Personal Programming Project:Implementation of crack mode I far field in Anisotropic elasticity with Molecular Statics

Praveenkumar Hiremath

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Abstract

In this work,I have modelled crack far field,crack propagation for three crack systems and, the stress intensity factor(SIF) K_{IC} and material behavior(ductile or brittle) under mode-I loading on anisotropic elastic medium of α-Iron are observed, using molecular statics. Here,plane strain problem along the crack front direction has been considered for the modelling. For this purpose,a new "`displace_atoms`" style(CrackAniso) was introduced in LAMMPS. EAM potentials(Mishin Cu EAM1 PRB(2001)63:224106-by G.Ziegenhain(2007), Fe2.eam.fs [4]) are used as inter-atomic potentials. The observations of this work are validated through the use of some already done works on α-Iron.

Contents

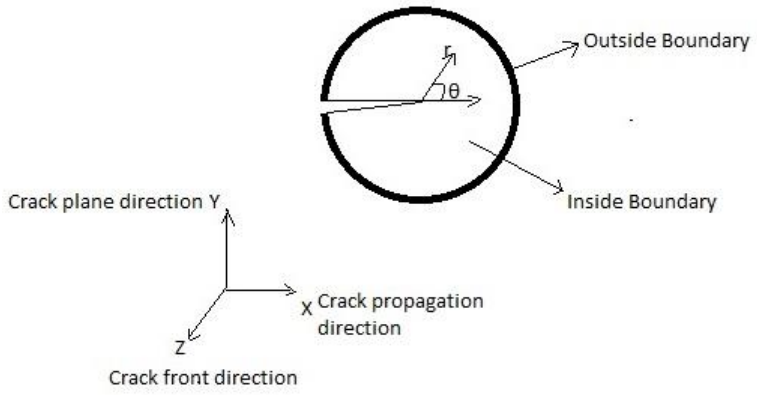
1 Introduction

α-Iron has body-centred cubic crystal structure with anisotropic elastic behaviour. The atomistic simulations of crack propagation mechanisms help us to predict the nature of fracture exhibited by a material in different situations. Use of correct inter-atomic potentials is very essential for predicting the true nature. But existing potentials of α-Iron are not so reliable because they don't predict few properties with enough accuracy. The potentials used in this work justify this unreliability.

2 Crack system

A crack system is represented by the set of three orthonormal vectors namely, crack propagation direction(say X-axis[o,p,q]),crack plane direction(say Y-axis [u,v,w]) and crack front direction(say Z-axis[a,b,c]) such that
$[a, b, c] = [o, p, q] \times [u, v, w]$

Figure 1: Crack System



3 Anisotropic elasticity

In anisotropic elasticity,the elastic properties of the material are don't have rotational symmetry. The stress-strain relationship in anisotropic medium is given by,$\sigma_{ij} = C_{ijkl} * \epsilon_{kl}$ where σ_{ij} is second order stress tensor,ϵ_{kl} is second order strain tensor and C_{ijkl} is a fourth order tensor called stiffness tensor.

3.1 Compliance matrix

$\epsilon_{kl} = S_{ijkl} * \sigma_{ij}$ relates strain with stress where S_{ijkl} is compliance tensor with $S_{ijkl} = {C_{ijkl}}^{-1}$. Both stiffness and compliance tensors contain 81 elements in general. The symmetry in strain and stress tensors, results in stiffness and compliance tensors with 36 independent components. These fourth order tensors can now be written in the form of 6X6 matrices with <100> type axes. Again these matrices are symmetric matrices and hence the components are now 21. For a BCC structure, there are only three independent components namely c_{11},c_{12},c_{44}(elastic constants) and s_{11},s_{12},s_{44}(compliance constants) because, $c_{11} = c_{22} = c_{33}; c_{12} = c_{13} = c_{21} = c_{23} = c_{31} = c_{32}; c_{44} = c_{55} = c_{66}$. All the other components are zero in <100> type axes(referred to as original coordinate system). The components of tensor S_{ijkl} can be written matrix form S_{mn} using following table(Tensor coefficients to matrix coefficients).

