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Atomic theory of Fracture and Quantization of Fracture Toughness

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Abstract

This research work is an atomic theory of fracture and quantization of K_{ic} Fracture toughness. Especially in ceramics. It shows the atomic level aspects of fracture process from the stress intensity factor or fracture toughness, K_{Ic}. The crystalline structure, the atomic positions and lattice points, and how nanomaterials show atomic level fracture process as well as nanoceramics exhibit Quantization of fracture toughness and other nanomaterials show higher stress intensity factor, K_{Ic} than microsize equivalents of those nanomaterials. This is a deep treatment of the fracture process with a survey of present status of fracture, the application of the fundamentals of fracture toughness for the atomic theory of fracture, the data evidence for confirmation of the theory and some extension for its applications in biomaterials, electronic materials and cutting tools for manufacturing. This is a rigorous and clear treatment of the atomic theory of fracture.

INTRODUCTION

Fracture of materials has been an important area of research for applications in materials usage in various applications as well as life-cycle determination and improvement in various contexts. It includes fracture of metals in usage and also improvement of toughness of ceramics as the mechanical, physical and functional properties of ceramics foretell wide usage but ceramics have moderate fracture toughness. Nanoceramics have good fracture toughness and the theory of fracture would be apt in these materials and also for improvement and tailoring of properties of all nanomaterials in addition to ceramics. Semiconductor materials and biomaterials would allow us to throw light on these materials for a better understanding of their scope and opportunities.

We could apply the fundamental basis of fracture mechanics, toughness and mechanical properties. In nanomaterials, biomaterials etc and their properties can be analysed for favourable results. This would create the opportunities for applications of these materials as well as exploit the full scope of crtitical applications and the understanding of some classes of new materials and availability of new tools, methods of materials characterization not to mentions new methods of materials synthesis to tailor and improve properties for various applications.

Thus in view of the preludial note, it becomes natural to review the relevant materials including composites before we Develop the theory of fracture especially for brittle ceramics in addition to other materials now that carbon materials and other new classes of materials are being developed/investigated for applications, The following section reviews the literature reports of fracture properties of different materials.

STATUS AND BACKGROUND

With the advent of nanotechnology, biomaterials, the electronic materials developments, the properties of these has led to large number of research studies. The authors research measured high fracture toughness in Aluminia-zirconia nanocomposites. The paradigm shift in materials is to tailor properties, compositions of materials instead of design applications based on available materials with their properties The fracture properties addresses integrity of materials in various applications.

Novel properties and tools.

Silicon[44] undergoes brittle to ductile transformation at high temeperature. Plastic deformation, slip bands and dislocations are formed. Slip banda are formed, also crack tip stress intensity causes strain gradient ahead of crack tip, hence half planes and dislocations are formed at regular intervals. The [5] article provides a textual exhibition of all possible fracture surfaces- it is a sort of fracture atlas. The perfect depiction of fracture surfaces of single crystals is like a theoretical treatment, of course, we then understand real world fracture surfaces. There is crack growth over time and continuous values in K_{Ic} for metallic materials is illustrated in this atlas in keeping with the atomic theory of fracture. Nanocrystalline[30] metals are brittle at very fine nanosize grains, larger grain size nanometals are ductile and at intermediate nanosize have a combination of ductile and brittle behaviour. Increase in fracture toughness continuously with decrease in nanosize but due to manufacturing defects only, mechanism of ductility is affected by manufacturing defects in whose absence nanosize increases toughness, this is valid for metallic nanomaterials Synchrotron[15] X-rays can do imaging and diffraction simultaneously. It is possible to obtain information of a volume of material at the crack tip .Multiple materials can be investigated three dimensionally. Stress intensity and fracture toughness can be investigated and quantization could be investigated.

Biomaterials

Dentin[9] – dental implant fails in a brittle manner through cleavage fracture unlike metals. Cracks start due to multiple causes including biological, chemical and fatigue but only along atomically dense planes. With understanding of fracture, materials selection with techno-financial gains is possible. Biomaterials[31] can have multiple functions in one implant leading to improvements in quality of life. Even hierarchial materials and hybrid micro-nano open promising avenues in biomaterials. Ti stems cannot be replaced by tissue engineering. Understanding fracture can enable a deeper approach to mechanical properties in biomaterials including micro, nano etc. Crack-bridging[13] from smaller cracks ahead of main crack in dentin prevents growth of crack, failure etc. Mineralization in collagen prevents microcracking and aged tooth fail quickly. Understanding of fracture at nanoscale, namely atomic theory of fracture and strain gradient at crack tip but crack tip could get rounded before next decrease in toughness – microcracks can form over time and stress intensity decrease are possible approaches to prolong dentin life,

Polymers and Metals

Polymers fracture without features except with second phases[6]. Fracture feature sizes in second phase show fracture information. But we can use optical birefringence to see video like depiction of fracture process. Atomic theory of fracture portends continuous values in fracture toughness with material variations. In rubber[46] and blends – elastomers, cavity forms during fracture. When the rate of loading is high there is adiabatic heating and melt forms. Elastomers fracture is not much related to stress intensity approach, especially in rapid load to failure .Metallic glasses are both amorphous and have non-directional bonding, but turn into nanocrystalline regions under cycling loading but not during monotonic loading. In cyclic loading region at crack tip crystallises into metal but in monotonic loading crack tip is blunted because of crystalline regions forming and growing in high stress intensity at crack tip These crystalline regions cause crack bridging. Metallic[1] glasses have only 4% deformation to fracture. There is formation of shear bands and branching in fracture surface. Crack bridging by nanosize crystalline regions that sre forming at crack tip. Metallic glasses are almost brittle if not actually so since crystalline regions forming at high stress intensity. Computer modelling[19] of nanotwinned metals shows large ductility. Non-directional bonding means there is no quantization of stress intensity. Nanotwinning[22] in copper leads to high fracture toughness. Other properties are higher, large defects and twinning lead to high properties. Nanotwinning is slightly different mechanism for high fracture toughness.

