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IMPLEMENTATION OF MODIFIED VIRTUAL INTERNAL BOND METHOD TO INVESTIGATE FRACTURE SIMULATIONS IN BRITTLE MATERIALS.

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***Abstract*—Modified virtual internal bond method with an integration of atomistic scale and continuum scale. In this method the domain is presumed to be consisting of material points which are randomly distributed and connected through virtual bond the stress-strain response is controlled through defined potential function. In this paper an attempt is made to derive the stress and strain expression within the frame work of hyper elastic model by using energy stored in normal and shear bond thus the obtain stress and strain expression are used to write Vu-mat subroutines provided in Abaqus environment. In order to prove the robustness of the code several standard cases of fracture problems are solved the obtained results in respect of crack propagation reasonable agreed with a published literature thus existing modified virtual internal bond method can be used as a fracture studies where complex loading.**

Keywords—: Bond energy potential, Virtual internal bond,Crack propagation,Brittle material

I. INTRODUCTION

The Modified virtual internal bond (MVIB) is a micro-macro constitutive modeling method for solids. Virtual internal bond model Developed by Klein and Gao. Every solid consists of randomized material particles on micro scale it may be billions of the particles consists in small solid part.These material particles are connected with virtual internal bonds. The macro constitutive relation is directly derived from the interactions between particles. This type of modeling method is that the micro fracture mechanism is directly converted into the macro constitutive relation so that the VIB can simulate fracture behaviors without any separate fracture criterion. Different methods are available to find the crack behaviour. The first is based on molecular dynamics (MD) method. The other two based known as cohesive bond theory for modeling fracture and the virtual internal bond analysis the molecular dynamics method uses the interatomic potentials to simulate millions of atoms with appropriate boundary conditions, the choice of the interatomic potential and availability of supercomputing facilities to model around 10^{23} items to simulate $1cm^3$.of solid are critical parts of this approch.[1] The cohesive surface approach is based on defining discrete cohesive surface.[2] It need to separte fracture criteria.In this paper Modified virtual internal bond was used. This bond density potential is converted into the continuum mechanics.Bond density potential allows to change peak stress and softening phase by adjusting of some parameters.by using this parameter it possible to obtain stress strain curve of different materials. By using visual studio software build the user defined material for the Abaqus software. This Fortran file is linked to the Abaqus software after that different analysis carried out by using the new materials. It is required to link three software to each other.

II. CONSTITUTIVE MODEL

In the VIB microstructure, material particles in a micro element are considered to be connected to each other through the randomized micro bonds. In this VIB formulation, the strain energy density of a micro element is calculated.

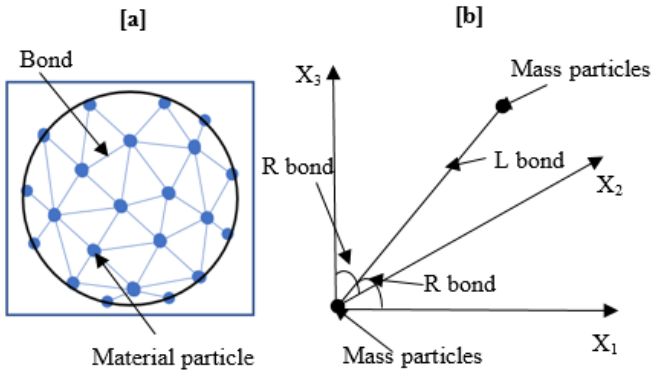

Fig 1. (a)Virtual Internal Bond Model (Randomly oriented Particles) (b) L bond and R bond in sphere coordinate

The interaction laws between the particles would determine the macroscopic properties of the any material. [3] In the VIB model interaction between the particles are nonlinear. In this constitutive model there are two interactions assumed first is L-bond and R-bond this is linearly elastic. [4] Potential stored in a single L-bond can expressed as follows:

$$U_L=\frac{1}{2}kl^2=\frac{1}{2}k(\ell_0\xi_i\,\varepsilon_{ij}\eta_j)^2 \quad (1)$$

Where, k is the L-bond stiffness coefficient; *l* is the stretch of the L-bond.

