Mechanical behavior of materials

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Week-1

Lecture-5

Atomistic basis of elasticity

Mechanical Behavior of Materials (Hindi)

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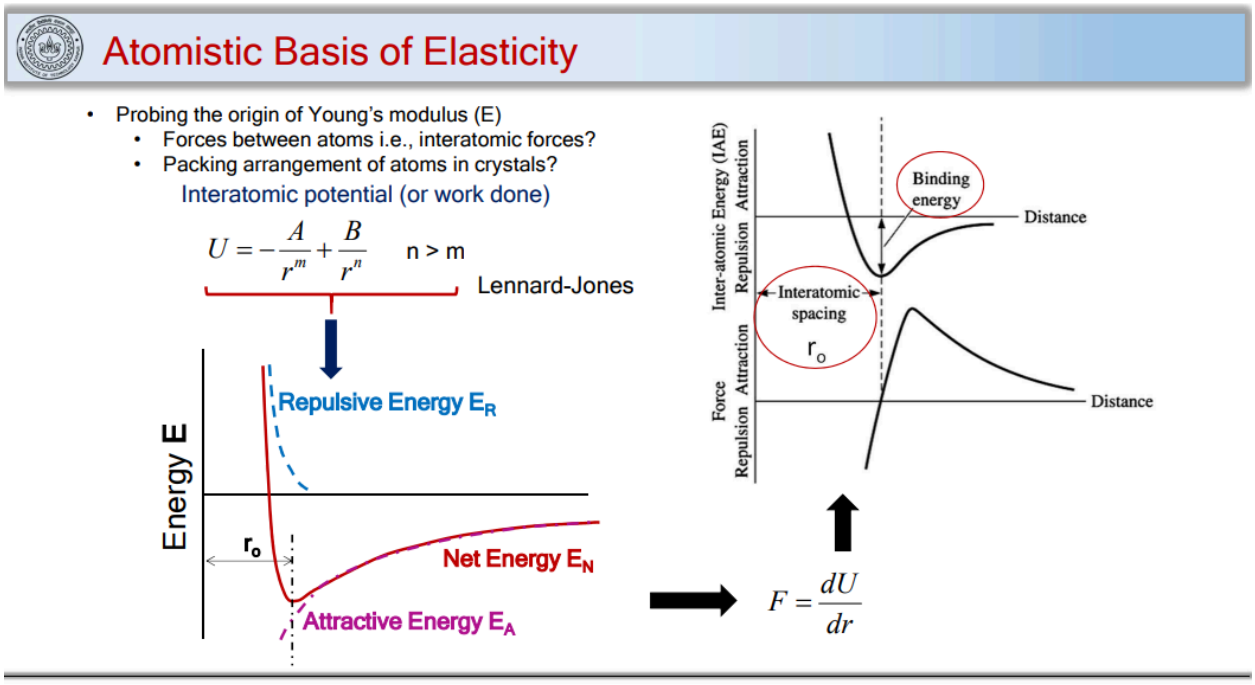


Namaskar aap sabka phir se swagat karta hoon. Is part mein hum dekhenge ki atomistic basis of elasticity kya hai, yaani elasticity ka atomic origin kya hai. Humne dekha tha ki elastic model jo hai hamara, ya hum usko Young's modulus, tensile deformation kar rahe hain, to hum usko Young's modulus kehte hain, na stress Strain ka jo slope hai linear region ka, to Young's modulus ka, yeh modulus ka atomic origin kya hai? Atomic origin agar hum jaanenge to,. humne baat ki thi material ki, tab wahan par humne baat ki thi ki different wahan pe bonding hai, to us bonds mein different forces bhi honge. Jo forces hain atoms ke beech mein, isko hum interatomic forces bhi kehte hain. Ye jo interatomic forces hain, wahi is Young's modulus ka origin hain.

Hum isko abhi ek simple, saral mathematical derivation se bhi dekhenge. Aur ye jo interatomic forces hain, ye aapka Young's modulus ko to effect karte hi hain, par aapka material kaise bond hai yaani kaise packed hai aur atomic arrangement kya hai material ki, ya crystal mein woh bhi Young's modulus ko affect karte hain. Ye bhi hum jaanenge is video mein.