Acoustic[2] emission happens before actual fracture and is a premonition for upcoming fracture. A strong interface is seen between lamellar intermetallic compound and matrix in Ti-Al-Mn alloy.the interface increases i.e. adds to fracture toughness. Morphology of lamellar intermetallic has a predominant effect in increasing toughness. Delamination at interface relates to high K_{Ic}. Delamination is like breaking atomic bonds in crack formation. In-situ[28] straining in Al-Cu – Mg alloy showed that dispersoids slow down fracture and that dislocation buildup, voids etc. can lead to necking. Crack propagation is slower. So it is likely that there is higher ductility and toughness compared to other brittle materials. In metallic[8] materials fatigue loading and crack produce grain growth in the surrounding region upto 150nm This is so in nanocrystalline copper. When nanograins coarsen the metal resembles conventional metals. Metals are similar in fracture even in fatigue loading.in nanostructured form. Hydrogen[45] in metals affects only cyclic loading by creating plastic zone at crack tip. Monotonic loading does not show effect of hydrogen. Stress intensity is boosted under hydrogen at crack tip. When iron[23] is melted to form Iron, if strontium, aluminium and silicon are present then Intermetallic structure is obtained. Composition affects fracture but in some alloys intermetallics increase fracture strength.

Material[26] is deformed to nanosize. Higher energy leads to smaller nanosize and crack propagation is less. Finer nanosize increases toughness in atomic theory of fracture but there is no quantization of fracture toughness. A review[28] of failure in nanostructured metallic materials showed increase in strength but lowering of ductility. Involved analysis of processing and design likely to lead to better nanometallic materials. Nanosize increases toughness but no quantization.

Ceramics and Semiconductors

Silicon[3] single crystal crack tip has no significant plastic deformation. The type of fracture is cleavage i.e. similar to ceramics. We do see a few extra half planes ⊥r crack tip at stress intensity region near crack tip, strain gradient from crack tip stress intensity should lead to bond breaking , so extra half planes ⊥r to crack tip appear as in figure 1.

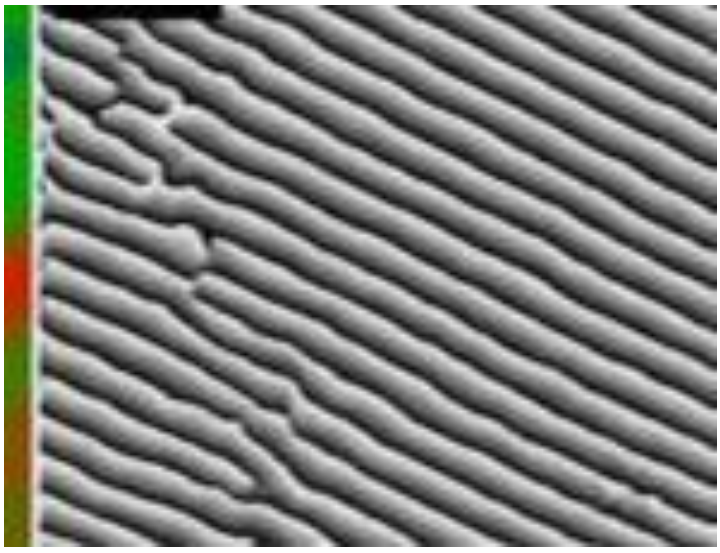

Figure 1. HRTEM image with NM – Numerical Moire Methods showing atomic extra half planes.

HRTEM image with NM – Numerical Moire methods. Annealing [10] closes crack tip in Si, Ge, SiC and AL_2O_3. While stress intensity is quantized, annealing can increase life though at higher processing cost. Even atomically sharp crack can be processed in these non-metallic, non-polymeric magterials and related technological gains follow from them. Indentation[11] and the crack tip by hardness indenter have compressive stresses and the dislocation field is due to compression used to create crack. Dislocations in compressive force field shield the crack tip. Computer model and HRTEM produce same estimation of compressive field at crack tip. If initial crack in silicon wafer is by compression, K_{Ic} quantization and compressive field add to technological gains.

Good estimation[16] of K_{Ic} in Nanoscale diamond except one method/value. All brittle materials can be studied for K_{Ic} with this computer model. Further studies for diamond nanosize variation in nano –regime would lead to better picture of atomic theory of fracture. Consistent results by 4 methods seem to be interesting computing approach to nano-diamond. Yttria[17] and alumina were doped in zirconia. Hardness nearly constant and maximum in 3% Y-TZP. Fracture toughness shows clustering nearly at high, very high and very low values even though change in yttria content is continuous but toughness values are clustering. SiC[18] is added to alumina Al_2O_3 to the extent of 2.5 to 7.5% sintered at 1550□C. Stress intensity fracture toughness is practically, exactly at 3MPa√m. There is no shift even with so much SiC, so all samples at one value of quantization of toughness. Hence there are no changes even with 7.5 % SiC – a hint of atomic theory of fracture and quantization of K_{Ic}. Al_2O_3[25] nanoceramic had best cutting tool performance but had chipping. Si_3N_4 lesser performance but low temperature superplasticity of surface of tool decreases life. Hence if superplastic temperature can be increased than tool would have better life. However[42] my PhD research has shown very high toughness at 5nm Al_2O_3- ZrO_2 composite and likely good candidate for cutting tool.

Grain [34] boundary sliding and addition of zirconia, ZrO_2 and gb migration to increase fracture toughnes. While plastic deformation is the objective in the paper, the stress intensity is higher n nano-nano ceramics. Finer nanosize and quantization and the resulting mechanical integrity are not being focussed in this study. Toughening[35] in nanoceramics similar to microscopic ceramic mechanisms. At nanoscale, gb sliding, gb migration, gb diffusion, rotational deformation, gb rotation all are in place to increase fracture toughness. In this study grapheme increases the fracture toughness of nanoceramic to a bigger multiple. SPS Spark Plasma Sintering[36] provides valid method to sinter nanoceramics to nano/nano composite or monolith. Consistent report of high fracture toughness but lack of theoretical model for the same. Atomic theory of fracture and quantization of fracture toughness is valid model for nanoceramics.