The energy potential stored in the R-bond is:

$$U_{R1}=\frac{1}{2}r\beta_1^2=\frac{1}{2}r(\xi_i\,\varepsilon_{ij}\eta_j')^2 \quad (2)$$

$$U_{R2}=\frac{1}{2}r\beta_2^2=\frac{1}{2}r(\xi_i\,\varepsilon_{ij}\eta_j'')^2 \quad (3)$$

$$U_{R3}=\frac{1}{2}r\beta_3^2=\frac{1}{2}r(\xi_i\,\varepsilon_{ij}\eta_j''')^2 \quad (4)$$

Where r is the R-bond stiffness coefficient; U_{Ri} (i = 1,2,3) is the energy potential of the R-bond corresponding to the coordinate-xi such that bi is the rotation angles of L-bond

towards coordinate- xi. Hence, the energy potential within a two-coupled particles i _ j could be expressed as:

$$\eta' = \xi \times (\overrightarrow{x_1} \times \xi) \quad (5)$$

$$\eta'' = \xi \times (\overrightarrow{x_2} \times \xi) \quad (6)$$

$$\eta''' = \xi \times (\overrightarrow{x_3} \times \xi) \quad (7)$$

$$W_{IJ} = U_L + U_{R1} + U_{R2} + U_{R3} \quad (8)$$

$W_{IJ}$is the total bond energy potential.

$$W = \int_0^{2\pi}\int_0^{\pi} U_L D_L(\theta,\emptyset)\sin\theta d\theta d\emptyset + \int_0^{2\pi}\int_0^{\pi} U_{R1} D_{R1}(\theta,\emptyset)\sin\theta d\theta d\emptyset + \int_0^{2\pi}\int_0^{\pi} U_{R2} D_{R2}(\theta,\emptyset)\sin\theta d\theta d\emptyset + \int_0^{2\pi}\int_0^{\pi} U_{R3} D_{R3}(\theta,\emptyset)\sin\theta d\theta d\emptyset \quad (9)$$

Where, $D_L(\theta,\emptyset)$ is the distribution function of the normal bond, $D_L(\theta,\emptyset)(\theta,\emptyset)\sin\theta d\theta d\emptyset$ is the number of normal bonds in the unit volume between $(\theta,\theta+d\theta)$ and $(\emptyset,\emptyset+d\emptyset)$ in the sphere coordinate system, $D_{Ri}(\theta,\emptyset)(i=1,2,3)$ is the distribution function of the shear bond related to x_i coordinate Based on the hypoplastic theory, the elastic tensor can be obtained from Equation10.

$$C_{ijmn} = \frac{\partial W}{\partial \varepsilon_{ij}\partial \varepsilon_{mn}} = \int_0^{2\pi}\int_0^{\pi} k\xi_i\xi_j\xi_m\xi_n D_L(\theta,\emptyset)\sin\theta d\theta d\emptyset + \int_0^{2\pi}\int_0^{\pi} r\,\xi_i\eta'_j\xi_m\eta'_n D_{R1}(\theta,\emptyset)\sin\theta d\theta d\emptyset + \int_0^{2\pi}\int_0^{\pi} r\,\xi_i\eta''_j\xi_m\eta''_n D_{R2}(\theta,\emptyset)\sin\theta d\theta d\emptyset + \int_0^{2\pi}\int_0^{\pi} r\,\xi_i\eta'''_j\xi_m\eta'''_n D_{R3}(\theta,\emptyset)\sin\theta d\theta d\emptyset \quad (10)$$

Let the distribution function be unit, i.e. $D_L = D_{R1}(\theta,\emptyset) = D_{R2}(\theta,\emptyset) = D_{R3}(\theta,\emptyset) = 1$, then the corresponding relationship between bond stiffness and material constants can be derived as,

$$k = \frac{3E}{4\pi(1-2\nu)} \quad (11)$$

$$r = \frac{3(1-4\nu)E}{4\pi(1+\nu)(1-2\nu)} \quad (12)$$

Where,E and *ν* are the young's modulus and the Poisson's ratio of material respectively. Quantitatively describe the relationship between the bond distribution density and bond deformation, the following phenomenological relationship is proposed.

$$D_L(\theta,\emptyset) = \exp\left\{-C_1\left[\frac{2\beta}{(1+\nu)\varepsilon_c}\right]^{n_{c1}}\right\}\exp[-C_2\left(\frac{-l}{\varepsilon_c}\right)^{nc2}$$

$$D_R(\theta,\emptyset) = \exp\left\{-C_1\left[\frac{2\beta}{(1+\nu)\varepsilon_c}\right]^{n_{c1}}\right\} \quad (13)$$