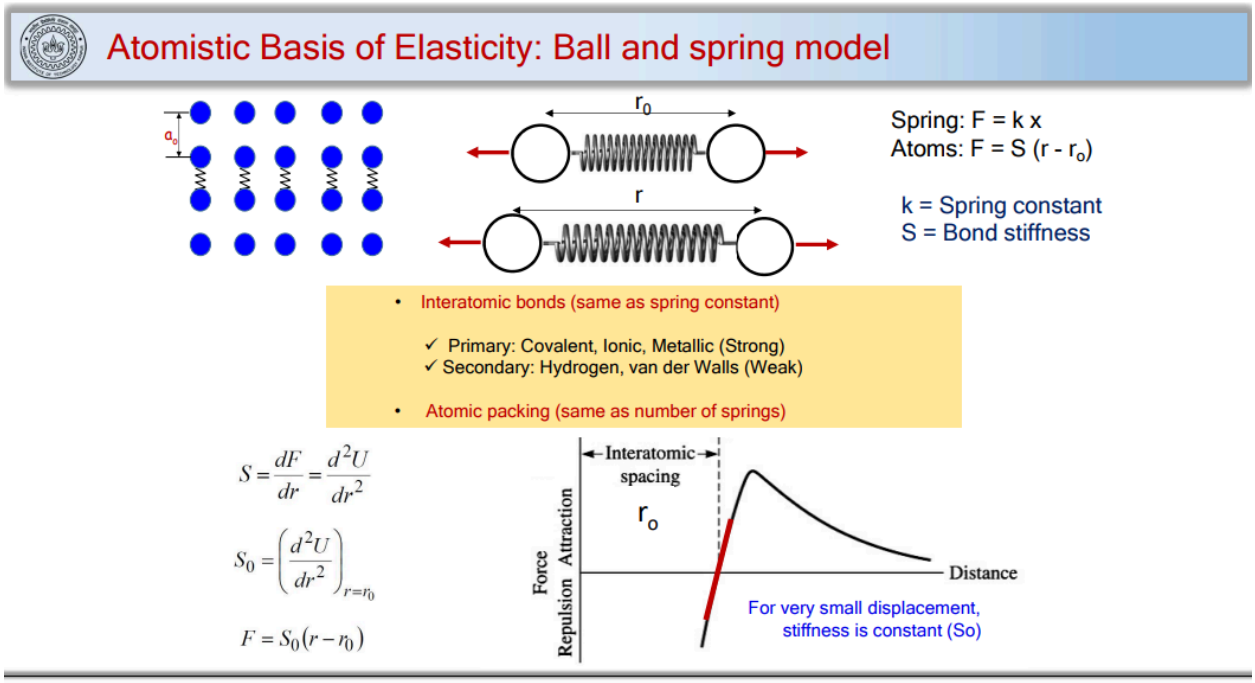
To sabse pehle hume dekhna hai ki interatomic potential kya hai. Jaise humare paas do atoms hain, un do atoms ko hum paas laane ki koshish kar rahe hain. Agar humare paas do atoms hain, aise hum unko paas laane ki koshish kar rahe hain, to ye jo potential hai, jo energy change hogi ya work done hoga, isko hum interatomic potential kehte hain. To ye ek simple interatomic potential hai, jisko hum likhenge (- **A**/r^n + **B**/r^m), jahan pe n > m hota hai. Kyunki hum chahte hain ki jab do atoms close aayein to energy negative rahe. To isliye ye condition yahan pe satisfy honi chahiye jab do atoms paas aa rahe hain. Hum isko kehte hain Lennard-Jones potential ya kabhi kisi books mein aapko dikhai dega isko 12-6 potential bhi kehte hain, kyunki m ki value 12 rahti hai aur n ki value 6 rahti hai. Isko hum 12-6 potential bhi kehte hain. Ye ek simple potential hai. To abhi isse hum jaanenge ki jab hum do atoms ko ya molecules ko paas la rahe hain to kya hota hai. To jaante hain ki wahan pe ek attractive energy bhi rahegi aur ek repulsive energy bhi

rahegi. To attractive energy hamari aati hai electron aur nucleus ke beech mein ya electron aur proton ke beech mein ya nucleus ki baat mein jo attraction rahega, woh rahegi.

Aur repulsion hamara rahega electron-electron ka repulsion, nucleus-nucleus ka repulsion, do atoms ke beech. To ye repulsive energy wahan se aati hai. Aur ye attractive energy in dono ke attraction se aati hai.