Tensor	11	22	33	23	32	13	31	12	21
Matrix	1	2	3	4	4	5	5	6	6

Here $S_{\mathrm{ijkl}} = S_{\mathrm{mn}}$ is given by

$$S_{\mathrm{mn}} = \begin{bmatrix} s_{11} & s_{12} & s_{13} & s_{14} & s_{15} & s_{16} \\ s_{21} & s_{22} & s_{23} & s_{24} & s_{25} & s_{26} \\ s_{31} & s_{32} & s_{33} & s_{34} & s_{35} & s_{36} \\ s_{41} & s_{42} & s_{43} & s_{44} & s_{45} & s_{46} \\ s_{51} & s_{52} & s_{53} & s_{54} & s_{55} & s_{56} \\ s_{61} & s_{62} & s_{63} & s_{64} & s_{65} & s_{66} \end{bmatrix}$$

3.2 Rotation of compliance matrix

The compliance constants are calculated from elastic constants by inverting the elastic constants matrix(6X6) using $S_{\mathrm{ij}} = C_{\mathrm{ij}}{}^{-}1$ or by using the following formulae:Compliance constants in <100>axes system(old)
$s_{11} = \frac{c_{11}+c_{12}}{(c_{11}-c_{12})(c_{11}+2c_{12})}$
$s_{12} = \frac{-c_{12}}{(c_{11}-c_{12})(c_{11}+2c_{12})}$
$s_{44} = \frac{1}{c_{44}}$
Then these compliance constants are required to be rotated in another coordinate system depending on the crack system. To obtain the compliance constants in rotated coordinate system, the following formula can be made use of [1]

$$s'_{\mathrm{ijkl}} = \sum T_{\mathrm{ig}} T_{\mathrm{jh}} s_{\mathrm{ghmn}} T_{\mathrm{km}} T_{\mathrm{ln}} \tag{1}$$

where
s_{ijkl} =Compliance constants in old coordinate system(i,j,k,l $\in$ [1,2,3])
s'_{ghmn} =Compliance constants in new coordinate system(g,h,m,n $\in$ [1,2,3])
$\mathrm{T_{pq}}$ are components of transformation matrix given by

$$T_{\mathrm{pq}} = \begin{bmatrix} X_1 & Y_1 & Z_1 \\ X_2 & Y_2 & Z_2 \\ X_3 & Y_3 & Z_3 \end{bmatrix}$$

with
$X_1 = o/\sqrt{o^2+p^2+q^2}; Y_1 = p/\sqrt{o^2+p^2+q^2}; Z_1 = q/\sqrt{0^2+p^2+q^2}$
$X_2 = u/\sqrt{u^2+v^2+w^2}; Y_2 = v/\sqrt{u^2+v^2+w^2}; Z_2 = w/\sqrt{u^2+v^2+w^2}$
$X_3 = a/\sqrt{a^2+b^2+c^2}; Y_3 = b/\sqrt{a^2+b^2+c^2}; Z_3 = c/\sqrt{a^2+b^2+c^2}$

Before and also after rotating the compliance matrix to required orientations, the following conditions are considered.
$pS_{\mathrm{ijkl}} = S_{\mathrm{mn}}$ where,
$p = 1$ for m AND n $\in$ [1,2,3]
$p = 2$ for m XOR n $\in$ [1,2,3]
$p = 4$ for m AND n $\in$ [4,5,6]

3.3 Plane strain condition

Since the problem under consideration is plane strain problem,plane strain conditions are imposed on the rotated compliance constants.

$$\begin{bmatrix}\epsilon_{11}\\ \epsilon_{22}\\ \epsilon_{33}\\ 2\epsilon_{23}\\ 2\epsilon_{13}\\ 2\epsilon_{12}\end{bmatrix} = \begin{bmatrix}s_{11} & s_{12} & s_{13} & s_{14} & s_{15} & s_{16}\\ s_{21} & s_{22} & s_{23} & s_{24} & s_{25} & s_{26}\\ s_{31} & s_{32} & s_{33} & s_{34} & s_{35} & s_{36}\\ s_{41} & s_{42} & s_{43} & s_{44} & s_{45} & s_{46}\\ s_{51} & s_{52} & s_{53} & s_{54} & s_{55} & s_{56}\\ s_{61} & s_{62} & s_{63} & s_{64} & s_{65} & s_{66}\end{bmatrix} * \begin{bmatrix}\sigma_{11}\\ \sigma_{22}\\ \sigma_{33}\\ \sigma_{23}\\ \sigma_{13}\\ \sigma_{12}\end{bmatrix} \tag{2}$$