Where,

$$\beta = \max\{\beta_1,\beta_2,\beta_3\}, \quad (14)$$

$$\beta_i = \left|\xi_m\,\varepsilon_{mn}\eta_n^i\right| \quad (15)$$

$\varepsilon_c = is\ the\ uniaxial\ compressive\ strain\ strength;$

$$l = \xi_i\varepsilon_{ij}\xi_j, \quad (16)$$

$c_1, c_{2,} n_{c1}, n_{c2,}$ *are* model parameters, which govern the characteristics of complete stress-strain curves. Different material corresponds to different set of model parameters.

III. CALIBRATION PROCESS OF MVIB MODEL PARAMETERS

In this constitutive formulation was converted into micro level to continuum level. Using this formulations VUMAT code was build.VUMAT code defines the user defined material to the Abaqus software which is linked together. It is useful for the all brittle fracture materials and thiswas developed for the explicit nonlinear analysis. Its required matching the stress strain curve to the experimental stress strain curve of the materialHence some properties are essential to know of any materials such as young's modulus, possion's ratio, tensile strain, and critical strain. In the bond energy potential four parameters was used for to obtain correct nature of the stress strain curve. In this HS10 materials was used and obtained stress strain curveHS10 is the high strength concrete.In the Calibration Process Robustness of the VUMAT code was tested.

A. Bond breaking process in MVIB model

The stress and strain expression within the frame work of hyper elastic model by using energy stored in normal and shear bond thus the obtain stress and strain expression are used to write VUMAT subroutines provided in Abaqus environment. when applied load on the element crack propagate this is shown by the element stretching. There are two phases in the stress strain curve. First is peak stress in this phase maximum stress was developed in the material after that material is fails and softening phase will be starting that condition. In the softening phase the stress is minimum and strain is maximum hence element of the material is starching. The following Fig2. shows the correct effect on the element of the stress strain.

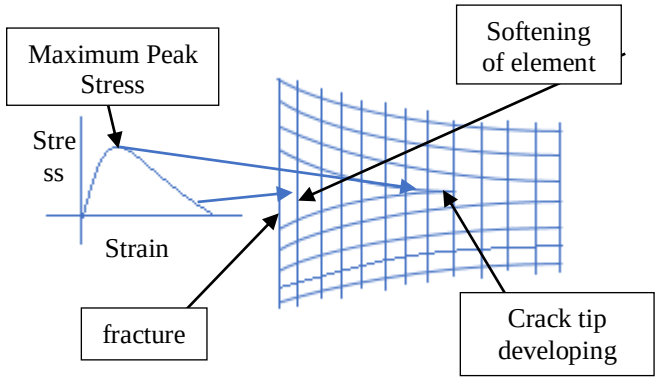

Fig 2. Bond breaking process in Modified Virtual Internal Bond model

The crack behavior also depends on the Mesh shape and size in the quadrilateral and triangular mesh element size is approximately same but It can be observed that qualitatively they both behave in similar fashion. The issue of mesh shape dependence on the softening behavior is a subject of investigate and another factor is loading rate and type in this Crack initiation and propagation behaviour is highly sensitive to the loading rate and type. Displacement boundary conditions are specified in ABAQUS/Explicit as varying from zero to maximum amplitude over step time.

B. Loading rate and type

The loading rate is very important factor in this case since it determine the nature of the results.Various factor that affected the simulation result include the elastic modulus E, the density and the overall simulation time T (step time). As the explicit integration scheme is conditionally stable, an appropriate choice of time increment Δt is critical to ensure stability. The stable increment can be approximately estimated using,

$$\Delta t = \frac{L_e}{C_d} \qquad (17)$$

Where, $L_e$is the characteristic length associated with each element (of the order of the element size) and $C_d$is the dilatational wave speed is given as,

$$C_d = \sqrt{\frac{E}{\rho}} (18)$$

$$\rho = \left(\frac{\Delta t \times \sqrt{E}}{L_e}\right)^2 \qquad (19)$$

Where,

E= Young's modulus

$$\Delta t = \text{Time Increment}$$

$$L_e = \text{length of element}$$

Loading rate or displacement: In this problem giving displacement and different boundary conditions are used to here different modes of fracture in used for analysis. Displacement calculated through the formula:

$$\text{Displacement} = C_t \times L_e \times mtimes \qquad (20)$$

Here C_t is the critical strain and l_e is length of element
This is used for the single material when using the composite material and one and more materials then,

$$\text{Displacement} = \left(\frac{C_{t1}+C_{t2}}{2}\right) \times L_e \times mtimes \qquad (21)$$

C_{t1}: critical strain of first material

C_{t2}: critical strain of second material

By using this formulation find out the mass density ρ Value of the material. In the Abaqus time step increment is taken automatic and step time period was taken unity.

