

Atomic and Quantization Theory of Fracture Toughness as Well as Electron Segmentation Theory for Mechanical Properties of Nanoceramics and Ceramic Nanocomposites

A. Thirunavukkarasu^{1*}, V. Deva Kannan²

¹Certified Partner, iPro, Internet Profits, Bengaluru, India

²Assistant Professor, Department of Metallurgical Engineering, Government College of Engineering, Salem, India

Abstract: A fundamental understanding of fracture toughness as well as other mechanical properties of Nanoceramics and ceramic nanocomposites has been arrived at now. The atomic and quantization theory of fracture toughness based on the comparability of nanograin size and interatomic distance has been expounded. The other mechanical properties including stiffness are based on large electronic segments in the interatomic bond when total no. of atoms is less in nanosize grains of ceramics. The electron segments are implicit in quantum mechanics due to indistinguishable nature of electrons and half – spins of electrons and its ramifications. The applications to ceramics coatings with less need for control of coating process and also human issues etc. and the large potential for flexible packaging materials in the immediate years is imminent upon the scene now. The possibilities including high mechanical integrity of ceramic makes a utopia of choices between nanoceramics even with metals and polymers in the transforms materials domain. The understanding of nanoceramics with near atomic theory and quantum mechanics on its one side while Hall-Petch and fracture toughness in conventional materials has bridges the continuum of theoretical framework from macro to atomic through nanoceramic and we have large potential in ceramic coatings and the immediacy of flexible packaging, the hype of nanoceramics is now a happening event for all roles from the field applications, engineering and technology to fundamental theoretical investigators. The mosaic is complete and visible picture for the implementation now.

Keywords: Nanoceramics, ceramic nanocomposites, fracture toughness, mechanical properties, electron segmentation, atomic theory of fracture, ceramic coatings, flexible packaging materials, Two-counter Mathematical Induction.

1. Introduction

Nano ceramics have high fracture toughness enabling their mechanical integrity in applications whereas conventional ceramics or not so. The ceramic coatings are even more suitable for Nanoceramics due to good mechanical integrity and other mechanical properties of Nanoceramics and ceramic Nanocomposites of the nano/nano type.

We can tailor thin dimension i.e. thickness of a thin film used for coatings and applied and industrial/other coatings. The

choice of mechanical properties and fracture toughness (K_{IC}) can allow a certain window of thickness of films usually related to process control or inability to control the process practically in implementation and they can be managed. We can coat in application with both best mechanical integrity as well as achieve the best property of coating in its specific application context.

Of course the thickness of coating in thin film form and its mechanical property/mechanical integrity (i.e. Its fracture toughness) must have a large economic impact during utility and cost control ramifications, smooth human performance during coating etc. also.

Normally ceramic coatings lack toughness. But nano ceramics in coating form have high toughness as well as hardness, strength, stiffness etc. so they can be candidates as ceramic coatings but also compete in applications usually involving metallic and polymeric coatings during the applications of latter two also.

Issues such as reliability and predictability (skills of human operators, process issues) are better with quantisation of fracture toughness (K_{IC}) with nano ceramics/composites. The mechanical, physical and functional properties of ceramics like a alumina – zirconia[1] ceramic have applications like oxygen sensor, cutting tools, bearings, automotive components, seals, catalytic products, electronic substrates, extruded products, slip cast products, high efficiency gas turbines, IC engines, membranes, biomedical products, ceramic toughening forms, catalytic and photocatalytic materials and corrosion and wear resistant coatings –but all these require mechanical integrity in applications whereas conventional ceramics need improvement in fracture toughness and that can come from nano ceramics./ceramic Nano/nano composites. Some of these applications offer scope for coatings as well as bulk nanoceramics and ceramic nanocomposites.

“Additionally organic/inorganic hybrid coatings such as the ones prepared through Solgel process have received a lot of interest during the early 21st century. Devices obtained through

*Corresponding author: athiru70@gmail.com

this low-temperature route display a large panel of bulk and surface properties that can then be modulated according to targeted needs. Moreover, this versatility enables solutions in various domains and industrial applications such as in microelectronics, optics, aeronautic, automotive and health contexts. When the targeted applications required polymer as substrate, the use of Solgel process takes its full interest as soft chemistry” [2] Worldwide ceramic coatings will be dollar 14.4 billion (I.e.0.01% of worlds GDP) in the year 2027 (as per April 2021 prices). While ceramic coatings will be 0.01% of world economy in 2027, when we consider coatings on flexible packaging materials [3] can go up to 0.23% of world GDP in 2024 itself.

“The principle of the technology is not difficult but controlling the process maybe” [4,]. This is valid for ceramic thin films. This is where variations in thickness of coatings, variations in processing without control and variations in human efforts aspect of thin ceramic film coating processes – all these together means that quantization and atomic theory of fracture toughness provides more scope and freedom in implementation of coatings in a consistent and controlled, predictable outcome in ceramic thin films. The thin-film toughness will be constant even if there are other variations in the technology that lead to difficulties and complications in the engineering implementation of the coating technology.

2. Literature Survey

A. Atomic and quantisation theory of fracture toughness

[5] Silica (SiO_2) nanoparticles of about 20 nm were made into a packing of about 100 nm. AFM nanoindentation and imaging was carried out to probe local mechanical properties [5] The probe scale included a few particles size and individual particle and even a fraction of a single particle size. Heterogeneous mechanical behaviour with location dependency was observed. The large discontinuous changes in atomic and quantisation of fracture toughness throws up large variations in local mechanical properties in different length scales in this study with some soft spots [6]. Alumina- silicon carbide was doped with magnesia (MgO), Ytria (Y_2O_3) and Ceria(CeO_2) to enable pressure less sintering - a liquid phase enables sintering. For Ceria doping, there was an increase in hardness while wear resistance increased to multiples compared to other nanocomposites with magnesia and yttria. The results for Ceria doping was due to residual compressive stresses, grain refinement and grain boundary strengthening. Ceria leads to densification compared to high-temperature processing but grain size was less leading to high fracture toughness. The small grain leading to high fracture toughness is fully manifested.

[7] zirconia (ZrO_2), Spinel (MgAl_2O_4) and Alumina (Al_2O_3) were processed for surface chemistry and ball milling to avoid agglomeration then characterised by dynamic light scattering – the processing leads to small and narrow distribution of particle sizes. After Spark plasma sintering an empirical model of grain growth was obtained. The results showed multiphase and 2-phase ceramics lead to slower grain growth. The hardness with grain size as a parameter lead to correlation with Hall-Petch

relationship. But fracture toughness (K_{IC}) had a lot of scatter. Except one zirconia sample all had grain sizes of some hundreds of nanometres. The failure included intergranular/transgranular and mixed modes. Grain boundary phases were present, hence no atomic theory of fracture even in near nanosizes. There are large range of grain sizes in different phases hence-a mix of sizes big and small means fracture toughness has large scatter disabling atomic theory of fracture even at near nano grainsizes. [8] The study involved Al_2SiO_5 , Kyanite and Al_2O_3 , corundum which were fabricated with high pressure and high temperature and their mechanical properties were studied. The hardness decreases as grain size decreases towards about 70 Nm but below 35nm (Pages 5 and 6) hardness decreases. The Kyanite grains change from more equant to more columnar shapes. Crack deflection in Columnar grains with aspect ratio 2 to 10 increases fracture toughness. Atomic and quantum theory easily predicts small nanosize increases K_{IC} , fracture toughness, and columnar grains with one small dimension has effect of smaller nanosize.

With high aspect ratio Columnar Kyanite grain, the smaller dimension is nano size when crack reaches grain boundary against thin head of forward grain, So the next grain boundary at the other end of the forward grain is only at short nanometre distance. Remember the next Grain boundary is a strong point mechanically but the volume of the present forward grain is comparatively weaker, so crack should propagate through volume of forward grain logically, .so stress intensity has to be high at Crack tip trying to enter volume of thin dimension ahead of crack tip so instead of breaking thin head of forward Grain, the crack gets deflected which increases K_{IC} , fracture toughness of nano size Kyanite with columnar grains of high aspect ratio from 2 to 10. Hence the thin dimension behaves like very fine nano size of kyanite leading to high fracture toughness K_{IC} just like fine nano size ceramic.

B. Electron segmentation theory

1) Modelling and mechanical properties of carbon nanotubes

[9] The elastic modulus, stiffness decreases with increase in thickness for most carbon nanotubes (CNTs) except highest chirality CNTs. Smaller diameter SWCNTs are more influential in increasing properties. This model with carbon atoms as nodes and interatomic interactions as beams – the whole SWCNTs are frames and the model results are in agreement with other models and experimental data., Small thickness and a small diameter mean less total number of atoms and hence there are a small number of large size segments in each interatomic bond, hence shifting and moving the electron cloud during deformation is difficult resulting in higher mechanical properties.