Since, plane strain condition is being considered, $\epsilon_{33} = \epsilon_{23} = \epsilon_{13} = 0$. $\sigma_{33} = f(\sigma_{11}, \sigma_{22}, \sigma_{12}); \sigma_{23} = f(\sigma_{11}, \sigma_{22}, \sigma_{12}); \sigma_{13} = f(\sigma_{11}, \sigma_{22}, \sigma_{12})$ are calculated. Then these are plugged in the above equation (2) to get general plane strain conditions for compliance constants. So now the conditions are(hand calculations):

$s'_{11} = s_{11} + (\frac{s_{13}*\delta_2}{\delta_1}) + (s_{14} * \gamma_1) + (s_{15} * K1)$

$s'_{12} = s_{12} + (\frac{s_{13}*\delta_3}{\delta_1}) + (s_{14} * \gamma_2) + (s_{15} * K2)$

$s'_{16} = s_{16} + (\frac{s_{13}*\delta_4}{\delta_1}) + (s_{14} * \gamma_3) + (s_{15} * K3)$

$s'_{21} = s_{21} + (\frac{s_{23}*\delta_2}{\delta_1}) + (s_{24} * \gamma_1) + (s_{25} * K1)$

$s'_{22} = s_{22} + (\frac{s_{23}*\delta_3}{\delta_1}) + (s_{24} * \gamma_2) + (s_{25} * K2)$

$s'_{26} = s_{26} + (\frac{s_{23}*\delta_4}{\delta_1}) + (s_{24} * \gamma_3) + (s_{25} * K3)$

$s'_{66} = s_{66} + (\frac{s_{63}*\delta_4}{\delta_1}) + (s_{64} * \gamma_3) + (s_{65} * K3)$

The 'δ's,'γ's and 'K's in the above equations are calculated as follows.

$\delta_1 = \beta_1 - (\frac{\beta_4*\alpha_4}{\alpha_1})$

$\delta_2 = \beta_2 + (\frac{\beta_4*\alpha_2}{\alpha_1})$

$\delta_3 = \beta_3 + (\frac{\beta_4*\alpha_3}{\alpha_1})$

$\delta_4 = \beta_5 + (\frac{\beta_4*\alpha_5}{\alpha_1})$

$\gamma_1 = (\frac{-1}{s_{44}}) * (s_{14} + (\frac{\alpha_2*s_{45}}{\alpha_1}) + (\frac{\alpha_4*s_{45}*\delta_2}{\alpha_1*\delta_1}) + (\frac{s_{34}*\delta_2}{\delta_1})$

$\gamma_2 = (\frac{-1}{s_{44}}) * (s_{24} + (\frac{\alpha_3*s_{45}}{\alpha_1}) + (\frac{\alpha_4*s_{45}*\delta_3}{\alpha_1*\delta_1}) + (\frac{s_{34}*\delta_3}{\delta_1})$

$\gamma_3 = (\frac{-1}{s_{44}}) * (s_{46} + (\frac{\alpha_5*s_{45}}{\alpha_1}) + (\frac{\alpha_4*s_{45}*\delta_4}{\alpha_1*\delta_1}) + (\frac{s_{34}*\delta_4}{\delta_1})$