C. Single element Analysis

Table I shows the material properties [3] of the concrete this was obtained by the experimentally in the research paper here directly applied following properties for the simulations.

TABLE I. MODEL PARAMETERS FOR NUMERICAL SIMULATION STYLES

Material Name	**High Strength Concrete (HS10) MaterialProperties**				
	E(Spa)	***V***	***Ct***	***Peak stress(Spa)***	***Density***
HS10	59.99e3	0.15	2.2e-3	71.09	5.999g m/nm^ 3

In this paper FEA analysis done in the Nanoscale. Hence Material properties required to convert in nanoscale table I shows the nanoscale material properties.

TABLE II. BOND ENERGY PARAMETERS ARE USED FOR OBTAINING CORRECT NATURE OF STRESS STRAIN.

Material Name	**High Strength Concrete (HS10) model parameters controls Stress strain curve**			
	C_1	C_2	n_{c1}	n_{c2}
HS10	1.2	0.2	2.0	2.0

In the Table II shows the calibrated material model parameters which was operated stress strain curve behavior, this was getting from no of trials.

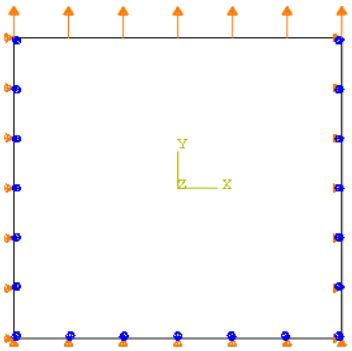

Fig 3. Single element with boundary conditions

Fig 3. shows the single element and x direction edge is fixed at y direction for displacement and rotation and y direction edge is fixed at x direction for displacement and rotation.

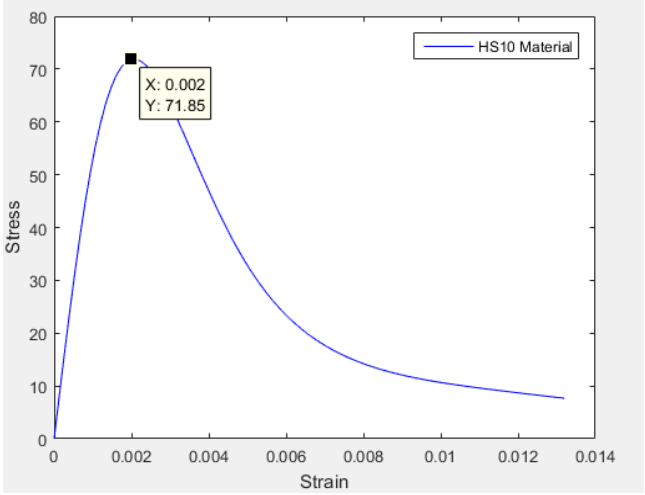

Fig 4. Single element Stress Vs Strain Graph for HS10 Material

After making the VUMAT Code complying is main process. When user defined material is ready or defined.it is required link to the Abaqus software this main task because without linking problems cannot be solved or simulation cannot be done. Hence this main phase, it is required correctly defined VUMAT Code and zero mistake is required. when VUMAT is made than it is required to test. After test it is shows the correct nature of stress strain graph of the given material. After successful of VUMAT test than this code used for large problems and one or more no of element.Fig 4. Shows the calibrated stress-strain curve for given material. This graph calibrated from the single element analysis this graph closely matched with experimental material properties

IV. Modelling and Simulation of Plate with a Hole, under Quasistatic Conditions

Firstly, taken the problem of plate with hole. The Fig5. shows the quad part of the plate with hole geometryDue to symmetricity taken one quarter part of the plate with hole geometry and also shows the boundary conditions. [5] This model given uniaxial boundary conditions. Boundary condition given in as shown in Fig 5.