To agar hum net energy plot karein — net energy plot karein — to hume is tarah se kuch ek curve milega. Aur humne dekha ki yahan par ye distance par sabse kam energy rahegi — aur negative energy rahegi. Energy pehle decrease ho rahi hai jab hum paas la rahe hain, aur ek samay ke baad repulsive energy dominate karegi, to ye energy yahan pe badhegi.

To ye jo distance hai in dono atoms ke beech ka, jahan pe energy lowest hai, usko hum kehte hain r_0. Aur jo force hai in dono ko paas laane ka, hum isko nikaal sakte hain agar hum iska differential r ke saath lein — to hume force bhi milega, in dono ko paas laane mein kitna force lag raha hai. Aur agar hum is force ko plot karein to hume force ka nature kuch is tarah se milega. To ye hamara interatomic energy ho gayi. Yahan pe humne dekha ki ye attractive energy dominate kar rahi hai, aur is region mein — yaani is distance se kam jab distance hum paas laayenge dono atoms ko — to repulsive energy dominate karegi. Aur yahan pe ek kuch equilibrium milega. Isko hum kehte hain interatomic spacing r_0, ya equilibrium distance between two atoms. In do atoms ke beech ka ek equilibrium distance. Aur ye jo energy hai jo sabse negative energy hai agar main iska magnitude dekhoon sbse negative energy milegi usko hm kehte hain Binding energy. To ye jo binding energy hai, to yaha pe hm dekhenge ki jb hm force ko plot kare yahan pe distance k hissab se agar hm is curve ko differentiate kare to hame ek force milega to yaha pe pehle dekhenge force pehle negative tha, aur ye yahan pe zero aayega. To jahan pe mera interatomic spacing hai, wahan pe mera force zero rahega. Aur phir ye badhega yaani attractive hoga aur ye yahan pe maximum value milegi. To is curve se hum jaanenge hamara elasticity se kya relation hai. Iske liye hume pehle jaana hai ki elasticity kya hai hum ek simple model introduce karenge us model ka naam hai Ball and Spring Model.



To hum jaante hain ki agar hamara koi crystal structure ya metal se alloy hai, usmein atoms hain, molecules hain, to hum ye jo balls hain, ye hamare atoms indicate kar rahe hain, aur ye jo springs maine mark kiye yahan par, ye springs mera bond jo hai do atoms ke beech mein, ye mark kar raha hai.

Abhi hum spring hi kyun istemal kar rahe hain? Kyunki hume elasticity ko derive karna hai, aur aap jaante hain ki spring aisi analogy hai — agar main usko stretch karta hoon to utna hi mujhe bal dena padega. Ye humne Hooke's Law mein bhi dekha tha.

To isliye, ye jo dono bonds ke beech mein — dono atoms ke beech mein — jo bond hai, usko hum spring se denote karte hain. Aur ye jo distance hai, yahan par maine a_0 (r not) mark kiya, ye hamara interatomic distance ya equilibrium distance hai.

To maan lijiye mere paas do atoms hain, aur unke beech mein ek spring maine laga diya. Ye spring mera bond ko represent karega. To un dono ke beech ka distance maine mark kar liya — ye interatomic distance r_0 maine mark kar liya. Aur agar main is bond ko stretch karta hoon, ek force lagata hoon — tensile force — to kya hoga? Ye bond stretch hoga.

To abhi maan lo in dono ka beech ka distance abhi change ho ke r ho gaya hai. Agar main release kar doonga — agar mera elastic deformation hai — to ye bonds, ye atoms phir se apni equilibrium position mein aayenge — r_0 par.

To ye spring model agar hum istemal kar rahe hain, to hum ek simple mathematical relation dekhte hain spring ke liye: **F = k * x** ye jo k hai hamara spring constant hai, aur x hai ki kitna displace ho raha hai ye bond — yaani ek hamara hoga yahaan pe is distance ke baad kitna displace ho raha hai.

Agar ye main atoms fixed maan loon, aur isko main stretch kar raha hoon, to ye kitna displace ho raha hai x direction mein. To x ko main replace karoonga yahaan par **(r - r_0),** yehi mera change

in distance hoga. Aur k ko main replace kar raha hoon yahaan par bond stiffness se. To analogy maine ek istamal ki atoms ke liye agar force dono atoms ke beech mein bond stiffness ke through measure karoonga, aur ye jo displacement hai ($r - r_0$) rahega. Ek simple model maine yahaan par introduce kiya hai. Agar main bonds ki baat karoonga, tab mere paas kaunse kaunse bonds hain? To mere paas primary bonds hain aur secondary bonds hain. Primary mein bonds aayenge covalent bonds, ionic bonds, metallic bonds ye hamare strong bonds hain.