[10] Molecular mechanics was used to obtain mechanical properties of SWCNT. Covalent bond are two types of Van der waal’s bonding are utilised to calculate the stiffness of SWCNTs, Van der waals can significantly reduce the Mechanical properties. The stiffness of SWCNT’s around 1.2 TPa and it agrees with experimental data. [11] A Finite element model with carbon- carbon bond as a beam between two carbon atoms gives the correct Young’s modulus. The Young’s

modulus Increases with diameter before saturating at about 1.5 nm diameter. The modulus is in the axial direction but the diameter is increasing so percentage of energy absorbed laterally increases and less energy is available for axial strain, hence Young's modulus increases in axial direction. This novel finite element method can also be extended to MWCNTs i.e. is multi walled carbon nanotubes.

[12] A continuum approach to Young's modulus and shear modulus of DWCNT will overestimate them for longer DWCNTs but gives good values for short DWCNTs only, for longer DWCNTs Van der wals has disproportionate role hence approximation is inaccurate. Critical buckling loads of zig zag CNTs depends on chirality of CNT. Axial Compression in DWCNT double walled carbon nanotubes has been applied to obtain the properties in this model [13] CNTs have 1TPa stiffness and 60 GPa strength as high strength for these materials but there are large experimental data variations. Armchair, zigzag and chiral configurations lead to variations in properties in molecular mechanic's model. Change in radius/diameter varies Young's modulus from 0.95 to 5.5 TPa and changes poisson's ratio from 0.15 to 0.29. At a fixed total number of atoms, we can systematically correlate all structure and properties with Electron segmentation theory, even then change in diameter will change the percentage of energy for axial strain and modulus. So we get large variations in properties in this study.

[14,] The mechanical properties of nanotubes are studied by FEM and ANSYS to analyse variations in reports of CNT properties. The Young's modulus varies with thickness, lengths and/element diameter. The results match with previous reports and will be useful for new nanocomposite materials and CNT. [15] Molecular dynamics and molecular mechanics are used to study the energy, structure mechanical and vibrational properties of armchair, zigzag and chiral types of SWCNTs. The bending modulus is higher than Young's modulus. A defect can decrease some properties but with less defects the bending is like twisting but Young's modulus is having only one dimension in action with linear strain. Hence a molecule like high bending modulus and lesser one-dimensional Young's modulus in SWNTs. The results include different forms of armchair, zigzag and chiral types of SWNTs. The study included energy variations with different configurations and "phase change" i.e. favourable configurations when radius of SWNT changes. The energetics means that as diameter changes particular configuration is favoured energetically for one particular region of radii of SWNTs. [16] the research focuses on SWNTs with 3-D FEM code using ANSYS in molecular mechanic's evaluation. The effects of diameter, length and Chiral angle on elastic modulus and poisson's ratio in the armchair, zigzag and chiral structures are investigated. For diameter over 2 nm and length over 36.5 nm, Chiral angle is only factor to decide tensile properties. As per Electron segmentation theory beyond a certain large number of atoms the electron segments are so small, so no further significant change in properties can be seen.

[17] Molecular dynamics (MD) and molecular statics (MS) are used for mechanical properties of single walled carbon

nanotubes SWCNTs). Tensile strength increases at smaller diameter of SWCNT/- but the electron segments are smaller and easier to break the structural C-C bond in larger size SWCNT, hence the strength is lower. The corroboration of electron segmentation is seen in this study.

2) *Experimental studies of mechanical properties possessed by carbon nanotubes*

[18] The decrease in CNT diameter used in aligned CNTs increases the mechanical properties. When CNT diameter increases with generally similar long CNTs, then two things are: - at low diameter the less number of atoms in CNT means less number of electron segments, but there is larger size of electron segment due to less number of atoms segments in one interatomic bond. Larger electron segment is difficult to strain into larger length etc. hence modulus and strength increases that is mechanical property increases. In addition, the process to align CNTs drastically increases mechanical properties of the material itself as the individual CNT mechanical properties increases and serves to increase material mechanical properties. Raman spectroscopy is used to characterise alignment of CNTs in composites of CNT/epoxy.

[19] Density, defect degree and moment of inertia influence intrinsic mechanical properties of vertically aligned CNTs arrays. This is in the context of compressive load and buckling behaviour. While diameter is considered in study, it is moment of inertia that indirectly has an influence on compression and Buckling. Density and defect degree are most important. In energy absorbing and damping applications involving crack initiation and crack growth as well as vibrations. The modulus and other mechanical properties as well as above- said experimental properties are indirectly involved with electron segmentation theory.

[20] The Young's modulus increases with diameter and saturates around 15 nm diameter. At high number of atoms in CNT the electron segment becomes small enough and further decrease in segment size is not significant anymore. In this study both analytical method and finite element method /are used to get young's modulus and shear modulus for SWNT, double walled CNT and MWNT. Shear modulus increases and saturates at ~20nm. Shear modulus is more sensitive to increase in number of tubules. Good conformity is seen with reported experimental values. Electron segments have lesser role in number of tubules in carbon nanotubes since van der waals forces are significant in plural number of tubules. [21] As the length of CNT increases the elastic modulus decreases. Larger number of atoms means more and smaller size of electron segments, hence easier to the deform & lower modulus is seen. It saturates at around 55nm. The experimental data validates the calculated Young's modulus.

[22] A carbon nanotube may be considered as being made by rolling up a hexagonal lattice of carbon. In a multi-walled nanotubes, the individual nanotubes inside a MWCNTs are loaded together because of Van der waal's forces. There also exists undetermined structure in some nanotubes with diameter less than 100nm and they are also carbon nanotubes. All these nanotubes have mechanical properties based on each sole or one of multiple nanotubes, the number of carbon atoms in CNT and

electron segments in the bonding (multiple electron segments in each interatomic bond) determine the mechanical properties. [23]. A carbon nanotube has a screw dislocation along the axis. The growth rate is proportional to the burger's vector i.e. to the chiral angle of tube. Other studies have said mechanical properties are related to the chiral angle. Hence, the chiral angle, burgers vector of screw dislocation is the linked chain causing mechanical properties. While at the fundamental level the mechanical properties are related to electron segmentation the actual properties or a modification of fundamental theory of electron segmentation. [24] The nanotube model with FEM showed the effects of diameter, length and tube chirality on the elastic properties. Elastic and shear moduli of both armchair and zigzag CNTs increased monotonically with increasing diameter. The findings are in good agreement with theoretical and experimental results that exist as of now. As in other studies the proportion of energy in diameter, direction increases. Hence actual elastic and shear modulus increase with increasing diameter (electron segments predict that moduli must decrease not increase with increase in diameter).

[25] This research focussed on tensile strength, Young's modulus and Weibull scale and shape parameters of MWCNTs synthesised by chemical vapour deposition (CVD) and then defects studied by TEM. To analyse failure of MWCNTs...The fracture was affected by structural defects in the form of discontinuous flaws like holes, kinks and bends and remnant catalysts and hence properties results changed. The process of thermal annealing improves properties as there is a removal of structural defects during thermal annealing, however the removal was incomplete. When a near complete removal of defects can be done then properties would near the trend based on electron segments deciding mechanical properties. [26] SWCNT has high tensile strength. Small diameter SWCNT has highest strength in keeping with electron segments being bigger in smaller diameter SWCNTs. Defects are considered as the reason for lower experimental strengths of CNTs. In smaller CNTs, the bigger electron segments would play an overpowering role in increasing the strength of smaller diameter CNTs. The chirality also affects the strength in addition to smaller diameter of CNTs... Hence future processing and production should consider this electron segmentation theory for mechanical properties of SWCNTs.

3) *Applications of carbon nanotubes based on their mechanical properties*

[27] A CVD modification process was used to produce long multi walled CNT ropes having a tensile strength of 210 MPa and elastic modulus of 2.2 GPa. The high strength and reproducibility favour the applications of these CNT ropes. It absorbs NH_3 . But there is a gap between CNT mechanical properties and rope properties. [28] The high strength, high stiffness and low density of CNTs holds out a big potential for this material. A need for a database of properties, defects, temperature, chemical environment, functionality, load cycling, lifetime etc has been asserted. Available studies are the tip of the iceberg and implications of more studies in the future. Even if diameter and length affect properties other factors have a role in applications as in the list in above sentences [29] With carbon

nanotubes that is an extreme improvement in properties in the context of civil engineering materials. Carbon nanotubes can be used in both concrete and also in the steel towards construction purposes. The carbon nanotubes compare favourably with other nanotubes, but there exists issues in manufacture of CNTs. [30] from various research studies we have some more aspects in CNTs. For bundles and ropes from CNTs, the mechanical properties depends on Van Der Waals between/individual neighbouring SWNTs and/or MWCNTs. For Heterojunctions of CNTs of varying diameters in conjoined two nanotubes, the taper joint i.e. the heterojunction, the overall properties of entire nanotube depend on taper and dimensions of heterojunctions joint. Individual CNT properties less important in bundles, ropes and heterojunctions. Also in Buckypaper the properties depend on number of layers, alignment of CNTs, Van Der Waals etc not on individual CNTs. However, there is a proportion between individual CNTs and electron segments for properties on one hand and the properties of bundles, ropes, heterojunctions and also Buckypaper.