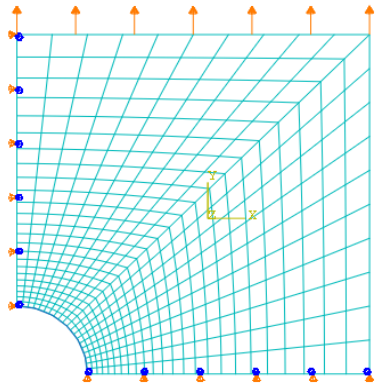

Fig 5. Boundary conditions and meshing of the Plate with Hole

This is uniaxial problem. Displacement and mass density was calculated using the above formulations. This is 2D model size of the plate is 1nm by 1nm and the radius of the circle is 0.2 nm. this problem was solved by using the user defined material. material properties taken from HS10 material. Mesh type is quad structured. At the hole side element count is increases and size of element is minimum. Element type the geometry was meshed with CPS4R (A 4-node bilinear plane stress quadrilateral, reduced integration, hourglass control.) element. The total no of element is 480.

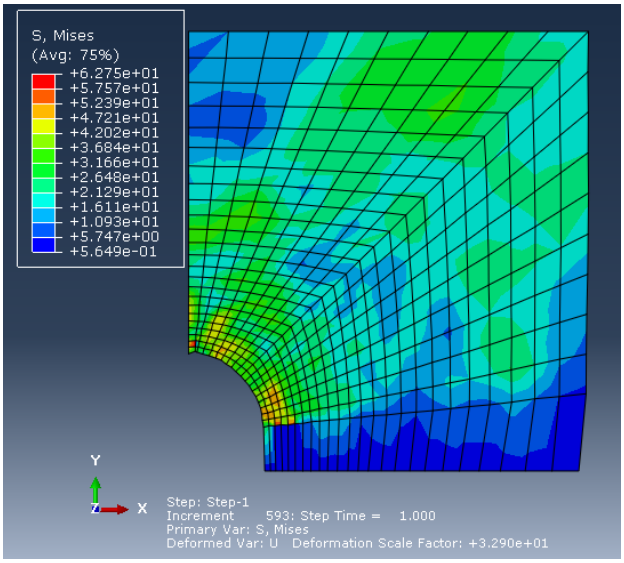

Fig6.Von mises plot of a plate with hole indicating crack propagation at the bottom of the plate.

In the plate with hole problem stress is flow from upper to bottom. Fig6. shows the typical result of von mises stress intensity at the hole edge. Increasing the applied load or applied displacement the domain near the hole edge enter the strain softening phase. Hence at that point stress is minimum. This indicates the crack initiation. Increasing the further load crack is also increasing.

V. Modelling and Simulation of theplate with different Pre-existing Crack

Form the view of MVIB, material consists of material particles in microscopic this material particles bonded with each other. with consist of potential energy between them. The interaction strength between material particles shown by the bond stiffness. when material particles separate from each other than bond stiffness can be gradually decreases. The reason of the macro crack is increasing the distance between the particles. In the model is unnecessary to treat the pre-existing crack as the free boundary as the traditional continuum mechanics-based methods do, which bring significant convenience for numerical simulation. To represent the effect of pre-existing crack, the intersected microelement is assigned an initial deformation large enough to make the bond stiffness negligible. After that study of the crack behavior is required for the macroscopic analysis. Hence in the model pre-existing crack is developed and studding the growth of the crack.[6] Study of the crack propagation is very important. It is required to correctly crack propagate as per the start point is preexisting crack tip. Here different preexisting model is studied.

A. Crack propagation process in the plate with preexisting horizontal and inclined crack

Two simulation examples are shown. Simulating specimens are a square plate with a horizontal/inclined predefined crack whose dimensions is 100nm x 100nm. Fig8. displays the boundary conditions.