Carbon based Materials

Graphene[24] with pre-crack tested for fracture toughness in molecular model methods. Estimated 3 to 3.5 MPa√m value is considered higher than true value for grapheme. Atomic theory of fracture while valid for ceramics and crystalline covalent bonding etc., the orientation of grapheme such as armchair, etc of graphene means that chirality and orientation of precrack especially to applied stress, than there is continuous variation of K_{Ic}. Fracture toughness is not probably quantized. Brittle fracture in nanomaterials as well as carbon materials is studied at atomic level by atom – molecule – bond approach and at macroscopic level by Molecular Dynamics simulation and then scaling it, we understand interesting issues. Constant developments are seen in this double-pronged effort. Stress[14] intensity quantization with less number of values for all nanosizes shows numerical computing can be much less with atomic theory of fracture and its stress intensity quantization. A review[27] of nano particles in epoxy such as CNT, Graphene, nanoclay, nanosilica etc shows nanosilica and CNT produce high properties. However if strength is very high, than the fracture toughness is lower. Many mechanism are there in toughness. Polymer and nano as a composite form is a different mechanism(s) of high mechanical properties and not directly related to atomic theory theory of fracture. But valid high properties are seen in these materials. Graphene study[29] shows single layer material has low fracture toughness and not possessing reliability in applications. Use of graphene multilayers has high fracture toughness (J-Integral) $39J/m^2$ for random crack path in individual graphene sheets and toughness is high. Processing issues and how many layers in multilayers of graphene are questions. When graphene is put in application, stress intensity, say in matrix of composite would be vital. Fracture[32] toughness of graphene ~4MPa√m is in a nanoindenter. Both intergranular and transgranular crack in computer modelling. While graphene has molecular bonding, its fracture toughness is low. Atomic theory of fracture in one atom thick materials is not apparent at this stage. But more rigorous study would be needed to analyse graphene and its properties especially in mechanical stress applications.

Carbon[33] materials in epoxy can add various types of properties. SWCNT provides electrical properties and MWCNT increases fracture toughness – they double it. Issues in processing for manufacturing versus high properties are analysed. Thermal[37] stresses in thin films on substrate are studied in this article. Addition of nanotubes as nanoinclusion in epoxy thin film on aluminium substrate is carried out. Interphase and surface of nanotube in epoxy matrix is important and is successful. At high thermal residual stresses – stress intensity could lead to failure in thin film material. Processing and geometry etc could be vital factors in this context. Remember nanotube is high modulus and epoxy low, so one cannot add more than 0.5% nanotube due to high stress intensity at interphase between CNT and polymer matrix.

The atomic theory of fracture is a valid model for directionally bonded, crystalline and 3d lattice based nanosize materials and is well grounded in various classes of materials and composites in this context, Single atom thick materials would need further development of approach to mechanical properties.

THE ATOMIC THEORY OF FRACTURE

There is a direct correlation between the strain gradient at the crack tip and the critical stress intensity, K_{ic} , which is the fracture toughness. But the value of the strain gradient (for a single inter-atomic distance) depends on the unit cell and its details.

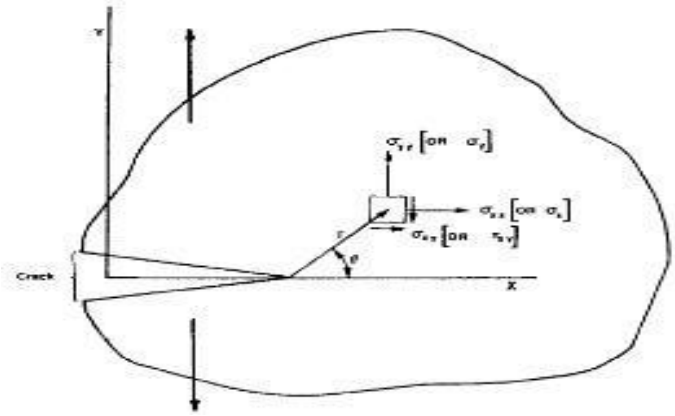

Figure 2. Arbitrary body with Arbitrary Crack and Arbitrary Mode I Loading.

For a body with crack of arbitrary size subjected to tension, bending or both, load is Mode I. The material is elastic and follows Hooke's law. Theory of elasticity can be used to calculate the stress field.

The crack tip stress field is at least biaxial and it may be triaxial if contraction in thickness direction is constrained. Hence, there will be stresses in at least X and Y direction, σ_2 and σ_y. From stress field solution, the stresses on a material element (Arbitrary body with Arbitrary crack and arbitrary mode I loading):

$$\left.\begin{aligned} \sigma_x &= \frac{K}{\sqrt{2\pi r}} \cos\frac{\theta}{2}\left(1 - \sin\frac{\theta}{2}\sin\frac{3\theta}{2}\right) \\ \sigma_y &= \frac{K}{\sqrt{2\pi r}} \cos\frac{\theta}{2}\left(1 + \sin\frac{\theta}{2}\sin\frac{3\theta}{2}\right) \\ \sigma_z &= 0 \\ \tau_{xy} &= \frac{K}{\sqrt{2\pi r}} \cos\frac{\theta}{2}\sin\frac{\theta}{2}\cos\frac{3\theta}{2} \end{aligned}\right\}.$$

Figure 3. Stress field at a crack tip from theory of elasticity

Both σ_x and σ_y exist.

For the case that θ +0 (plane through the cracked section) the shear stress τ_{xy} is zero.

It is convenient to confine the consideration to the plane through the crack with $\theta = 0$ in that case the functions of θ will be either 0 or 1, so that they essentially disappear (note also that x=r for $\theta = 0$)

$$\left.\begin{aligned} \sigma_x &= \frac{K}{\sqrt{2\pi x}} \\ \sigma_y &= \frac{K}{\sqrt{2\pi x}} \end{aligned}\right\}.$$

Figure 4. Stress field for Plane stress.

It appears that, at least along the plane Y=0 for which these equations hold the transverse stress, σ_{xy}= 0, equal in magnitude to the longitudinal stress σ_y. The stresses depend upon the distance x from the crack tip, note that at greater distances (larger x) the stresses are lower & is the stress intensity factor. Since stresses depend upon the distance between parallel atomic planes.