[30] SWCNTs have high mechanical properties and the large body of research literature contributed to substantial understanding of mechanical properties of CNTs. While applications are expected, a deeper theory is needed. The present article herewith electron segmentation theory could go down to the atomic level of mechanical properties of CNTs. We have a contribution to the theoretical understanding of not only CNTs, but also nanoparticles and nanoceramics and ceramic nano/nano composites with the electron segmentation theory as well as atomic & quantization theory of fracture toughness.

4) *Nanoindentation of a single nanoparticle (including graphene)*

[31] the research involves a theoretical model with grain boundary sliding and emission of lattice dislocations from Triple junctions. This discrete dislocation dynamics method leads to inverse Hall- Petch relation and shows qualitative coincidence with experimental micro hardness. This theory has good results in extremely small grain sizes. While mechanical properties involve electron segments and defects modify the results of electron segments in mechanical properties, here in hardness we have a indenter creating a flaw and obtaining hardness at a sharp tip of indentation which is less of bulk properties and more compatible to fracture toughness K_{IC} at a defect/crack tip. Hence hardness follows inverse hall – Petch relation and hardness decreases with smaller grain size. [32] This molecular dynamics study has a nanoindentation of single layer rectangular graphene with young's modulus and strength of 1TPa and 200 MPa respectively. The graphene has elastic and plastic regions in load- deformation curve. Young's modulus and maximum stress are material properties of graphene whereas other properties are influenced by indenter loading rate etc. are not so. The material properties of modulus and strength are part of the electron segmentation theory even though nanoindentation is not so. [33] C_{60} single crystal was grown and then characterised with nanoindentation and led to maximum stress strength that was 1/11 of the shear modulus. The shear strength was close to shear strength of defect free fullerite. A Finite element analysis was applied with the

indenter close to and realistic compare to actual indenter load $1/11$ of shear modulus/as shear strength.

[34] Nanoparticles can hold large stresses and provide large ductility. The maximum compressive stress and associated strain of SiC as a function of size of NPs (nanoparticles-NPs). Uniaxial compression was used in alumina, Al_2O_3 MD simulations. Lower size NPs are less prone to cracks and defects and have much higher properties before plastic deformation. While defects have a good role, smaller size NPs have less total number of atoms and hence larger electron segments in each interatomic bond in solid materials NPs hence, smaller NPs have higher properties in higher quantitative way in study. [35] Nanoindentation of single Nanoparticle was carried out in TEM. The load displacement curve was obtained and nanoparticles behave as elastic-plastic rather than brittle behaviour seen in microns size ceramic alumina (Al_2O_3) particles. We conclude that below a certain size, ceramic nanoparticle in elastic/plastic and matches grinding limit often reported in a ceramic science. My PhD thesis [1] had Alumina – Zirconia composite nanoparticles of 5.9 to 9.5 nm... When sintered to nanograins with one-dimension as low as 2.25nm. The composite nanoceramic has a fracture toughness of 29.5 $\text{MPa}\sqrt{\text{m}}$. Hence I have personally shown a ductile i.e. elastic-plastic mechanical behaviour of ceramic nanocomposite as the present reference reports with TEM Nanoindentation. The high fracture toughness and elastic plastic deformation are related to atomic and quantisation theory of fracture toughness. But the elastic modulus, strength etc of nanoparticle are based on electron segmentation theory being expounded at this instant of time. [36] The method of solgel coating with silica SiO_2 on polycarbonate is used to improve mechanical properties. As the thickness increases from 2.2–8.0 micro-- meter, the hardness increases from 30 HV to 250 HV. Say with 10% silica, it really means equivalent silica thin film with a thickness of about 220nm to 800 nm. But high porosity is the cause of lower hardness. So above 100nm no effect on hardness coating. Hardness of film only bulk hardness so above 100nm all coatings same. Since silica is amorphous we do not envision Hall-patch hardness either. The thickness in this study are near-nano but amorphous and near-nano as practically the same property as bulk.

[37] Diamond like Carbon (DLC) in single film made by sputter deposition has compressive stresses and only low thickness feasible to avoid cracking. Hence gradient in composition, constitution or properties are used for DLC thin films. Microhardness indentation and AFM imaging proved all gradient thin films have better crack resistance while also maintaining a high hardness of 4000 HV005. This is like a stacking of many thin films or nearly so, hence smaller thickness and larger electron segments lead to higher hardness even though compressive residual stresses also have a role in properties of DLC thin film. [38] The hardness and Young's modulus of nanocolumnar films of 500 to 1500nm thick films is measured. The effect of deposition, site, shape of deposition on mechanical properties of titania, TiO_2 films is studied. Zigzag layers have lower properties but prevent fracture and delamination. The nanoindentation also lead to force-

displacement curves. While electrons segments have a role in Young's modulus, the zigzag geometry of Nanocolumnar thin films has lower property as the full integrity of thin film may not be there.

[39] The nanoindentation of ZnO nanorod by sophisticated mechanism was carried out using nanomanipulation. The study resembled three-point bending test of this nanorod. It leads to an elastic modulus of 800 GPa and unloading curve and also creep. The study of this mechanical behaviour will be useful for design and applications for future nanodevices and so will be the electron segmentation theory. Very high elastic modulus 800 GPa shows larger electron segments in smaller number of total atoms in ZnO nanorods and leads to high elastic modulus. This is consistent with electron segmentation theory results in other nanomaterials and especially nanoceramics. Remember 800 GPa modulus is close to elastic modulus of even 1.2 TPa of SWCNTs that is near perfect structure and a near molecular material. To compare it with ZnO nanorod is advanced Nanoceramic materials. [40] The research has nanoindentation and nanopressurisation of graphene sheets. In this study load versus indentation for hardness and load versus deflection for mechanical properties has been carried out. Different shapes as well as different sizes and hardness of graphene but based on assumption of constant elastic modulus in this study is seen. But nanomaterials of graphene must have variation in modulus with size and shape variations as diagrams of the simulation given in this study report.

3. Mechanical Properties of Nanoceramics and Ceramic Nanocomposite

A. Scope of nanoceramics and ceramic nanocomposites

The mechanical, physical and functional properties even refractory nature make them ideal for a number of applications and even new Frontiers. In the materials domain and its engineering as well as other applications but their low fracture toughness compromises their mechanical integrity hence Nanostructured ceramics and ceramic nanocomposite's which have high fracture toughness can manifest structural integrity and reliability. The quantisation of fracture toughness of nanoceramics and ceramic nanocomposite enables quick fix applications in vast domain areas. They have reliability in spite of process variations and engineering ease of processing while providing scope for human-based variations in implementation including processing brings it into prime position in practical use and hence applications. The complete set of mechanical properties of nanoceramics and nanocomposites with the exception of fracture toughness are now understood through electron segmentation theory towards successful application of these materials. While electron segmentation is implicit in quantum theory it was an untouched part of the physics. The nanoceramics and a mechanical properties have bridged the chasm between fundamental quantum physics and its practical and the vast scope of nanoceramics having high properties and also the additional benefit of quantised fracture toughness are now inaugurating a new chapter in both nanotechnology as well as ceramics especially in the area of ceramic coatings. They will

only grow by leaps and bounds in the coming few years. The mechanical integrity of ceramics by themselves say in cutting tools as well as niche area of ceramic coatings which will even have a role in the practical applications of the polymers and also metals. There is now a vast scope for ceramic nanocomposites and nanoceramics and even a unique niche for some applications hence materials and their engineering applications catching up with the many years of potential applications predictions. These contemporary theories of atomic and quantization theory of fracture toughness as well as electron segmentation especially in ceramic coatings are clearly on the radar of vast industries with a theoretical basis bridging the fundamental quantum theory on one hand and the hope and scope of nanotechnology on the other hand with the developments near at hand and this is a happening field now and the immediate future years itself. The uncertainty in perfectly controlling processing especially in thin films and the variations in thickness of coatings but the strict need to produce same fracture toughness mechanical integrity in spite of process variations and variety in engineering context and environment –all of these call for application of atomic theory of fracture and quantisation of fracture toughness (even the skills involved could be an issue). Also the understanding of other mechanical properties from electron segmentation can be used to simulate/calculate mechanical properties in nanoscience regime and size of nanomaterial grains/particles/coatings which will play in tandem with fracture toughness to tailor coatings with good and required mechanical properties. When the coating is a nanoceramic as opposed to conventional micro-size ceramic then the temperature of processing will be less. But after coating you can reheat it that as a whole or as a surface reheat and ceramic coating will be sintered and if sintering coarsens the coating into micron size structure then the coating can have higher temperature of operation/service usage. In ceramic thin films, “The principle of the technology is not difficult but controlling the processing maybe so [41].

Thus the atomic and quantisation theory of fracture toughness as well as electron segmentation theory of mechanical properties together in nanoceramic coatings is a distinct niche for involved implementation in the near future and beyond too.

