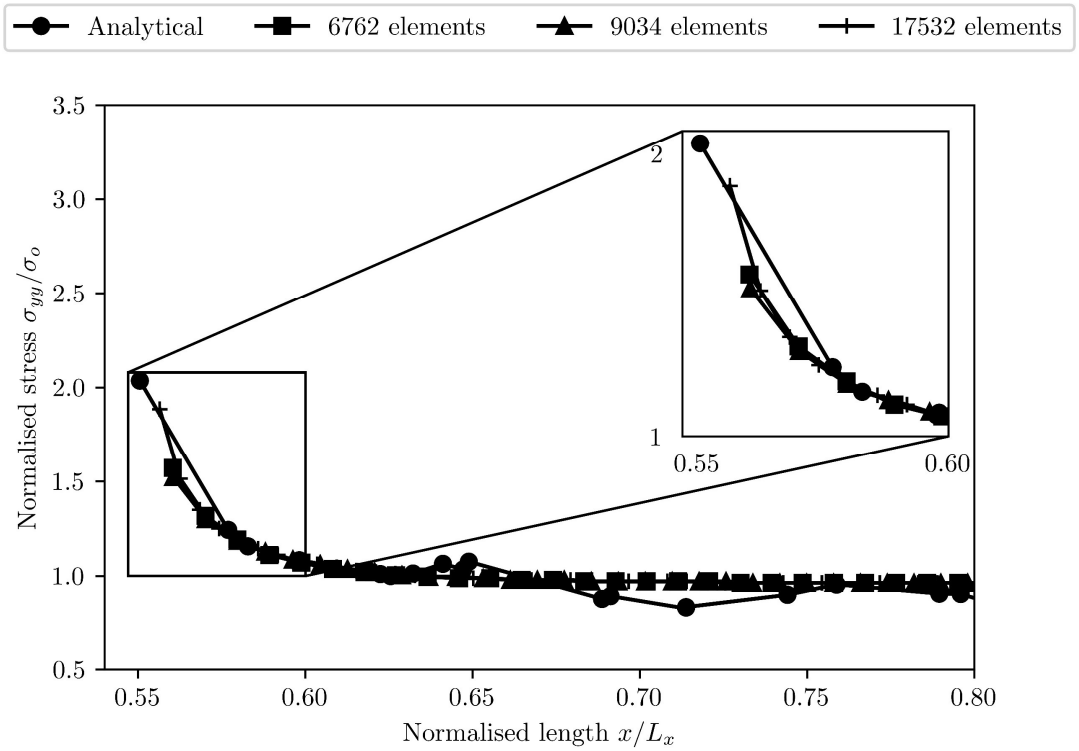

Fig.2 – Normalised stress field variation near the crack-tip in amorphous silica at remote strain 0.130

3. Conclusions

The stress field matches well with FEM ahead of the crack tip within the linear elastic region. This behavior is correctly predicted by BKS inter-atomic potential, which justifies its use. The critical SIF can be calculated at a critical state (remote strain of 0.130) by fitting the localized normal stress on the inverse square root relation. The calculated critical SIF is used to further calculate critical SIF in pure Mode II. The crack growth criteria can then be found by using either maximum tangential stress and strain energy density criteria.