The distance between parallel planes in one set of planes with its unique Miller indices along with the applied stress and its value at crack tip leads (Interplanar spacings have only particular set of values & hence it is quantized K_{Ic})

$$D_{hkl}=a/(\sqrt{(h^2+k^2+l^2)})$$

Figure 5. Interplanar spacing for planes with Miller Indices hkl

to certain strain gradient in the nano grain at the crack tip. In other words, the stress intensity at the crack tip is directly related to the strain gradient at the crack tip. So, with a specified value of interplanar distance for a particular crystallographic plane perpendicular to the crack at its tip, the crack will grow the fracture with one threshold value of stress intensity at the crack tip. Hence, stress intensity for fracture is directly connected to the value of the interplanar distance of that crystallographic plane.

For a crack tip at a nanograin boundary to grow crack across the adjacent nano grain only certain major crystal planes with thei own unique Miller indices, the value of the interplanar distances at zero stress, the planar distances are fixed and discrete and not a continuous collection of distances values but discrete or we could say the distances are quantized. So the values of fracture toughness, K_{Ic} is discrete and quantized for nanograins in materials. The distance between adjacent planes planes depends on the unit cell and miller indices of one particular set of planes that are perpendicular to crack tip.

In electron microscopy, the physical presence of planes is important for diffraction but the exact position of atoms in a given atomic plane with its Miller indices is irrelevant to the

diffraction pattern. But we have to break the interatomic bonds to get fracture at crack tip and then the crack propagates. So we need to analyze whether the exact position of atoms in the atomic planes present a the crack tip and perpendicular to crack tip, so the exact position of atoms could be relevant to stress intensity and fracture progress.

In smaller nanograins the distance from crack tip at grain boundary to interior center of grain is small, so we need higher stress intensity to propagate the crack across the nanograin to reach the opposing gran boundary, remember the grain boundary is stronger than interior of grain volume, so in general transgranular fracture is better route for fracture to propagate. So stress intensity and fracture toughness, K_{Ic} is higher for nanomaterials.

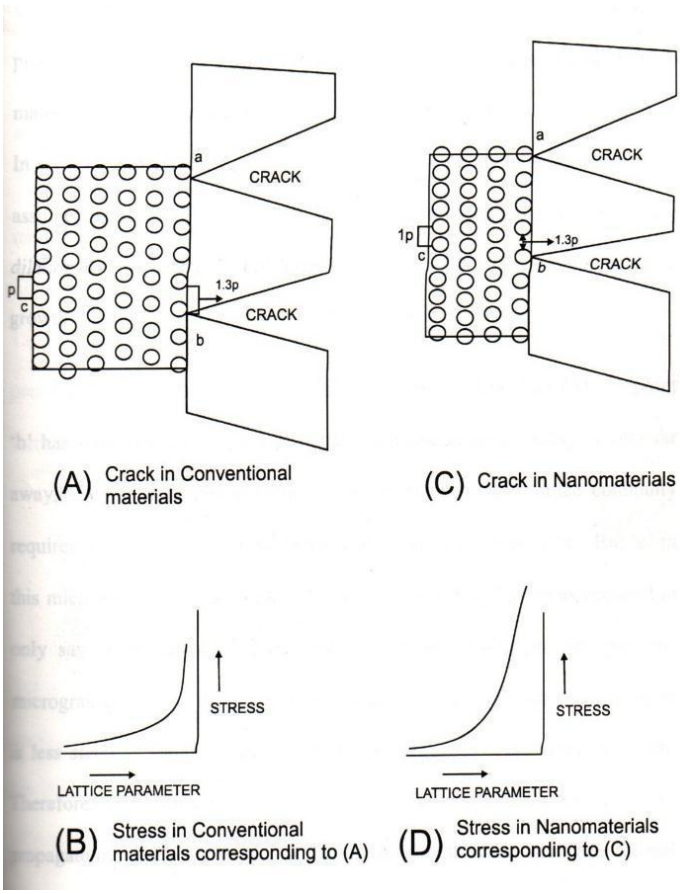

Figure 6. The stress at a crack tip for nanograin and conventional grain materials

The core of fracture is K_{Ic} namely stress Intensity what I extended is that the Stress Intensity Factor, the real meaning is the stress at the crack tip is very high as you move away from the crack tip, the stress level rapidly decreases, so in some way, the K_{Ic} corresponds to the gradient in stress it is highest at a sharp crack tip and decreases away from lattice parameter can be over the body of the grain of 100μm grain, but with 100nm size of a nanograin, in nanomaterial otherwise the K_{Ic} for failure of body will not happen in a nanograin .i.e. from crack tip to body of grain, the high stress at crack tip to low stress at a distance from crack tip, the fall in stress is steep i..e. a nanograin needs higher K_{Ic} for failure at crack tip. Of course, in microceramic materials, the grain boundary is stronger than body of grain, that is why we say Hall – Petch relation is higher strength and higher toughness for smaller grain size is more grain boundaries, so the material is tougher and/or stronger.

But in nanomaterial it is the opposite i.e. the grain is stronger and the grain boundary is weaker – only in comparison between body of grain and boundary of grains, that is the shift is not in absolute values but in relative terms i.e. only on comparison between the grain boundary and grain interior, we say the grain is stronger and grain volume is stronger, grain interior is stronger.

But what I did and what can be done is we put Boron or Zirconium at grain boundary (like in superalloys) and then grain boundary is strengthened and material is nano is strong, my Ph.D data shows that adding born increases the hardness of my ceramic nanocomposite, my Ph.D thesis data is evidence, in one case there was multiplier of increase in hardness of nanomaterial.

So by this process again the weak portion is interior of grain(even at room temperature not like high temperature super – alloys), so we show interest in stress intensity, at crack tip in the interior of the grain. We also know that a crack can start at the triple junction of three grains, etc.