$K1 = (\frac{\alpha_2}{\alpha_1}) + (\frac{\alpha_4*\delta_2}{\delta_1})$

$K2 = (\frac{\alpha_3}{\alpha_1}) + (\frac{\alpha_4*\delta_3}{\delta_1})$

$K3 = (\frac{\alpha_5}{\alpha_1}) + (\frac{\alpha_4*\delta_4}{\delta_1})$

with 'α's and 'β's as

$\alpha_1 = 1 - (\frac{s_{45}*s_{45}}{s_{44}*s_{55}})$

$\alpha_2 = (\frac{s_{45}*s_{14}}{s_{44}*s_{55}}) - (\frac{s_{15}}{s_{55}})$

$\alpha_3 = (\frac{s_{45}*s_{24}}{s_{44}*s_{55}}) - (\frac{s_{25}}{s_{55}})$

$\alpha_4 = (\frac{s_{45}*s_{34}}{s_{44}*s_{55}}) - (\frac{s_{35}}{s_{55}})$

$\alpha_5 = (\frac{s_{45}*s_{46}}{s_{44}*s_{55}}) - (\frac{s_{56}}{s_{55}})$

$\beta_1 = 1 - (\frac{s_{34}*s_{34}}{s_{44}*s_{33}})$

$\beta_2 = (\frac{s_{43}*s_{14}}{s_{44}*s_{33}}) - (\frac{s_{13}}{s_{33}})$

$\beta_3 = (\frac{s_{43}*s_{24}}{s_{44}*s_{33}}) - (\frac{s_{23}}{s_{33}})$

$\beta_4 = (\frac{s_{43}*s_{45}}{s_{44}*s_{33}}) - (\frac{s_{53}}{s_{33}})$

$\beta_5 = (\frac{s_{43}*s_{46}}{s_{44}*s_{33}}) - (\frac{s_{63}}{s_{33}})$

Here 's's are rotated compliance constants and 's''s are compliance constants with plane strain

condition.

3.4 Mode-I displacement field solutions

The displacement field solutions for mode I(plane strain) loading in linear anisotropic elasticity are given by [1]

$$U_{\mathrm{x}} = K_{\mathrm{I}}\sqrt{\frac{2r}{\pi}} * Re[\frac{1}{(\mu_1 - \mu_2)}[\mu_1 p_2\sqrt{(cos\theta + \mu_2 sin\theta)} - \mu_2 p_1\sqrt{(cos\theta + \mu_1 sin\theta)}]] \tag{3}$$

$$U_{\mathrm{y}} = K_{\mathrm{I}}\sqrt{\frac{2r}{\pi}} * Re[\frac{1}{(\mu_1 - \mu_2)}[\mu_1 q_2\sqrt{(cos\theta + \mu_2 sin\theta)} - \mu_2 q_1\sqrt{(cos\theta + \mu_1 sin\theta)}]] \tag{4}$$

The displacements U_x and U_y are calculated using the information provided in [1]. The displacements U_x and U_y are the atomic displacements,added to their previous positions in the anisotropic medium(time evolution of the system using CrackAniso style in 'displace_atoms' inside a time loop). This in turn results in the modelling of crack propagation in anisotropic medium.

4 "displace_atoms" command-CrackAniso style

The anisotropic displacement fields are employed in 'displace_atoms.cpp' file in LAMMPS source code. The syntax for the use of style CrackAniso is as follows displace_atoms group_ID style args units box
style=CrackAniso.
args=K,xtip,ytip,s_{11},s_{12},s_{44},Crystal_structure,Crack_Plane_x,Crack_Plane_y, Crack_Plane_z,Crack_x, Crack_y, Crack_z.
K=Stress Intensity factor/Incremental Stress Intensity factor.
xtip,ytip=x and y coordinates of crack tip.
s_{11},s_{12},s_{44}=Compliance constants(for BCC).
Crystal_structure=(BCC)1,(FCC)2,(HCP)3(FCC and HCP can also be implemented with the same procedure).
Crack_Plane_x,Crack_Plane_y,Crack_Plane_z=Crack plane direction (coordinates)
Crack_x, Crack_y, Crack_z=Crack propagation direction(coordinates)

5 Implementation-Algorithm

- The required inputs like type of crystal structure,compliance constants,crack system are taken through the LAMMPS input script.
- The compliance constants in rotated coordinate system,displacements U_x and U_y are calculated and atomic positions are accordingly updated in displace_atoms.cpp.
- LAMMPS input scripts through which inputs are taken is written for modelling crack system and crack propagation.
- The output of molecular statics run is observed in ovito and the mode of crack propagation is observed. If the dislocation nucleation at the crack tip preferred over the cleavage decohesion,for K_{IC},then the material is ductile. Otherwise, the material is brittle.
- The SIF value 'K' for which the dislocation nucleation occurs or cleavage decohesion occurs is considered as the critical stress intensity factor K_{IC} [6].