B. Atomic and quantisation theory of fracture toughness

1) Definition and outline of theory

The quantisation of K_{IC} is because Nanosize of grains in nanoceramics is comparable to interatomic distance in nanoceramic K_{IC} denotes the strain gradient from a crack tip to nearby and strained regions in nanograins. Since grain size is comparable to interatomic distance is the stress gradient at crack tip cannot be completely smooth and continuous change but only steps in change in interatomic distances when force for fracture increases. Hence we have quantisation in fracture toughness. The fracture toughness of nanosize grained ceramic with grain size of 5 nm to 100nm has quantised values of fracture toughness. There are only specific values of fracture toughness and identical K_{IC} in a band of 10–20 nm inside 100nm and less nanosize, but there are many quantized bands

of K_{IC} inside nanosize grains in ceramics up to 100nm grain size. For crack tip to make a fracture in the nanoceramic the stress intensity at the crack tip must have a large enough value i.e. Critical stress intensity, K_{IC} for the interatomic bonds at the crack tip to break then crack grows and then failure occurs. At size grains there are hundreds and thousands of interatomic distances i.e. inter-atomic bonds and hence hundreds of interatomic jumps are needed for crack to grow and turn into failure in microns size grain. But in nanosize ceramic grain there are small number of interatomic distances between crack tip and grain boundary of the forward grain of nanoceramic where crack stops after propagating itself across the nanograin of ceramic. As the nanosize of grain decreases, the stress intensity to fail increases to a high-value at the crack tip of the forward grain up to next Grain boundary. So the stress intensity is high at the crack tip but decreases to low value at nearby grain boundary. So at the crack tip the stress intensity should be very high near the crack tip to fail by breaking interatomic bond at the crack tip and into the first point of the forward grain to enable the propagation of the crack into the forward grain. With a large grain size, the stress intensity can gradually decrease away from the crack tip and yet the nearby interatomic bond can break. But in the small nano size ceramic grain the interatomic bond at crack tip of forward grain requires large stress intensity to break bonds if crack has to grow, the stress has to increase steeply within a short distance to break interatomic bond and hence K_{IC} , fracture toughness is high.

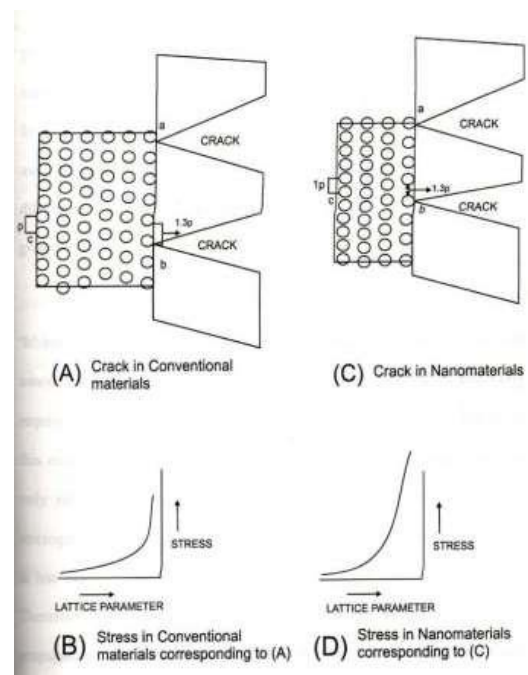


Fig. 1. The stress at crack tip for nano and conventional grain materials

For a little variation in nanosize grain length and already the stress intensity is high for failure though there is some change in interatomic distance as the crack grows to failure. The next grain boundary at the forward grain to crack tip distance and the interatomic bond length at crack tip are both comparable to each other. So once one interatomic bond snaps the stress intensity

at crack tip shoots up and second interatomic bond at forward grain breaks due to increase in stress intensity when first interatomic bond breaks. When grain size decreases the grain boundary distance at the forward grain decreases in a way comparable to interatomic bond length at the crack tip. So critical stress intensity makes a Quantum jump from one grain size of nanoceramic to a lesser nanosize of grain in same material nanoceramic. Remember interatomic bond length at crack tip is comparable to grain boundary distance of forward grain. So K_{IC} does not change for same little change in nanosize but when grain size changes by 10 or 15 nm the ratio of interatomic bond at crack tip and grain boundary size, the ratio makes a big change so that is a quantum jump in fracture toughness, K_{IC} . Since interatomic bond length at cracked tip is significant compared to grain size and stress intensity is high and toughness K_{IC} is already high so even if you slightly change the grain size i.e., slight increase in stress intensity at crack tip due to decrease in distance to next grain boundary at forward grain but increase in stress intensity is not enough to break bond i.e. K_{IC} fracture toughness does not change but when you change grain size by 10 or 15 nm, there is a real change in ratio of interatomic bond length at crack tip to distance of next grain boundary at the forward Grain so the fracture toughness K_{IC} makes a quantum jump else fracture toughness K_{IC} remains same for small change in grain size to enable snapping at interatomic bonds at crack tip and the crack grows. When ratio of interatomic bond distance at crack tip to nano grainsize has a significant change, then the K_{IC} fracture toughness makes a quantum jump. Else the K_{IC} value of nearby larger value of nano grain size ceramic continues. So the fracture toughness is quantised and as per atomic theory of fracture for nanoceramics and ceramic nanocomposites

forward Grain. But in microns size grain, there is gradual growth to failure by fracture and low stress intensity K_{IC} for failure. Whereas in nanograin there are only a few interatomic distances from Crack trip to next grain boundary at forward grain, .so stress intensity is very high in nanoceramics and to break less number of interatomic bonds at the crack tip. So High K_{IC} is needed for crack to grow. As the grain size of nanoceramic decreases there is smaller number of interatomic distances for crack to propagate. A few nanometre decrease in grain size means the same K_{IC} for failure by fracture toughness method. Only when nanosize decreases by 10 nm or 15 nm, then large decrease in number of interatomic distances in forward grain of present crack tip when the crack tries to propagate to failure. This new high K_{IC} continues for some amount of variation in nanograin size in ceramic. Until you reach a new level of big decrease in grain size of nanoceramic the K_{IC} is same when you do have a big decrease in grain size of narrow ceramic then again K_{IC} changes i.e. increases in a big significant way. Hence we have atomic theory of fracture and quantisation of fracture toughness in fracture of nanoceramic and ceramic nanocomposites. The fracture toughness of nano grainsize ceramic with grain size of 5 nm 100nm has quantised values of fracture toughness. There are only specific values of fracture toughness and identical K_{IC} in a band of 10-20 nm inside 100nm and less nanosize but there are many quantised bands of K_{IC} in nanosize grains in ceramic having up to 100nm grain size

2) *Mathematical induction with two dimensional method having two variables for Fracture Toughness quantization and atomic theory*

Table 1
Fracture toughness for nanosize grains and interatomic distance

Nanograin size	Grains size/Interatomic distance	K_{IC}
147	459.38	3.3
141	440.63	3.5
134	418.75	3.6
125	390.63	3.5

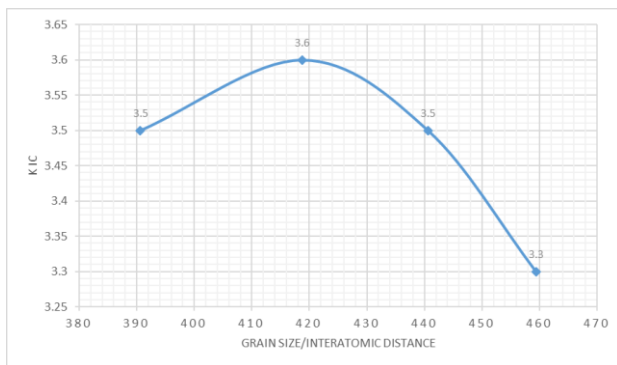


Fig. 2. The (grain size/interatomic distance ratio) in nanograins

In fig. 2, the process of quantization has started at 125 to 134 nm itself. When you analyse this from another angle (grain size D/interatomic distance) ratio is the number of interatomic distance from crack tip to the next grade boundary at the

Table 2
Nanosize and fracture toughness in Nanoceramics of ($Al_2O_3 + SiC$)

S. No.	SiC(%)	D1(nm)	D2(nm)	$K_{IC}(MPa\sqrt{m})$ with Math Relation Calculation in ()
1	5 to 7.5	146	135	3.5 (3.422)
2		142	152	3.3 (3.423)
3	0 to 2.5	120	130	3.5 (3.42)
4		130	138	3.6 (3.530)

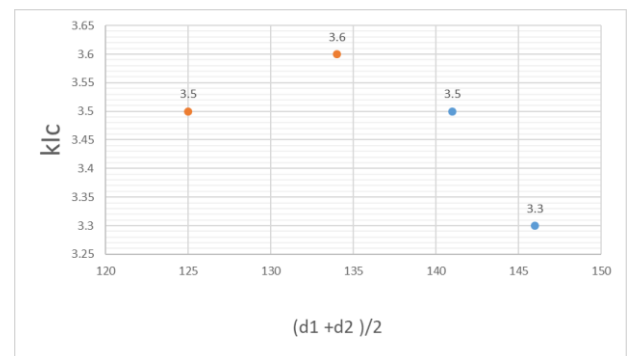


Fig. 2.1. The slowdown in Fracture toughness change as nanosize of grain decreases

We carry out mathematical induction on more than one counter specifically two counters i.e. 2-dimensional mathematical induction to prove that in multiple bands of grain size less than 100nm, all have quantisation of K_{IC} i.e. fracture toughness. Use first counter for each band of quantized, single

value of K_{IC} inside each band of nanograin sizes. Hence prove entire nano range of grain size between 5 nm up to 100nm. All have quantised values of fracture, K_{IC} .