(a)

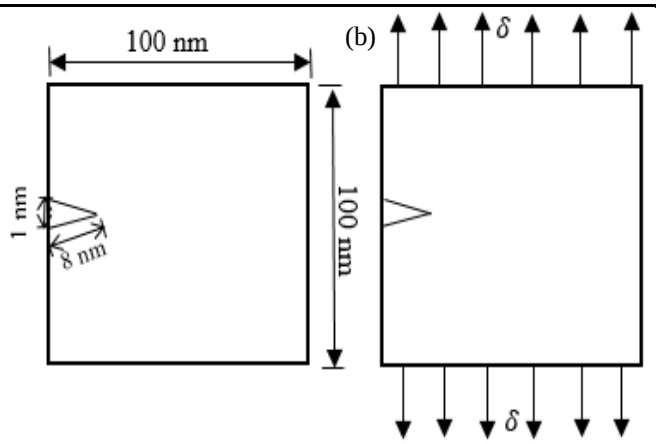

Fig7. Plate with Horizontal edge crack (a)Dimensions of the plate (b)Boundary conditions

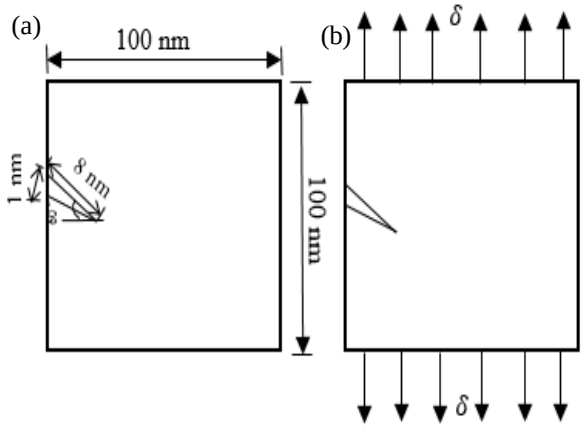

Fig 8. Plate with inclined edge crack (a)Dimensions of the plate (b)Boundary conditions

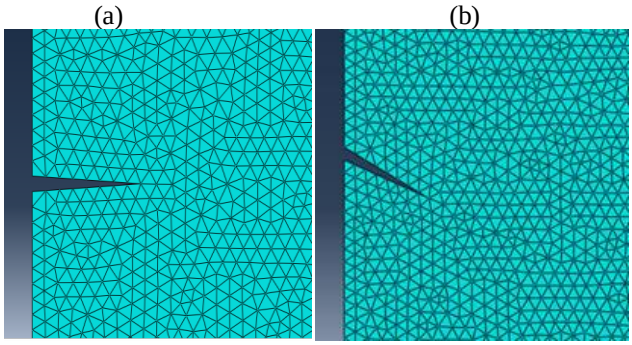

Fig9. Meshed Model(a)plate with horizontal edge crack (b) plate with inclined 60^0preexisting crack

In the Fig9. shows triangular meshed model. Element type the geometry was meshed with CPS3 (A 3-node linear plane stress triangle.) element. The element size is required very fine for the above model for higher accuracy is ensured. the element size is usually required to be finefor thepresented method if a higher accuracy is ensured.smaller the element size then the more accurate the outlineof intersected elements arrangement approaches to thecrack geometry therefore, the more accurate thesimulation.