6 Molecular Statics in brief

Molecular mechanics makes use of Newtonian mechanics to describe the behavior of a system. Molecular dynamics is the modelling of physical systems using molecular mechanics at temperatures other than 0K. But molecular statics is carried out at 0K.

6.1 LAMMPS input script

The crystal structure is built in the required orientation and is divided into outside and inside regions. The inside region is again divided into three sub-regions namely, upper left, lower left, right regions. The outer boundary is fixed and the inside region is displaced and relaxed. A small region is defined in front of the crack so that the crack propagation can be analyzed. The inter-atomic potentials are defined by different potential files. The crack tip advance is monitored by calculating maximum potential energy. The position of atom for which the potential energy is maximum is the crack tip position for that iteration. The value of SIF for which there is drastic change in crack tip position, is taken as the Critical Stress intensity factor K_{IC}.

6.2 K_{IC} calculation

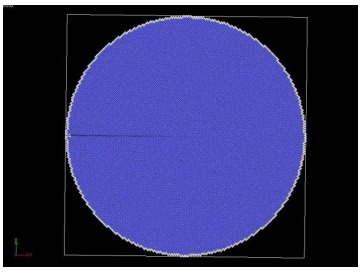
$K_{\mathrm{IC}} = InitDeltaKLammps + DeltaKLammps * (Step)$ (OVITO visualization) where 'Step' is the step for which there is drastic change in xtip value/crack nucleation is observed in ovito. InitDeltaKLammps is the initial guess for the SIF,DeltaKLammps is the increment given to initial guess.
$K_{\mathrm{IC}} = InitDeltaKLammps + DeltaKLammps$ (Graphical)

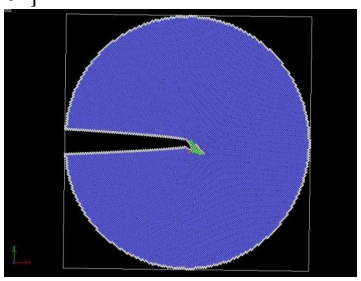
7 Results and Discussion

7.1 For Crack system (100)[001]

In this crack system, the crack propagation direction is [0-10],crack front direction is [001] and crack plane direction is [100]. The crystal structure data file is named as "atoms.crack.100_001.Fe"(read_data command in LAMMPS input script). The value of K_{IC} is 1.3657 $MPa.\sqrt{m}$,calculated using my implementation. I found out the nature of crack to be Brittle and at K_{IC},crack starts to propagate in (1-10) plane Figure 2. through my simulation. The work of Möller and Bitzek [5] shows that the value of K_{IC} for this system is 1.35 $MPa.\sqrt{m}$. The cracks on plane(100) are brittle in nature. Depending on the crack front direction, the crack either stays in (100) plane or kinks out onto (110) plane with the evolution of time. In this case, for the [001] crack front, the crack kinks out onto (1-10). This simulation result is in agreement with the work of Möller and Bitzek(2014).

Figure 2: Crack system (100)[001]





7.2 For Crack system (110)[1-10]

In this crack system, the crack propagation direction is [00-1],crack front direction is [1-10] and crack plane direction is [110]. The filename given to the crystal structure file is "atoms.crack.110_1-10.Fe". My implementation yields K_{IC}= $1.1499 MPa.\sqrt{m}$.Through my simulation, I also found out that the crack is Ductile in nature and at K_{IC} dislocation is emitted in 112 plane and then crack tip blunts Figure 3. The value of K_{IC} is 1.14 $MPa.\sqrt{m}$ as per the work of Möller and Bitzek [5].