Now to make fracture across the interior of grain, the high stress at crack tip when it extends interatomic distance at crack tip, when stress then strain and crack tip interatomic distance increases. To increase the interatomic distance from 1p to 1.3p i.e. 30% increase in lattice parameter, then bond in unit cell, breaks and then crack propagates leading to fracture of material. But we add crystal structure in this theory i.e. 1p increases to 1.3p, and then bond in unit cell breaks- say in cubic unit cell, a = b = c=p=a and then 1p becomes 1,3p, but in other unit cells, not cubic a≠b≠c≠p necessity, so in a,b & c directions the 1p to 1.3p is same need to break bond in unit cell, to break interatomic and fail to make crack propagate to failure. But even in cubic unit cell, there can be other atomic planes and other atomic directions i.e. Miller indices of planes and crystal directions so in edges of cubic unit cell, we need to go from 1p to 1.3 p i.e. 30% increase in lattice parameter for crack & failure. But interatomic distances along (111) plane or we may have a break in unit cell between parallel planes of (111), so depending on direction and habit plane of crack, for 1.3p along (111) plane for interatomic bond in unit cell to break and hence crack and failure in the material.

So actual value of stress intensity to fail, can change based on position and direction of crack and hence depending on atomic planes & directions, combine with volume of grain in nanograin and hence the K_{Ic} for failure in nanomaterial, the K_{Ic} can be dependant not just on size of nanosize grain but also usual position in trijunction of grains in nanomaterial and its relation to usual pattern of crack propagation in some crystal planes and crystal directions and so how much is the K_{Ic}, increasing from micrograin to nanograin, then there is a picture of atoms,

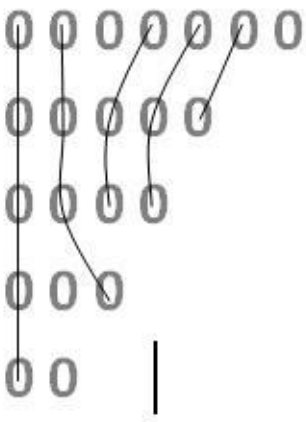

Figure 7. Arrangement of atoms in a strain Gradient at a crack tip.

Now in a cubic unit cell, we take a crossection cut say (111) plane or (100) plane then we have draw atoms like regular 2 – D array,

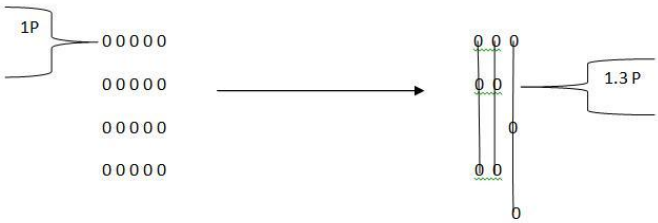

Figure 8. Arrangement of atoms with a strain in a nanograin close to fracture- from no strain in a nanograin to with a strain in a nanograin.

Crack tip with interatomic distance 1.3p and 30% strain in unit cell along say a b or c edges of cubic unit cell then fail at 1.3p, interatomic distances and failure at K_{Ic} say 150 MPa$\sqrt{m}$.

But same cubic unit cell and same crack tip in nanograin boundary say, at a tri-junction of three grains.

Then increase in inter atomic distances in cubic unit cell from 1p to 1.3p means we have to strain 30% not at 100µm grain size, but we have to strain 30% strain in 100nm grain from trijunctions grain boundary to interior of nanograin in just 100nm distance from crack tip, so a steep increase in strain i..e. higher K_{Ic} for volume of nanograin for crack to fracture and propagate the crack into volume of grain and hence failure of material, remember we have boron or zirconium to strengthen grain boundary so only way for material to fail is to propagtate crack in the volume of nanograin i.e.. intra-granular crack in volume of nanograin i.e. intra-granular crack in volume of nanosize grain, so K_{Ic} at nanosize is high, so fracture toughness of nanomaterial is higher.

So this is cubic unit cell a=b=c=a and increase in unit cell edge from 1p to 1.3p, but even in unit cell of cubic we can have other atomic planes and atomic directions, we can even have more than one atomic species, say we have interpenetrating cubic structure of two atomic species in some materials.

So instead of (111) plane being most dense with shortest interatomic distances we can have other atomic planes and other crystalline planes and directions, and throw in more than one atomic species in even an interpenetrating cubic structure, the K_{Ic} can be different. In one direction or plane increase a to from 1p to 1,3p for interatomic bond to break and crack into failure.

But in another crystal plane or direction or the interatomic bond between unlike atoms in 2- species cubic structure can be broken not at 1.3p, but say 1.2p or even 1,5p i.e. higher or lower strain of interatomic bond to break and hence failure and crack to propagate.

So even I ncubic unit cell, the atoms don't need to have square lattice so instead of :

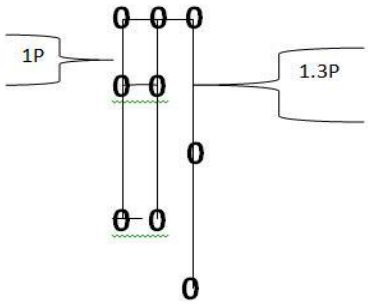

Fig 9 (a)

We can have:

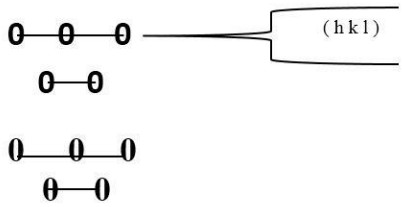

Fig 9 (b)

In same (hkl)

Planes, the actual positions of atoms in adjacent (hkl) parallel planes can be out of step so to go to;

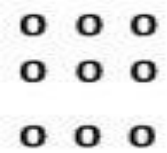

Fig 9 (c)

Figure 9 (a), (b) and (c). Atoms arranged as straight line points or atoms in zigzag arrangement for fracture material due to various crystal structures

Instead it can be as :

Same (hkl atomic planes but adjacent planes have atom poitions non – square i.e. not exactly one above another atoms in adjacent atomic (hkl) planes and understood non-square 2D lattice crossection only when:

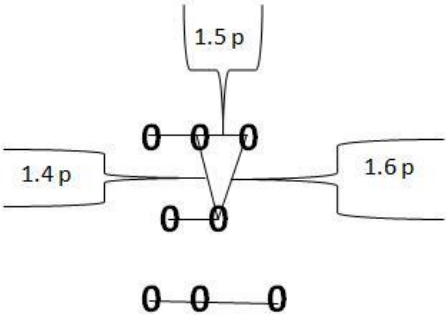

Figure 10. Strain in nanograin and changes in bond length in a triangle of atoms in lattice

So n triangle of atoms "a", "b" & "c" the interatomic bond can break at "a" – "b" = 1.5p or it can break interatomic bond for "c" – "b" to be 1.6p or it can break interatomic bond at "a" – "c" of triangle "a" – "b" – "c" to be 1.4 p for interatomic bond in (hkl) plane to break for K_{Ic} to increase and make material of nanosize grains to be of higher toughness and /or to be higher strength so with non-square "p":

Here "a" – "c" = 1.4p

But "b" – "c" = 1.6p > 1.4p

Of " a" – "c" , because crack tip is closer to "b" – "c" but more far away far away from " a" – "c" so

"a" – "c" < "b" – "c" i.e. we have a stress intensity near the crack tip which crack tip is to the right of

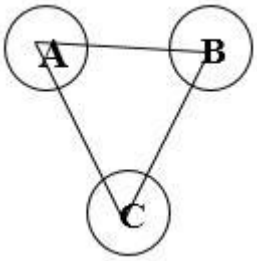

Figure 11. Triangle of atoms in a crystal lattice of nanograins to consider strain at a crack tip.

and hence we have failure due to stress intensity.Arrangement of atoms in parallel (hkl) planes, "a" – "b" – "c" triangle need not be an equilatral triangle, it can be isosceles "a" – "b" – "c" triangle, it can even be a scalene triangle with all of "a" – "b", "b" – "c" and "c" – "a" – all three disgtances will be unequal when stress intensity K_{Ic} for failure and fracture in (hkl) plane parallel planes, for fracture to take place in volume of nano grain and hence failure of nanoceramic.

This is the situation in a higher regular cubic structure A=B=C=p, but with other crysal systems and also 2 or 3 or even more than 3 atomic species and the direction and $(h_2k_2l_2)$ plane on which crack tip is there and further in what direction the crack grows and fails the material in volume of naograin, so what is K_{Ic}, the parallel planes In some (hkl) planes with different positions of atoms and also different species of atoms, so it is not a square type of 2D arrangement of one atomic species , it can be more than 1 atomic species and non-square arrangement of atoms and variations of atomic species etc so , it is an experimental science of fracture and we heard that crack surfaces actually have self- similar fractal structure with non-integral dimensions of fractals at crack surfaces.

We started with a simple square arrangement of 1 atomic species in + or – (hkl) plane to start K_{Ic} increases from micrograin to nanograin and hence nanomaterials are tougher and/or stronger, now we go into multiple atomic species and multiple crystal planes and/or multiple crystal planes and/or multiple crystal directions for analysing fracture and mechanical properties for transgranular crack and failure in a nanoceramic material. In fact, my Ph.D data is for a ceramic nano-composite with two types of grains of both alumina and zirconia in an Al_2O_3/ZrO_2 ceramic nanocomposite and the hardness data shows that the toughness is high in ceramic nanocomposite of alumina/zirconia i.e. Al_2O_3/ZrO_2 nanocomposite of ceramics. We have strengthened the grain boundary with Boron addition. The imaging contrast and fringes in TEM images could give a proof of stress intensity iin just stress & strain both being in a gradient state in a crack tip leading to fracture. There can be strain contrast and there can be diffraction contrast, what I need is strain, say at the crack tip. See fig. 12

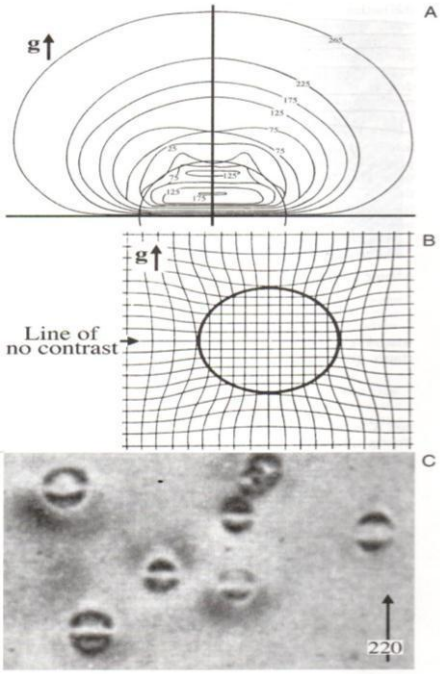

Figure 12. Strain/Distortion in lattice and strain contrast image for experimental observation in TEM to see strain gradient in a crack tip.

There is a line/area of dark vs bright line/area along the line of equal strain and maybe at the boundary between strain region

& no-strain region region in material/phase structure.

The shape and size of dark region in FIG12 is the region of strain contrast – the region where there is a strain and distortion in lattice parameter variation at the transition from particle to matrix. The dark band is a "strain field" comparable to the strain gradient in the crack tip leading to K_{Ic} and fracture and failure as per fracture mechanics.

High fracture toughness of ceramic nanocomposite such as in Alumina- Zirconia is the application and proof of this theory. High fracture toughness of nano ceramics maybe other metals is likely but sure in ceramics. Quantum confinement in nano is a parallel track for high mechanical properties of nanomaterials of 20 nm size grains and less size. However we we cannot rule out a synergy between my atomic theory of fracture and with quantum confinement – both methods and mechanisms may synergize together and such a possibility and reality cannot be completely ruled out.

In materials with nanosize grains, then crack has to propagate across the interior of nanograin provided grain boundariy has been strengthened with boron, so the stress gradient from crack tip at grain boundary to propagate to the center of grain – a short nanosize distance needs higher stress gradient to progress and propagate across the interior of grain i.e. K_{Ic} of nanograin is higher for fracture to take place, see fig 5.)