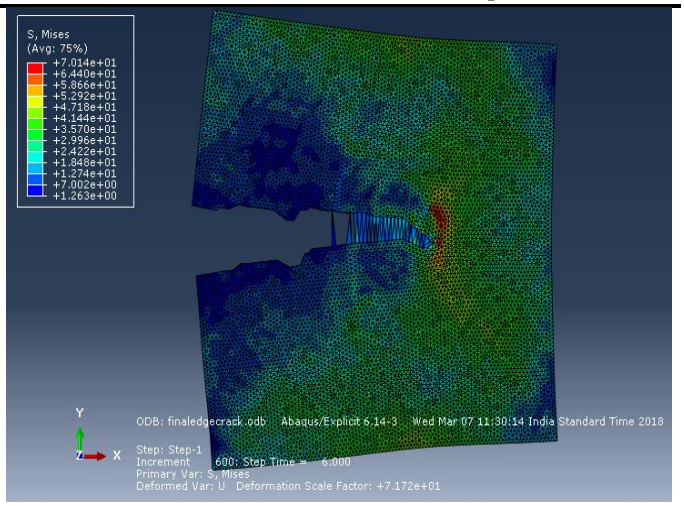

Fig 10.Von mises plot of a plate with edge crack indicating crack propagation

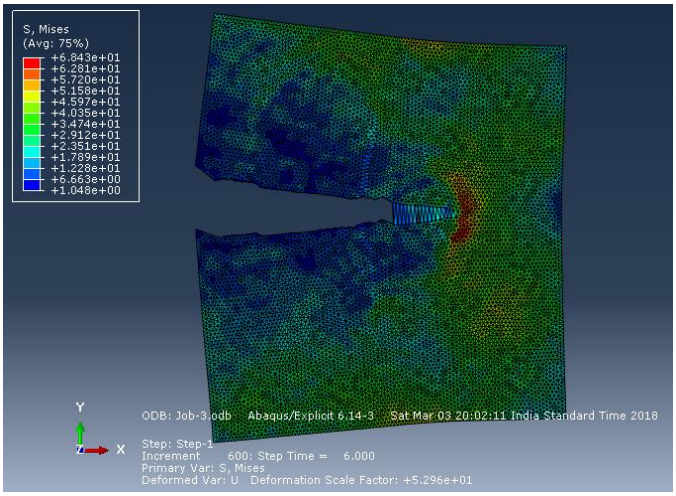

Fig 11.Von mises plot of a plate with Inclined 60^0 pre-existing crack indicating crack propagation

The preexisting crack can be modelled as by assigning initial displacement of the two edges. After submitting the job,In the Fig 10 and Fig 11 indicating the crack propagation. Crack was propagated as the horizontally. In the inclined crack model crack start form the predefined crack tip when force is increasing than crack also increasing the crack is goes perpendicular to the force this is correct nature of the crack. These simulations show the fracture propagation in the model.

B.Crack propagation process in the plate with preexisting notch.

In this setting fracture mechanics plays a central role, as it provides useful tools which allow for an analysis of materials

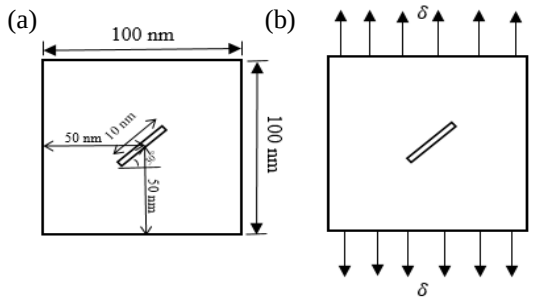

Fig 12. Plate withinclinedCrack at center(a)Dimensions of the plate (b)Boundary conditions

Fig.12 shows the boundary conditions and dimensions of the plate with notch, this is rectangular plate having preexisting notch. This notch inclined at 30^0

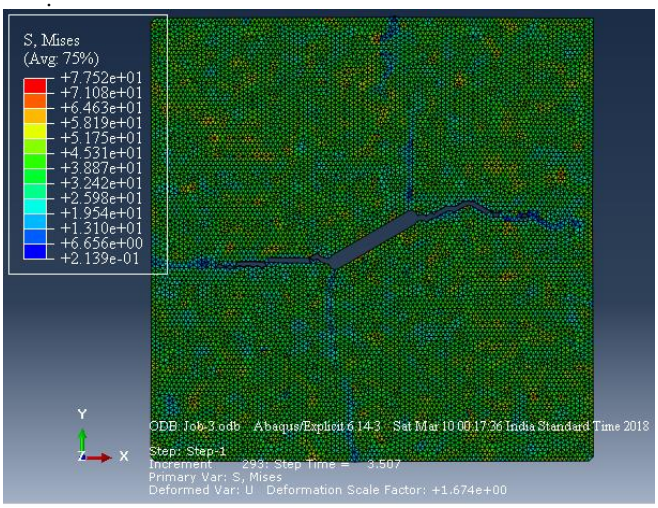

Fig 13.Von mises plot of a plate with Inclined pre-existing crack indicating crack propagation

This is plate with notch problem behavior of the Crack propagation was studied. When using the userdefined material after simulation crack path was propagated on the both side of notch this nature of the crack was studied in the fig 13. In this way we can examine the performance of the presented method.The simulation results suggest that the presentedmethod can simulate the crack propagation process andcan reflect the features of fracture propagation inmaterial.

VI. Conclusion

InitiallyModified Virtual internal bond calibrated parameters are implemented to obtain simulated stress-strain response as close as possible to experimentation. The concept of Modified virtual internal bond model is successfully implemented through VUMAT subroutine under Abaqus environment a unique way of virtual internal bond parameters calibration is propose. The obtained results for the standard fracture problem like plate with hole, edge crack, inclined crack gives the crack path propagation. In reasonable agreement with the contain published literature, thus the techniques can be further applied to studies issues related with fracture under complex loading and intercept boundary conditions.

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