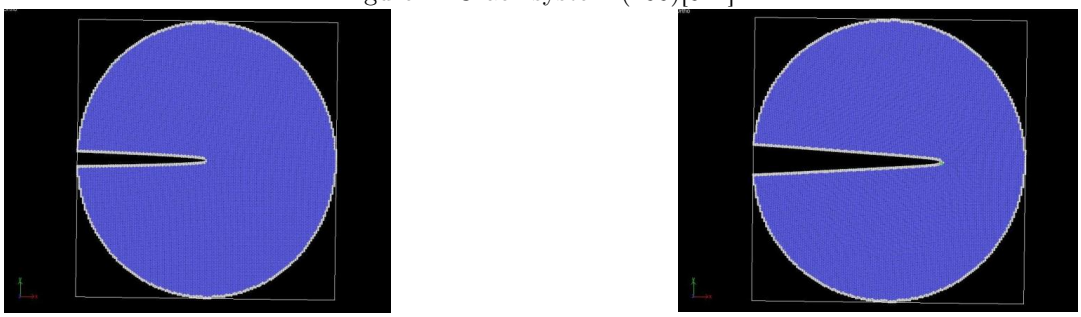
Till K_{IC},the crack tip is sharp. When K_{IC} is reached,the crack tip blunts and emits dislocation in 112 plane showing ductile nature. This simulation result is also in agreement with the work of Möller and Bitzek [5].

Figure 3: Crack system (110)[1-10]

7.3 For Crack system (100)[011]

In this crack system, crack propagation direction is [0-11],crack front direction is [011], crack plane direction is [100]. The crystal structure filename is "atoms.crack.100_011.Fe". My implementation yields the value of K_{IC} as $1.075 MPa.\sqrt{m}$. My simulation also shows that the crack is Brittle in nature and after K_{IC},for all potentials stays and propagates always in (100) plane Figure 4. The value of K_{IC} is found out to be 1.07 $MPa.\sqrt{m}$ in the work of Möller and Bitzek [5].

Figure 4: Crack system (100)[011]



8 Conclusion

From the above results, it is clear that for (100) plane cracks, the K_{IC} is higher for [001](1.3657 $MPa.\sqrt{m}$) crack front direction than for the [011] (1.075 $MPa.\sqrt{m}$) which is in agreement with the paper. The average value K_{IC} for [011] crack front is 1.08 $MPa.\sqrt{m}$. The simulation value for this is 1.075 $MPa.\sqrt{m}$. The crack in plane (100) with crack front [011] always propagates in the (100) plane as mentioned in the paper. Thus, the results for crack systems (100)[001],(100)[011] and (110)[1-10] from paper of Johannes J Möller and Erik Bitzek are reproduced by the simulation. Thus,I have reproduced the results for three crack systems(crack plane)[crack front] from my

simulations. I have validated my code using research paper of Johannes J Möller and Erik Bitzek. Other references that I used for this project are [2] and [3].

References

[1] Kin S Cheung and Sidney Yip. A molecular-dynamics simulation of crack-tip extension: the brittle-to-ductile transition. *Modelling and Simulation in Materials Science and Engineering*, 2(4):865, 1994.

[2] Alan Hinchliffe. *Molecular modelling for beginners*. John Wiley & Sons, 2005.

[3] SG Lekhnitskii. Theory of elasticity of an anisotropic body, 1981. *Grand Forks, BC, Mir*, 2011.

[4] MI Mendelev, S Han, DJ Srolovitz, GJ Ackland, DY Sun, and M Asta. Development of new interatomic potentials appropriate for crystalline and liquid iron. *Philosophical magazine*, 83(35):3977–3994, 2003.

[5] Johannes J Möller and Erik Bitzek. Comparative study of embedded atom potentials for atomistic simulations of fracture in α-iron. *Modelling and Simulation in Materials Science and Engineering*, 22(4):045002, 2014.

[6] James R Rice. Dislocation nucleation from a crack tip: an analysis based on the peierls concept. *Journal of the Mechanics and Physics of Solids*, 40(2):239–271, 1992.