For 5 to 7.5% SiC in alumina, for 11 nm change in grain size of alumina, the fracture toughness is constant at $3.5 \text{ MPa}\sqrt{\text{m}}$. Both SiC and grain size changes nanosize decreases but K_{IC} is constant with two big factors changing. Also for 130 and up to 138 nm change in nanosize, K_{IC} , is constant at $3.6 \text{ MPa}\sqrt{\text{m}}$. Similarly, for change in nanosize of grains from 142 up to 152 nm and also 120 up to 130 nm, the fracture toughness is constant at values of $3.3 \text{ MPa}\sqrt{\text{m}}$ and $3.5 \text{ MPa}\sqrt{\text{m}}$ respectively. Thus quantisation of fracture toughness is indicated and now we confirm it with mathematical induction.

$$K_{IC} = 0.59 \left(\left(\frac{E}{H_0 + \left(\frac{K}{\frac{\sqrt{d_1 + d_2}}{\sqrt{2}}}} \right)} \right)^{\left(\frac{1}{8} \right)} \left[\left(\left(\frac{HV}{\sin(\gamma_1)} \right) \left\{ P^{\left(\frac{1}{3} \right)} \right\} \right) \right]^{\left(\frac{3}{4} \right)} \left(\frac{d_2 - d_1}{10} \right)$$

- E = elastic modulus
- H0 = Intrinsic hardness of grain
- K = Strengthening constant
- HV = hardness Vickers, GPa
- γ_1 = Vickers indenter angle = 68 degrees
- P = load, N

The results are largely in agreement with research data in above table 2.

So we will accept the general trend that K_{IC} , is higher for smaller nanosize of grain in nanoceramics

Theorem (two –dimensional induction)

Let S (m,n) denote a statement involving two variables m and n. Suppose

- (1) S(1,1) is true
- (2) If S (k,1) is true for some positive integer K, then S (K +1,1) is also true
- (3) If S (h,k) holds for some positive integers h and k, , then S (h,, k +1) is also true.

Then S (m,n) is true for all positive integers m,n.

- (1) S (1,1) is true.

or Alumina samples from 2 up to 6 nm in my PhD thesis [1],

had constant fracture toughness of around $23 \text{ MP}\sqrt{\text{m}}$

- (2) S (K, 1) then S(K +1, 1) is also true.

Suppose S (K +1, 1) is true, then say the band 120 nm to 130 nm $(d_1 + d_2)/2 = 125 \text{ nm}$ is assumed to be true. Then S(k+1,1) is the band from 130 nm to 140 nm, hence $(d_1 + d_2)/2 = 135 \text{ nm}$, then K_{IC} must be quantized. The expression for K_{IC} is given, Then 1st term;

1st term

$$\left(\left(\frac{E}{H_0 + \left(\frac{K}{\frac{\sqrt{d_1 + d_2}}{\sqrt{2}}}} \right)} \right)^{\left(\frac{1}{8} \right)} \right)$$

2nd term

$$\left[\left(\left(\frac{HV}{\sin(\gamma_1)} \right) \left\{ P^{\left(\frac{1}{3} \right)} \right\} \right) \right]^{\left(\frac{3}{4} \right)}$$

$$K_{IC} = 0.59 \left(\left(\frac{E}{H_0 + \left(\frac{K}{\frac{\sqrt{d_1 + d_2}}{\sqrt{2}}}} \right)} \right)^{\left(\frac{1}{8} \right)} \left[\left(\left(\frac{HV}{\sin(\gamma_1)} \right) \left\{ P^{\left(\frac{1}{3} \right)} \right\} \right) \right]^{\left(\frac{3}{4} \right)} \left(\frac{d_2 - d_1}{10} \right)$$

So, $(d_{p+1} + d_{q+1})/2$ increases to 135 nm.

$$\text{So} \left(H_0 + \left(\frac{\sqrt{d(p+1)+d(q+1)}}{\sqrt{2}} \right) \right)$$

Means denominator increases, so 1st term increases

In 2nd term for K_{IC} , for $d(k+1)$, $p(k+1)$ is same but $\delta_0 = (HV/\sin(\gamma_1))$ – it increases for higher grain nanosize, by inverse Hall- Petch relation. Higher grain size has higher δ_0 related to higher hardness,

So 2nd term $(\delta_0 X P^{(1/3)})^{(3/4)}$ increases due to higher hardness. The premultiplier in K_{IC} is 0.59, so

$$K_{IC} = 0.59 \times (1^{st} \text{ term}) \times (2^{nd} \text{ term})$$

and both 1st term and 2nd term for $(k+1)$ increase, so K_{IC} increases in 2nd term, so $K_{IC}(K+1,1)$ is also true. Our data for 130nm to 138 nm in Table 2 shows an increase and also quantized K_{IC} in 2nd band also i.e. $S(k+1, 1)$ is also true .

(3) If $S(h,k)$ holds for some positive integers h and k , then $S(h, k+1)$ is also true.

In h_{th} band with grain size range of dh_1 to dh_2 then,

$$K_{IC} = 0.59 \left(\left(\frac{E}{H_0 + \left(\frac{K}{\frac{\sqrt{dh_1 + dh_2}}{\sqrt{2}}}} \right)} \right)^{\left(\frac{1}{8} \right)} \right) \times \left[\left(\left(\frac{HVh}{\sin(\gamma_1)} \right) \left\{ P^{\left(\frac{1}{3} \right)} \right\} \right)^{\left(\frac{3}{4} \right)} \right]^{\left(\frac{3}{4} \right)} \left(\frac{dh_2 - dh_1}{10} \right)$$

is true.

The $S(h, k+1)$, it also increases. i.e.

$$K_{IC} = 0.59 \times (1^{st} \text{ term}) \times (2^{nd} \text{ term}) \text{ also increases}$$

Also increases the band is same and grain size is within same band. So K_{IC} is constant,

$(K + 1, D)$ is within same band of $S(h,k)$. So K_{IC} -depends only on lower limit of $D(h+k)1$ and higher end $d(h+k)$ i.e. $S(h,k+1)$ is within same band $S(h,h)$ i.e. $K_{IC}(h,k)$ formula is same for $K_{IC}(h,k)$ as well as K_{IC} in side $d(h+k)1$ and $d(h+k)2$.. Here the data in all bands is based on expression for K_{IC} and it is valid for all bands in nanosize and is seen in data in Table 2 for large data in nanorange, from 2nm, 6nm [1], to even 150 nm. As per K_{IC} relation the Fracture Toughness is monotonic from 2nm to 150nm and is valid at both 2nm and 150nm ends of nanosizes of ceramics, thus $S(m.n)$ is valid in $S(h,k+1)$. Hence K_{IC} is quantized and same i.e. $S(h, k+1)$ is true.

Whether, it is 1st grain size or middle grain size or largest grain size in h_{th} band, $S(h, k)$ is same as $S(h,k+1)$. So “ h ” denotes band and “ k ” denotes a nanosize of grain within h_{th} band, so for entire band, $S(h,k)$ true automatically means , $S(h, k+1)$ is true . K_{IC} depends only on start grain size and last grain size in h_{th} band of quantized K_{IC} . Hence atomic and

quantization theory of fracture toughness is proved by two-dimensional Mathematical Induction.

4. Other Mechanical Properties Excepting Fracture Toughness

A. Electron segmentation theory

1) Outline of electron segmentation theory

Electrons are indistinguishable and have $(1/2)$ spin i.e. plus half or minus half not 1, 2, 3 Spin – not integral spin, so you should rotate on electron orbital for two rotations to come back to same Point i.e. $1/2$ Spin., the only way for this is that the Orbital of an electron is segmented i.e..1 orbital is divided up into multiple segments and when you rotate the orbital, all the divided parts of orbital are anti-correlated and not directly correlated. So when segments in one orbital are Anti-correlated you need to rotate the orbital for two rotations to come back to same point. i.e. to come back to same configuration at same point with same appearance, electrons globally is being rotated 360° or two pi radians but the segments inside the electrons are each segment– half of all segments are rotating in opposite direction across the electrons global rotation by 360° or two pi radians i.e. it has spin half. Remember the single orbital has two electrons of opposite spin to each other even if space of second electron is not filled up in orbital. the orbital space itself is rotated, as two electrons would, but they are half occupied. The electrons in the segments are themselves indistinguishable, hence we have the theory of electron segmentation which includes the electrons in bonding orbital where there is bonding between two atoms [41], Thereafter on segments in the interatomic bond affect the bond stretching in mechanical strain and further more when strain breaks the bond between atoms then there is fracture. This is the essence of electrons segmentation affecting mechanical properties other than fracture toughness, the latter depends on the presence of a crack for failure, it is related to K_{IC} and crack growth. The other mechanical properties are correlated to electron segmentation.