Aur secondary bonds jaise hydrogen bonds, van der Waals bonds ye weak bonds hain.

Aur jab main bonds ki baat kar raha hoon, to yah bond aap samajh sakte hain jaise maine yahaan par to ek hi bonding dikhaya, to ye bhi ek bond ho gaya, ye bhi ek bond ho gaya, ye bhi ek bond ho gaya. To ye ho gaya mera bonds, ye ho gayi meri bonding, aur ye saari bonding meri stiffness contribute karegi.

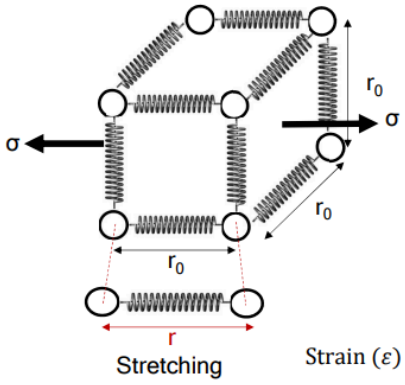
Aur ek cheez hai ki atomic packing. To yahaan par to maine simple ek simple cubic lattice diya hai. Par meri atomic packing to aise bhi ho sakti hai hexagonal ki tarah. Agar meri atomic bonding hexagon ki tarah hogi to yahaan par bhi ye stiffness aur interatomic bond jo bhi present hai ye stiffness ko contribute karega.

To agar main stiffness define karu with respect to change in stress upon change in length, isko hum maaneinge stiffness. Atoms ke liye likha hai: agar hum isko differentiate karein r se, to mujhe stiffness milni chahiye.

To wahi equation humne yahaan par liya hai, aur humne jaana hai ki $\mathbf{dF/dr = d^2U/dr^2}$ — yah hume interatomic potential se mil sakta hai. Agar hum second derivative lein interatomic potential ka, to mujhe stiffness milega.

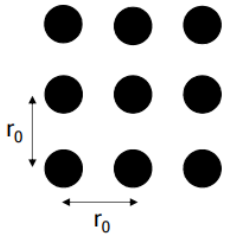
Humne last slide mein likha tha ($r - r_0$). Yahaan pe to agar hum — ye mera force tha with respect to distance, aur ye mera interatomic spacing ya interatomic distance tha — agar hum isko differentiable maan lein, ye almost straight line hai. But jab hum differentiable hain to ye distance r, ye bahut kareeb hai — bahut small hai. Kyun small hai? Kyunki humne jaana tha ki elastic deformation mein atomic jo displacement hai, wo small hai, isliye hum yahan par jo baat karenge, small displacement ki baat karenge around interatomic space. To yahan par yahi likha hai ki hum bahut small displacement ki baat karenge. Ab agar hum yeh small displacement ki baat kar rahe hain, to jo slope aayega hum isko straight line consider kar sakte hain. Aur hum stiffness hai, slope hai, yeh constant hai. To agar hum slope nikaalenge to hume slope yahan se le sakte hain, ya stiffness yahan se nikaal sakte hain. To agar hume interatomic potential pata hai — likhta hoon main yahan — agar hume interatomic potential pata hai to hum stiffness measurement karte hain xRD measurement se hume lattice parameters milte hain, aur is lattice parameter se hi hum interatomic nikal sakte hain.

Atomistic Basis of Elasticity



Strain $(\varepsilon) = \dfrac{r - r_0}{r_0}$

$F = S_0(r - r_0)$



Stress per bond/atom (σ) = F/r_o^2

$\sigma r_o^2 = S_o (r\text{-}r_o)$

$\sigma r_o^2 = S_o r_o \varepsilon$

$\sigma/\varepsilon = S_o / r_o$

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To agar hum force apply kar rahe hain, jaise hum stress apply kar rahe hain, yahan par maan lijiye mera crystal hai, yeh atoms hain, aur yeh spring hai, aur maine force yahan par apply kiya, ya stress apply kiya, to yeh measurement se hume lattice parameters milte hain, aur is lattice parameter se hi hum interatomic nikal sakte hain.