Fracture toughness is basically a measure of the ability of a crack to propagate further based on the stress concentration developed at a crack tip. A material has two types of cracks one in the interior of grain and other at a grain boundary, in order to explain the K_{Ic} in conventional grains and nano grain

Materials one can assume that the lattice parameter is "p" in an undisturbed grain and that a dilation to 1.3p leads to breakage of bond in the lattice leading to crack growth.

In a conventional micro size grain as shown in Fig 6. the point 'p' has some dilation i.e. 1.3p,but the opposite grain boundary is very far away, say six atom lattice points away. At point 'c', the lattice continuity requires a dimension of normal lattice parameter i.e.. 1 at point 'x' from the crack tip and lower away from crack tip. And also transverse stress is equal to longitudinal stress. Then just as there is a regular decline in stress away from the crack tip there is also a regular decline in strain away from the crack tip. At the atomic level in a nanomaterial with crack, there is a strain gradient from high to low away from the crack tip.

But 'c' in this micrograin in Fig 6 is only six lattice points away , say as opposed to only,say 4 lattice points away (since nanograins are smaller in size than micrograins) away in nanograins in Fig.6 .) , therefore the stress gradient is less steep ss shown in Fig.6 , for a microsize conventional grain. Therfore, the critical stress intensity i.e. K_{Ic} required for the crack to propagate must be less i.e. K_{Ic} or fracture toughness is less in a conventional micrograin material and more in a nanograin material.

For a crystalline material, there is only certain value of interplanar distance for a set of parallel planes having unique miller indices. Correspondingly, only a certain threshold value of stress intensity at the crack tip, will lead to fracture to propagate across the grain to the opposite grain boundary.

Of course, there could be different sets of planes perpendicular to crack tip and planes of different miller indices might require different values of stress intensity for the crack tip to propagate the crack.

A given material is likely to have a certain set of atomic crystal planes with fixed values of interplanar distances. So the value of K_{Ic} can change with particular set of planes that are perpendicular to crack tip. And the nanosize of grain also is important for higher stress intensity in smaller nanograin and lower stress intensity in in the bigger micrograin. But at the exact point of crack tip at grain boundary, the interplanar distance translates to size length of interatomic bond and a particular interatomic strain at point of crack tip and the bonding fractures to two unbonded atoms at crack tip. This value of strain requires higher stress intensity for a smaller nanosize grain but requires only a lower stress intensity for a bigger microsize grain.

The strain to break interatomic bond at crack tip is fixed for one particular nanomaterial with one particular crystal structure. But to attain that strain at crack tip requires lower stress intensity in bigger grain but needs a higher stress intensity for a smaller size nanograin.

But this interatomic distance at the crack tip depends on the interplanar spacing of the crystal parallel planes that are perpendicular to crack tip. While stress intensity changes with size of entire nanograin, the crack propagation depends on strain in interatomic bond i.e. interplanar distance right at the exact crack tip. So the value of the stress intensity is magnified highly at the crack tip depending on the interplanar distance for the planes perpendicular to crack tip at the point of first two atoms and their bond length at the crack tip itself. While the size of nanograin plays a role in stress intensity for fracture, K_{Ic}, the first bond length i.e. interplanar distance magnifies the stress intensity of the volume of nanograin. In other words, K_{Ic} is practically dictated by the interplanar distance of the atomic planes that are perpendicular to the crack tip at nanograin boundary.

So the strain to break the bonding between parallel planes at crack tip is not continuousas there are only certain finite types of crystal planes in a crystalline material and they have only discrete values of interplanar distances for respective crystal planes. The strain for fracture to propagate at the point of crack tip is highly dependant on interplanar distance i.e.. interatomic bond length. It is this interatomic distance that magnifies the effect of entire nanograin size on stress intensity to fracture .i.e. K_{Ic}. So the interplanar distance is some type of multiplier of nanosize effect on K_{Ic}. But this value of multiplier is not continuous as the available crystal planes, their interplanar distances are available only at certain values and discrete, so the value of the multiplier is discrete and quantized not continuous correspondingly, the K_{Ic}, the critical stress intensity takes only certain quantized discrete values and cannot vary continuously with change in nanosize of the nanograins in a nanomaterial. Of course, this is only for nanomaterial being 100% nano and not for mix of micro and nano grains.

But we do say, bonding in metals is not directional but is based on electron gas of bonding electrons and for atonic nuclei positioned at lattice points In metal crystal structure as a bravais lattice having lattice parameters, unt cell etc.., on the other hand in nanoceramics, there is covalent and/or ionic bonding in general. So we can study quantization of K_{Ic}, and its relation to interatomic and interplanar distances, in parallel planes, with a certain Miller indices ⊥R, crack tip at nano grain boundary. Of course we can refine this with a look at unit cell, unit cell parameters and lattice points in u nit cell, the actual position of lattice points of next neighbour atoms in adjacent parallel planes can be zigzag rather than in a straight line, which however we know from the miller indices of parallel planes.

We look at correlation of K_{Ic} in nanomaterials with size of nanograins and how K_{Ic} changes with change in size of nanograins, is there a quantization of K_{Ic} when size of grains changes in nanoceramics. Also for metals of nanograin size, do they have lower correlation or continuous changes in K_{Ic} with change in nanosize of grains in metallic nanomaterials.

We see continuous changes, variations in K_{Ic} in metals, nanosized materials and quantized discrete changes in K_{Ic} in nanoceramics.

At room temperature grian boundary is stronger than grain volume. So crack path/propagation is likely through volume of grain and not along grain boundary.i.e. crack in nanometals and nanoceramics is transgranular(volume of grain) and not intergranular(not along grain boundaries)

At room temperature, grain boundary is stronger than grain volume, so crack propagation /path islikely through volume of gain and not along grain boundary. But we have inverse Hall-Petch relation in nanoceramics and not direct hall petch relation like conventional metals have in similiar situation. Toughening in nano ceramics similar to microscopic ceramic mechanisms. At nano scale grain boundary sliding, grain boundary migration, grain boundary diffusion, rotational deformation, grain boundary rotation all are in place, to multiply fracture toughness. But we invoke the data in Ali Asadi et al to apply intergranular fracture and prove atomic theory of facture and to show quantization of K_{Ic} in nanoceramics.