In conventional materials mechanical strength and failure is dependent on voids and cracks to decide mechanical properties during defamation. But defects are less important. In nanoceramics, they deform by grain boundary sliding and just about one dislocation in each nanosize grain of ceramic. The number of electron segments affects mechanical properties of nanoceramics due to variation in nanosize of grains in ceramics so electron segment is precisely the determinant of mechanical properties in nanoceramics. But fracture toughness depends on pre-existing crack and/or crack propagation pathway in ceramic nano materials and there is a facile near straight line path for crack to propagate and cause mechanical failure. But other mechanical properties depend on interatomic bond and bond to break up in strength and stiffness of a nanocomposites when the number of atoms in a carbon nanotubes or nanosize grain or Nanosize thickness thin film changes then the mechanical properties except fracture toughness vary in a monotonic way with number of atoms in grain/ nanotube /nanosize thickness thin film. Basically electrons are indistinguishable particles.

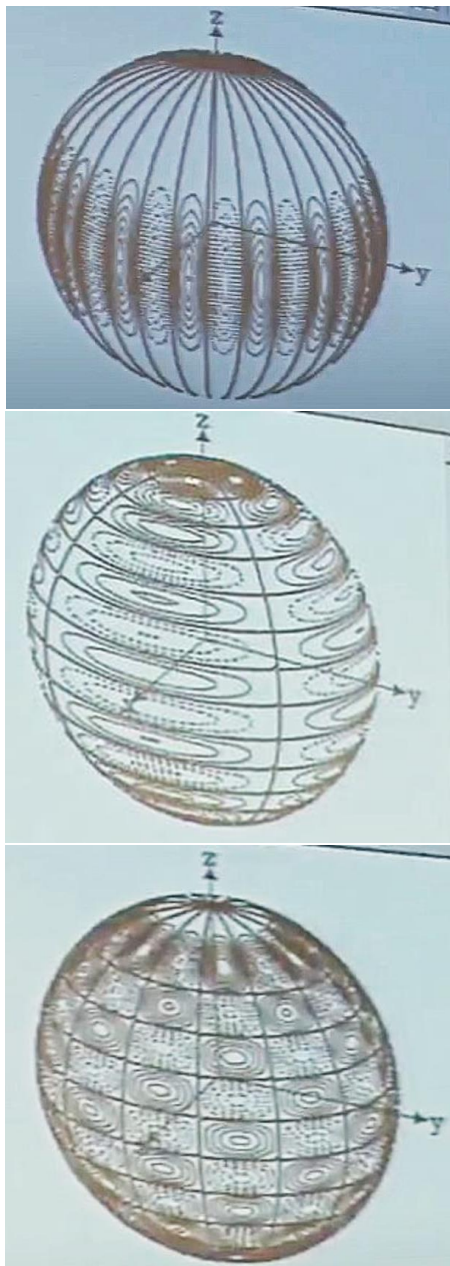


Fig. 3. Some types of electron segments

When there is a bond, double bond or triple bond in the unit cell of a grain of nanoceramic or nano/nano ceramic nanocomposite, then electron bonding region of orbital can have electrons segments. The modulus and strain and stress during application of stress and when mechanical failure occurs electrons, bonds or modified and stretched and compressed and finally lengthened or shortened to the point of snapping, breakage fracture in the tensile strength and compressive strength. So it is electron segmentation which plays a big role in mechanical properties (except fracture toughness which has a crack present and then crack grows to failure. The electron segments in conventional microns size materials has very thin electron segments due to large number of atoms in a microns size region. But in a nanograin the number of atoms is less – and the electron segment is bigger and also electron segments enlarge at a rapid rate as the nanosize of grain decreases from

hundred or 50 nm down to 20 nm or even 5 nm itself. Hence the electron segmentation comes into strong play in covalent/ionic bonding in nanoceramics with big influence and role in mechanical properties other than fracture toughness. Also in metallic bonding and macro molecules of polymers, the electron sea in metals and macro size molecules of macromolecular polymers do not lend themselves to electron segmentation theories. (Though even gold is not highly metallic in Nanosize particles of gold in nanogold). Thus we lay out the electron segmentation theory in the mechanical properties of nanoceramics and ceramic nanocomposites of nano/nano type where all grains are nanosize and no fiber/ no particulate in the ceramic.

2) *Nanotube diameter and electron segmentation*

When diameter of nanotubes of same length changes the yield strength tensile strength, hardness, elongation, the elastic modulus all except fracture toughness must increase but changing circumferential sharpness, Stress concentration mean that properties increase not decrease by electron segmentation

3) *Nanotube length and mechanical properties*

When Length of nanotube changes with all of them having same diameter – but their length changes, then yield strength, ultimate tensile strength, hardness, elongation and elastic modulus – all except fracture toughness – all decrease with increase in length of Carbon Nanotube.

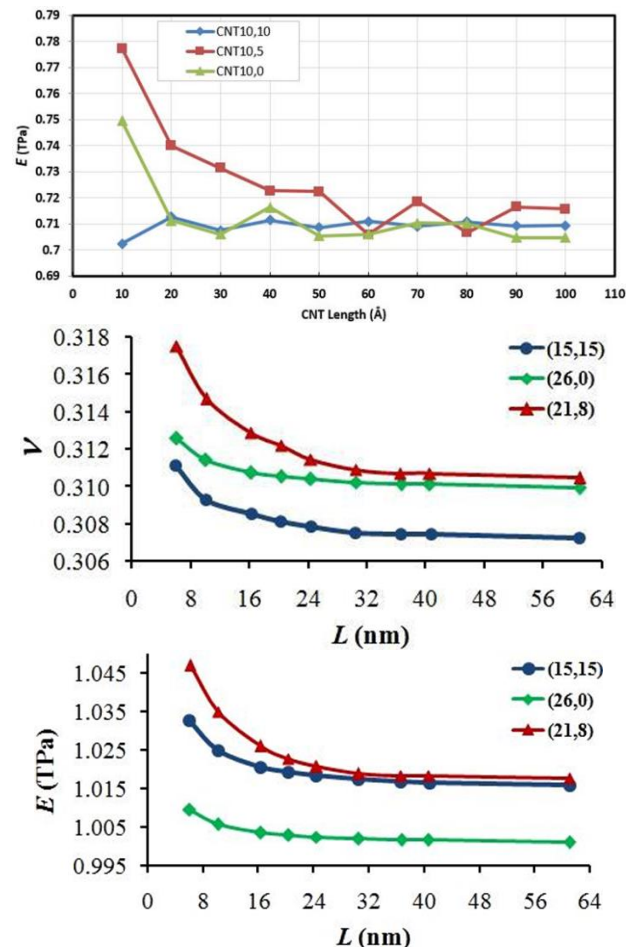


Fig. 4. Changes in Elastic Modulus and Poisson's ratio for carbon nanotube with length change. Nanotube length vs. mechanical properties

4) *Discussion of nanotubes*

In graphene when the speed of indenter of graphene increase /the modulus as well as maximum stress decreases. The graphene has multiple atoms and multiple electron segments where interatomic/ carbon-carbon bond. When speed increases the same number of electron segments in one bond or getting more energy per unit time to extend “C-C” interatomic bond to extend them. Later they also break the “C-C” bond. When the number of electron segments is constant, it is easier to deform more and also to quickly increase energy i.e. maximum stress also decreases because more energy for each electron segment in fixed, time, therefore modulus and maximum stress decrease. When we deformed on a tensile test the material is strong. When the metal has a shockwave in an explosion breaks up even more and smaller pieces in all directions i.e. higher rate the material appears bigger. So also when speed on graphene increases it appears weaker and as lower elastic modulus and lower maximum stress for weaker situation. But in the last experiment the larger indenter has already created a hole in graphene and it is breaking individual “C-C” Bonds in the circular circumference of the indenter with “C-C” bonds at the edges of indenter as well as deeper points in the centre of the indenter. This is breaking the graphene into many pieces and not just deformation. So like an explosion has higher energy but many pieces so also the modulus and stress is not the story, the material is going into separate pieces, so apparent modulus and the maximum stress appear higher. The graphene is not one piece having lost its mechanical integrity by the large and and quick indenter. Hence the last experimental modulus is anomalously high. During the process of slow and systematic defomation, the electron segments show that modulus and stress are lower at quicker speed of indenter Also as size of indenter increases modulus and maximum stress decrease. Again bigger indenter gives more energy and hence more like a large number of hands pulling apart one rope in a tug of war, so modulus and maximum stress or less. The interconnectedness of electron segments many of them in one “C-C” bond explains that each bond has components of entire graphene film and all of its atoms and not just two atoms in each bond the latter does not explain the show in the elastic part and even lower plastic part of defamation in its “C-C” bond as applied indenter is opposed by elastic modulus of each “C-C” bond and also increases the maximum stress of each “C-C” bond. It is electron segments that explain one connected nature of entire graphene film in all experiments and variations in graphene film indentation at nano dimensions of Indenter as well as material [32]