To agar hum force apply kar rahe hain, jaise stress apply kar rahe hain, yahan par maan lijiye mera crystal hai, yeh atoms hain, aur yeh spring hai, aur maine force yahan par apply kiya ya stress apply kiya, to yeh change ho raha hai r, agar yeh badh raha hai to hum strain define kar sakte hain.

Hum aise strain define kar sakte hain: yeh mera final stretch length hai, aur yeh mera initial stretch length hai, aur agar main isko initial stretch length se, matlab initial atomic spacing se divide karunga to mujhe mil jaayega strain.

Yeh mera strain main yahan se nikaloon. Aur maan lo mera atomic structure hai, maan lijiye ki dono side yani d dimension mein mera r_0 same hai, ya interatomic spacing same hai. Ek simple model hum use kar rahe hain isliye hum consider karenge ki r aur r_0 yahan par same hain.

To stress mera kya aayega? To stress mera aayega force jo maine apply kiya apne cross-sectional area par. Agar yeh wahi area main consider kar raha hoon, yahan par main force apply karoonga is cross-sectional area par, to yeh cross-sectional area aayega mera A_0 (a not) square.

Aur is case mein agar main dekhun ki equivalent number of atoms kya hai — equivalent number of atoms to yeh mera / yahan se aaya 1/4, yahan se aaya 1/4 atom, yahan se aaya contribution, yahan se aaya mere paas total 4 atoms hain. Mera yahan par number of equivalent atoms 1 ho gaya.

To stress experienced by one atom or per atom mein likhta hoon yeh mera terminology aa jaayega — **F / r_0^2.**

To F humne jaana ki yeh **$F = S_0(r-r_0)$** yeh humne define kiya tha spring ball model se. Aur F ko hum nikaalenge yahan se sigma in A_0 square.

To yeh stress per bond per atom yeh abhi explain kiya maine. Yeh aayega **F / A_0** square.

Aur agar yeh terms main yahan par replace karta hoon F ki jagah sigma in A_0 square, aur **$s_0 * (r - r_0)$** ko main yeh term **$(r - r_0)$** ko likh sakta hoon **$r_0 * \varepsilon$** (strain), to yeh yeh terminology mere paas aa jaayegi.

Aur main yeh kuch rearrangement karunga, strain ko is side leke aata hoon, to sigma upon ε aayega, aur s_0/r_0 aayega.

To yeh jo term hai abhi aap isko jaan sakte hain, yeh jo term wahi mera elastic modulus hai.

Sigma upon epsilon wahi maine define kiya tha, aur yeh mil gaya mujhe bond stiffness model simple way se — stress upon strain. Aur yahi mera aayega, s_0 upon r_0.

Aur maine bola tha ki s_0 bond stiffness aayega kis par depend karega? Bond stiffness depend karega ki mere bonds kya hain — primary bonds se, secondary bonds se, ya dono ka mixture hai. To yeh mera bond nature par depend karega.

ε (strain) aur r_0 mera depend karega atomic arrangement par.

To elastic modulus mera kis ka function ho jaayega? Mera elastic modulus agar main material ke properties ke perspective se dekhoon, elastic modulus mera function hoga bonds ka aur atomic arrangements ka.

To humne simple ek relation dekha hai elastic modulus ka — bond stiffness aur atomic distance.

Elastic Modulus

Material	Elastic Modulus (E), GPa
Metals	
Al	67
Cu	128
Fe	208
Zn	69-138
Ni	207
Ti	120
Ceramics	
TiO_2 (rutile)	283
Al_2O_3 (alpha)	380
Cr_2O_3	>103
Partially stabilized ZrO_2	205
Fully stabilized ZrO_2 (cubic)	97-207
Cr_3C_2	373
Cemented carbides	96-654
Diamond	1000
Graphite	27
PVC	0.003

Metal /Alloy	Modulus of Elasticity (GPa)	Thermal Expansion Coefficient (10^{-6} m/(mK)
Al	70	22.2
Brass	97	18.7
Cu	110	16.6
Mg	45	25
Ni	207	13
Steel	210	12
Ti	107	8.6
W	407	4.3

Thermal expansion Vs Modulus of Elasticity

Modulus of Elasticity Vs Melting point???

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To yahan par kuch materials hain — bahut saare engineering materials hain — hum dekh rahe the ki metals hain, ceramics hain, polymers hain.