In this publication, fracture is transgranuaalr, it means nanoparticles inside the volume of μ -Al_2O_3 have big role in toughness of this nanocomposite. Fracture mode changes from intergranular mode to transgranular mode due to addition of nano – SiC particles. So whereas earlier micrograin was strong and micro grain boundary weak so fracture mode was intergranualr. Now with addition of MgO and SiC the grain boundary is strong with nano –SiC in grain boundary, hence transgranular fracture takes place. The volume of micro Al_2O_3 grain is weak and K_{Ic} depends on nano –SiC in volume of microscopic grain of Al_2O_3. So the toughness value corresponds to that of effect of nano- SiC, so K_{Ic} values can be taken to correspond to the effect of nano – SiC. So it is valid data for the atomic theory of fracture and quantization of K_{Ic} in nannoceramics. (Nano SiC aee at both grain boundary as well as inside the volume of microsized Al_2O_3 grain, 500ppm MgO is only sintering additive (So MgO role is only at grain boundary) so entire K_{Ic} value is dependant only on effect of nano-SiC at both grain boundary and volume of grain also. So K_{Ic} values can be directly linked to nano – SiC. And fracture mode in practice like nano –SiC fracture.

In, Marek Blanda-et al SiC is added to Al_2O_3 to extent of 2.5 to 7.5 % sintered at 1550 □C Stress intensity factor is practically at 3MPa√m. No shift with even so much SiC, so all samples at one value of quantization in K_{Ic} hence no changes, even with SiO- a hint of atomic theory of fracture. Inevitably during fracture, the crack tip will encounter an high stress intensity requiring nanograin when the crack propagates to result in fracture failure. Unless the stress intensity is high, the crack tip cannot propagate to fracture failure, across that high stress intensity nanograin.

Table 1. Processing nanosize and fracture toughness in nanoceramics

T (°C)	SiC(%)	d(nm)	K_{Ic} (MPa√m)
1650	5	146	3.5
	7.5	135	
	0	0	3.6
	2.5	138	
1600	5	152	3.3
	7.5	142	
	0	0	3.5
	2.5	130	

The research experiments in processing of nanoceramic composites with nano SiC in microscopic Alumina – Al_2O_3 show quantization of fracture toughness in nanoceramics clearly. The " Table 1. Processing nanosize and fracture toughness in nanoceramics" shows nanosize and values of fracture toughness in nanoceramics..

At 1650 °C, for a change of 11nm in size of nano SiC, the fracture toughness is constant at 3.5MPa√m even though volume of SiC increases as well as nanosize decreases. Whereas both factors should increase fracture toughness, the K_{Ic} is constant. At the same temperature, for addition of 2.5 % nano SiC the fracture toughness holds steady from pure alumina to 138nm SiC at exactly 3.6MPa√m. for the next 2.5% increase in SiC the K_{Ic} quickly drops to 3.5MPa√m but again hold steady for more of SiC even though nanosize decreases and even amount of nano – SiC increases, but K_{Ic} holds steady again. Yet more SiC beyond 7.5%, then quickly K_{Ic} drops. So there is quantized values of K_{Ic} with two levels of fracture toughness holding steady at the quantized values of K_{Ic}.

The perusal of data for similar processing of nano – SiC in alumina at 1600 °C shows identical steady values first between 0 & 2.5% SiC and then a quick drop and again steady value of fracture toughness from 5 to 7.5% nano – SiC at quantized values of 3.5MPa√m and 3.3MPa√m in two steady constant levels for SiC additions increase of 2.5% SiC within the same value of each fracture toufghness. Of course, there is rapid decrease in K_{Ic} between 2.5 and 5% SiC and also after 7.5% SiC. In the two plateau regions of K_{Ic} both amount of

SiC increases and nanosize is also becoming finer but the quantized values of fracture toughness hold steady. While the intrapolated values of nanosizes of nanosize SiC in Alumina could have an error of 10% or so, the difference in values of nanosizes of SiC in two plateau regions of K_{Ic} would have negligible error only. Of course, while nanosize is becoming finer and volume of nano – SiC increase the fracture toughness is constant. The other mechanical properties have multiple trends depending on the property being measured but there is no steady plateau in same compositions where fracture toughness holds steady at the quantized levels.

Applications of Atomic Theory of Fracture

Possible applications could be materials selection with a certain nanosize for fracture toughness and no need to use smaller, finer nanosize in polysilicon for electron devices in semiconductor fabrication and also correct nanosize for a certain required values of fracture toughness (such as ceramic cutting tools) in nanoceramics, nanometals and also nanomaterials for Biomaterials applications. In both of these, we can minimize cost in semiconductors processing as well as cost in biomaterials and also in cutting tool applications.

Quasicrystalline materials have more than or equal to 3 elements and they have individual phases of combination of two types of grains of two ternary compounds of the same elements in quasicystalline materials . so their K_{Ic} is close to nano because, even though these two types of phases it has very, very small regions of 2 individual phases and we know that there is a natural disordered structure of atoms at a grain boundary, the gb itself can be 2 to 5nm itself. So quasicrystalline material could be like the grain boundary of a nanomaterial, in a nanomaterial the grain boundary can be weaker than volume of nanograin. Also quasicrystalline are close to amorphous materials also. So K_{Ic} of quasicrystalline materials and grain boundary of nanomaterial could be lower. Of course in nanomaterial ceramic, if we add boron & zirconium to grain boundary then grain boundary could be stronger than grain volume so in nanoceramics quantization of K_{Ic} is observed.

CONCLUSION

The atomic theory of fracture and quantization of fracture toughness holds steady at the quantized levels. Thus atomic theory of fracture and quantization of fracture toughness in nanoceramics is clearly true. Nnaometals have an increase in fracture toughness with decrease of nanosize but there is no quantization of fracture toughness as such due mainly to the nature of metallic bonding with “gas” of electrons and no clear directional bonding in metals. Other naterials have effects of nanosize on fracture without the clear quanization in nano ceramics, The atomic theory of fracture and its fundamentals are clearly manifest in these materials with a sound theoretical understanding and clarity.

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