5) *Silica thin film and nano indentation of single Nanoparticle*

“Though there have been plenty of experimental studies on both crystalline and amorphous thin-film there are very few theoretical and simulation studies. In particular, a systematic investigation of the film thickness and substrate density dependence of mechanical properties in amorphous thin-films is still lacking despite their obvious technological importance. In most of the studies the main focus is bestowed upon the electronic and magnetic properties. However it is equally important to investigate their mechanical properties as devices must be reliable they must have structural integrity, and they

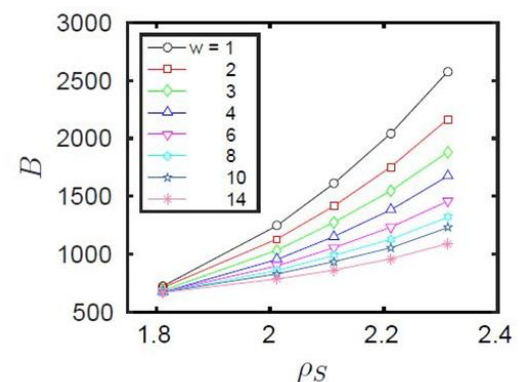
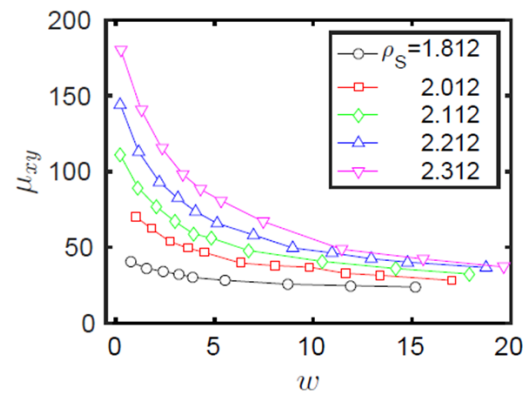
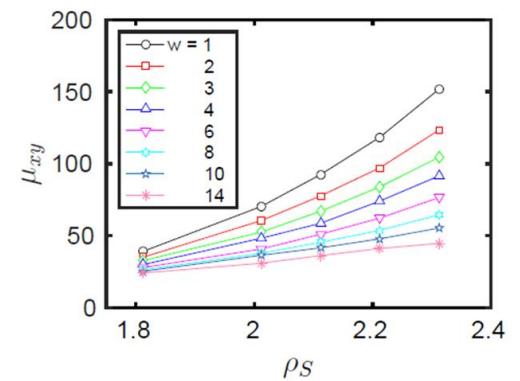
must retain that integrity over their lifetime, mechanical failures must not occur”. [42]. The global thin film semiconductor deposition estimated at US dollar’s 16 .1billion in 2020 and projected to reach US dollar 39.1 billion by 2027 i.e. 0.03 % of world GDP (dollar 130 trillion being the GDP of the world in 2027) by 2027.

6) *Nanosize thin film and mechanical properties*

Table 3
Properties of nanosize silica thin film for a substrate density of 2.312 [42]

Mechanical Properties		Film thickness (proportional to total number of atoms)
Shear Modulus(μ_{xy})	Bulk Modulus (B)	
90	1500	5
55	1300	10
50	1100	15

Thickness nanosize SiO₂ thinfilm vs. Mechanical properties [42] i.e.



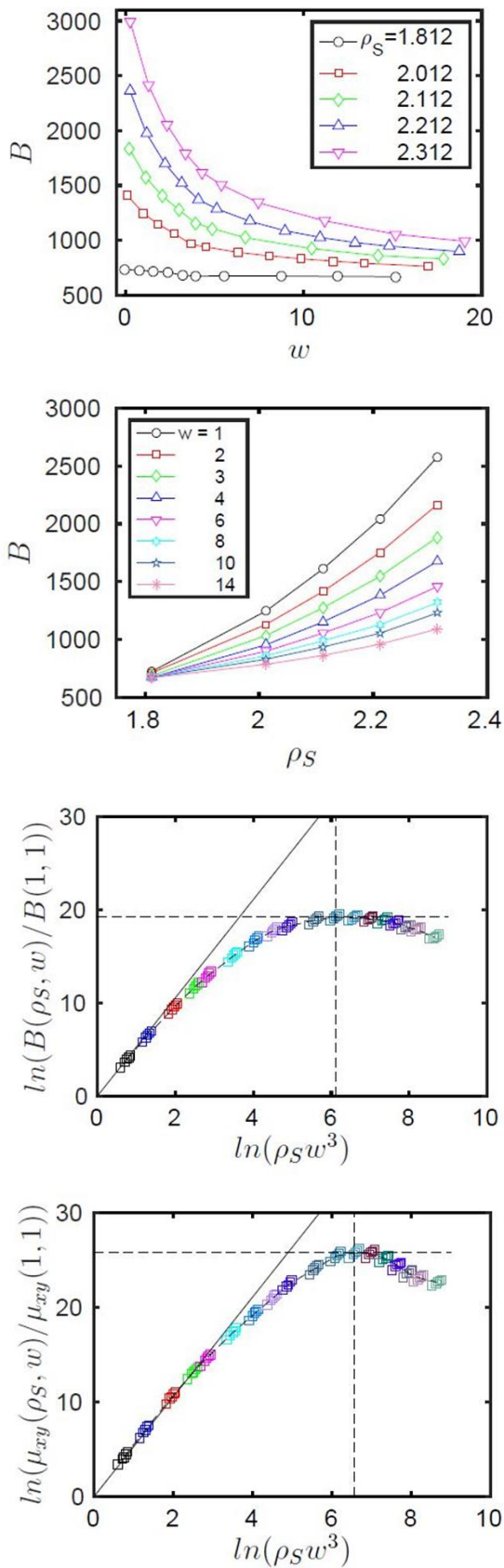


Fig. 5. Silica thin film Bulk Modulus and Shear Modulus as well as Mathematical fitting of Thin film properties

When thickness of thin film with nanosize thickness changes, then all mechanical properties-yield strength, ultimate tensile strength, hardness, elongation elastic modulus all except fracture toughness changes in a decreasing trend as nanosize thickness of thin film increases and. when the thickness of nanosize thickness silica thin film increases then the shear modulus and the bulk modulus decreases. The other dimensions are constant but thickness increases hence total number of atoms increases. This means the number of electrons segments in each inter-atomic bond in silica thin film increases. Hence the size of each electron segment between two bonded atoms (having multiple electron segments) decreases, hence to stretch as well as compress interatomic bond between two atoms is easier and requires less force, Pressure in shear modulus and bulk modulus. Even if it's only a change of shape in shear modulus the bonds and atoms and relative positions and spatial locations have to be shifted, hence shear modulus also decreases as thickness of silica thin film increases. The increase in thickness increases the total number of atoms and hence the number of electrons segments in any interatomic bond increases. For the same bond between two neighbouring atoms when total number of electron segments increases the size of each electron segment in each bond decreases. So, shifting the electron cloud in the orbit as is involved in the bonding between two atoms that are bonding-shift the electron clouds to change interatomic distances and spatial positions of bond in bulk modulus and shear modulus respectively is easier so force required is less. Therefore, the shear modulus and bulk modulus decreases as thickness of silica thin film increases. Alternatively, the silica thin-film of nanosize thickness is comparable to nanosize grains in nanoceramic as well as ceramic nanocomposite. So we prove that as size of nanograms in ceramics increases then shear modulus, Bulk modulus and other mechanical properties except fracture toughness of nanoceramic decreases as nanosize increases-but within the nanosize range of about 5 nm up to 100nm for grain size of nanoceramics. The bonding of ceramics compare to bonding in silica glass even though ceramics are crystalline and glass is amorphous. The electron segments depends on thickness of nanosize film and total number of atoms in nanograin of ceramic only and not on the crystalline or amorphous nature of ceramic or glass respectively. Thus as size of nanograins in ceramics increases the mechanical properties decreases. This has also been seen in the increase in nanotube CNT length increase leading to decrease its mechanical properties. Thus, the electron segmentation theory stands proved conclusively and is fully evident in multiple studies. The theory of electron segmentation is confirmed and concluded.

7) Silica thin film of nanosize thickness and proof of electron segmentation by Mathematical Induction

From [43] we derive a relation of shear modulus & bulk modulus from data in numerical plot [42].

$$\begin{aligned} \text{So,} \\ \mu_{xy}(\rho_s, w) &= \rho_s w^3 + \mu_{xy}(1,1) \\ \& B(\rho_s, w) &= \rho_s w^3 \times B(1,1) \end{aligned}$$

So μ_{xy} & B are exactly same relation mathematically with

respect to ρ_s & w

So if we prove μ_{xy} then relation of B is also proved.

$$S(m,n) = \mu_{xy}(\rho_s, w) = \rho_s w^3 \times \mu_{xy}(1,1)$$

Theorem 5.1 (Two – dimensional Induction version I) [43]

Let, $S(m,n)$ denote a statement involving two variables, m and n .