Yahan par elastic modulus humne plot kiya, aur humne dekha tha ki elastic modulus GPa mein measure karte hain. Metals mein hum baat karenge aluminium, copper, iron, zinc, nickel, titanium, aur inka corresponding ek elastic modulus hai aur ceramics me baat karenge ki TiO_2, Al_2O, Cr_2O_3 polymer me PVC hai.

To agar aap dekhenge metals, ceramics, aur polymers mein to metals mein elastic modulus hai, yeh jo ceramics se hai, yeh iski tulna mein kam hai, aur polymers se zyada hai.

To hum yeh jaanenge, jaise abhi maine bataya tha ki metals mein hote hain metallic bonds, ceramics mein hote hain covalent aur ionic bonds. Aur yahan par covalent elastic modulus kam hota hai, aur ceramics mein dekhenge covalent aur ionic bonds metallic bond se strong hote hain.

To yahan par hum dekhenge ki iska elastic modulus zyada hota hai metals ki tulna mein.

Agar metals tulna me hm dekhenge, metals mein hi tulna karni ho, to jaise aluminium hai — yeh bhi FCC hai, copper bhi FCC hai, aur nickel bhi FCC hai. In teeno mein atomic arrangement same hai, agar aap dekhenge, par iska elastic modulus different hai.

Teeno mein nickel ka elastic modulus zyada hai copper ke comparison mein, aur aluminium ke comparison mein copper ka elastic modulus zyada hai.

To aap dekhenge ki agar main elastic modulus ki baat karoon, to elastic modulus ko main melting point se agar main plot karoon, to aapko ek straight line milegi.

Jiska melting point zyada hai, uska elastic modulus bhi zyada milega.

To main aapko exercise deta hoon ki aap yeh elastic modulus aur melting points nikaalein different metals ke periodic table se, aur dekhein ki aapko elastic modulus aur melting point mein kya relation milta hai.

Aur ek cheez hai, jaise agar main elastic modulus ki baat karoon, aur coefficient of thermal expansion ki baat karoon.

Coefficient of thermal expansion hota hai ki agar main material ko heat kar raha hoon, to usmein ek change aayega uske length mein ya uske dimension mein change aayega.

Woh dimension kaise change ho raha hai, woh hum measure karte hain. Matlab kis rate se change ho raha hai, yeh measure karte hain coefficient of thermal expansion se.

To agar aap dekhenge, jaise jaise mera modulus of elasticity badh raha hai — jaise aluminium ka 70 GPa hai, aur tungsten ka 407 GPa hai, to uska thermal expansion bhi aapko us tarah se dikhai dega.

Jiska zyada elastic modulus hai, uska thermal expansion kam hoga, matlab woh zyada badhega nahi. To ek inverse relation aapko milega.

To yeh bhi main aapko ek exercise deta hoon ki agar aap elastic modulus aur coefficient of thermal expansion, jisko α se denote karte iska ek relation aap dhoondhiye, saare metals ya alloys periodic table se apni nikaaliye, aur inka ek relation dhoondhiye ki yeh kaise, kyun aise behaviour dikhata hai.

Yeh thoda sa jaanenge. Humne pehle baat ki thi interatomic potential ki. Mera distance hai, aur yeh mera interatomic potential.

Agar mere do materials hain, yeh material one hai, aur ek main material two leta hoon jisme interatomic potential aise change ho raha hai, jahan par yeh jo binding energy zyada hai, yeh mera material two ho gaya.

Jahan par binding energy zyada hai, yahan aap dekhenge ki material two jo hai, aur material one hai, iska melting point zyada milega ek ki tulna mein.

Aur iska coefficient of thermal expansion agar aap dekhenge, yeh kam milega melting point ki tulna mein.

Aur in dono ke saath hum baat karenge jab elasticity ki — elastic modulus do ka ek ki tulna mein zyada milega, kyunki iski binding energy zyada negative hai.

To yeh aap relations periodic table se saare metals ya elements nikaal sakte hain.

To humne dekha ki thermal expansion aur modulus of elasticity ka kya relation hai, aapko dhoondhna hai.

Aur modulus of elasticity aur versus melting point ka maine to bola ki ek straight line dikhata hai, yeh aapko verify karna hai.

Aur is point se main yahan par rukta hoon, aur is class mein humne jaana ki elastic modulus ka origin kya hai, jo bond stiffness, atomic spacing ya equilibrium distance se aata hai bonds ke beech mein aur atoms ke beech mein.

Dhanyavaad!