Suppose

- (1) $S(1,1)$ is true
- (2) If $S(k,1)$ is true for some positive integers, then $S(k+1, 1)$ is also true
- (3) If $S(h,k)$ holds for

Some positive integers h and k , then $S(h, k+1)$ Is also true.

Then $S(m,n)$ is true for all positive integer m,n .

Now:

- (1) $S(1,1)$ is true
 $\mu_{xy}(1,1) = \rho_s w^3 \times \mu_{xy}(1,1)$
 $\rho_s = 1, w = 1$
 So RHS = $\mu_{xy}(1,1)$
 LHS = RHS $\rightarrow S(1,1)$
 Is true.

- (2) $S(k,1)$ is $\mu_{xy}(k,1)$
 $\mu_{xy}(\rho_s, w)$ is true for
 $\rho_s = k$ and $w = 1$ then

(at $w = 1$ Figure 5 show that $\mu_{xy}(k,1)$ is true)

$$\mu_{xy}(k,1) = k \times w^3 \times \mu_{xy}(1,1) \text{ is true.}$$

Then $S(k+1,1)$

$$\mu_{xy}(k+1,1) = (k+1) \times 1^3 \times \mu_{xy}(1,1)$$

The relation $\mu_{xy} = \rho_s w^3 \times \mu_{xy}(1,1)$

Is linear w.r.t ρ_s

The graphs in figure 5 in [43] shows it is true & linear w.r.t. ρ_s .

Hence $\mu_{xy}(k+1,1)$ is true if $\mu_{xy}(k,1)$ is true.

- (3) If $S(h,k)$ holds

For some positive integers h & k , $S(h, k+1)$ is also true.

$$S(h,k) = \mu_{xy}(h,k) = \rho_{sh} \times (w_k)^3 \times \mu_{xy}(1,1)$$

$$S(h,k+1) = \rho_{sh}(w_{k+1})^3 \times \mu_{xy}(1,1)$$

Data is from fig. 5 [43] show that,

$$S(h,k) = \mu_{xy}(h,k) = \rho_{sh} \times (W_k)^3 \times \mu_{xy}(1,1)$$

Is true. So $S(m,n)$ is true from graph based on value at $S(h,k)$. So same $S(m,n)$ applied to $S(m,n)$ as $S(h,k)$ and then $S(h,k+1)$ is also true with same relation for μ_{xy} & B at $(h,k+1)$.

So based on graph $S(h,k)$ is true implies $S(h,k+1)$ is also true.

So $S(m,n)$ i.e. $\mu_{xy}(m,n)$ & B(m,n) are both true for all m,n .

As per data in figure 5 [43] the μ_{xy} & B value and variations based on ρ_s & w mean that when thickness, w increases, then μ_{xy} and B both decrease at nanosize values of thickness w .

Hence electron segmentation theory is valid for μ_{xy} , the shear modulus and B, the bulk modulus and further for mechanical properties of nanoceramics and ceramic nanocomposites.

5. Results and Discussion

We have fixed values of properties of materials in conventional materials. But ceramics have low fracture toughness in conventional ceramics. However, with nanomaterials including ceramics, we can tune the properties with value of nanosize in ceramics of nano/nano structure which have high toughness. We can obtain mechanical integrity. While we can tune nanosize to some extent and hence vary the value of nanoceramics properties. But processing and technology implementation with issues in controlling the nanosize towards the objective of obtaining targeted properties. Here we have a quantization, so even if there is a little variation in structure, the properties are about the same. The fracture toughness changes with value of nanosize, but “in steps” of value of toughness so can allow freedom in engineering implementation while ceramics like alumina show fracture toughness of 30 MPa \sqrt{m} to 3.3 MPa \sqrt{m} for grain size changing from 3nm to 150nm (respectively). We can tune our property without having too much engineering and human control. “We can have the cake and eat it too”. The property tuning and its practical ease both are done effectively.

Quantum theory has implicit concept of electron segmentation and in nanosize we have the material and its properties explained well with a bridging of the chasm between fundamental quantum mechanics which has electron segments implicit in it and the understanding of the basis of variation of properties from 5nm to 100nm. We have inverse Hall-Petch relation in nanoceramics and we have conventional Hall- Petch in micronsized ceramics and also electron orbitals theory in quantum mechanics. We have bridged the theory to explain the nanoceramic properties between Hall- Petch and Quantum Mechanics to explain tuning of properties in nanoceramics and ceramic nano/nano composites. Now we understand the past engineering, the foundations of quantum mechanics and in the process we understand the theoretical basis of nanoceramics and we have a method to implement it in engineering and technology of such nanofilms and nanosize coatings and even thin films in semiconductor processing. We now understand the continuum from atomic/subatomic to the macro. We also have practical solutions. We are now ready to takeoff into real-world applications from the research and development and technology issues too,

We now can confidently implement quantization of fracture toughness as well as electron segmentation of mechanical properties for thin films, say in ceramic coatings. Also in ceramic nanosize coatings in flexible packaging coatings and further thin films in say, semiconductors where polysilicon is

nanostructured in semiconductor and memory devices where the latter includes ceramic thin films. We can make thin films of nanoceramics in wear, in polymers if not get involved in some of the areas of other material classes of polymers and metal thin films, since nanoceramic thin film now has mechanical integrity of good fracture toughness. The other properties are also higher higher and tunable too.

The electron segment size and mechanical properties can change and can be used to obtain high properties. We can understand the properties, the quantization of toughness can maintain mechanical integrity and be used to decide the toughness. The existing body of research data can be used to implement easy and effective engineering solutions and we now know and have a composed picture to assemble a mosaic of all nanosizes and all properties and so, we can usher in the bold new era of practical nanotechnology in vast areas – we know what and how to do. The promise of nanotechnology is now materializing and imminent upon all of us –and all it is.

We have applied the concept of electron segments implicit in quantum mechanics and the properties of nanoceramics. We already have flexible packaging materials; we have thin films of metals even polymers bulk as well as films. We have semiconductor materials having certain nanofeature sizes and structures. We can pick and choose, mix and match the applications, the classes of ceramics with the classes of polymers, metals and semiconductors certain types of materials and applications. We have a true utopia in the materials world all the way from theoretical quantum mechanics and applications and human factors in types of materials, engineering methods and people's issues too, this is win-win from all aspects due to nanotechnology.

The electron segmentation theory with ((nanosize of grain) \times density) vs properties even that a linear change with a mathematical relation and also quantization of fracture toughness with (nanograin size to interatomic bond ratio) calculation, we now have two measurable parameters in addition to foundations of quantum mechanics as well as literature and data with volumes of studies in the past few decades and now we are ready to finish the task with the potentials of nanotechnology.

We can make coatings and with technology and human factors and the use the classes of nanoceramics and polymers and metals and large areas of engineering and applications that is as Feynman said "Plenty of room at the bottom" in the context of nanotechnology.

The two types of quantitative relations for fracture toughness and the other for elastic modulus with other mechanical properties is a new basis as we go from Hall- Petch plus K_{IC} in conventional materials and atomic quantum mechanics. We understand it above 100nm and below 5nm too.

We have now mixed the engineering and materials science in conventional materials with the atomic – subatomic quantum mechanics using the implicit electron segments in quantum theory all in the context of complete set of mechanical properties of nanoceramics. We now communicate between mechanical and functional properties in the theory as well as practical usage of all these types of properties in various

sciences and engineering. We can understand the compartments and their correlations through the needs of nanomaterials and their mechanical properties basis and usage too.

The quantization of fracture toughness and electron segments in quantum mechanics applied to mechanical properties of nanoceramics shows that quantum theory has vast scope and quantization of even mechanical properties in nanoceramics that the science is vast now more than ever and it can play a powerful role in vast areas of nanoceramics as well as the way it is bound to influence metals and polymers and even practical areas of nanometals and many thin films even more powerfully. The science has expanded from theory to engineering with human issues too in application areas.

The dynamics of nanoceramics are apparent and having mechanical integrity they can mix and match with polymers and metals. The potential of flexible packaging materials using nanoceramics and it could happen in a big way in the next few years itself means the compartments of classes of materials can mix and innovations can happen anytime in immediate years and in thin films also there can be growth in the nanoceramics and involve innovators and people will be involved in multiple classes of materials by even the same persons.

6. Conclusion

Atomic and quantization theory of fracture toughness and electron segmentation theories for nanoceramics and ceramic nanocomposites with possible innovative applications of ceramic thin films due to their own mechanical integrity and the immediate impact in flexible packaging applications with the powerful new versions of quantum theory(s) in both fracture toughness as well as other properties of mechanical nature of nanoceramics with electron segments of quantum mechanics while now the classes of polymers, metals and nanoceramics can now be directly comparable and also closely related if not competing.

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