KATILARIN ELEKTRONİK YAPISININ BENZETİŞİMİ

Elektronik Bant Yapıları-2

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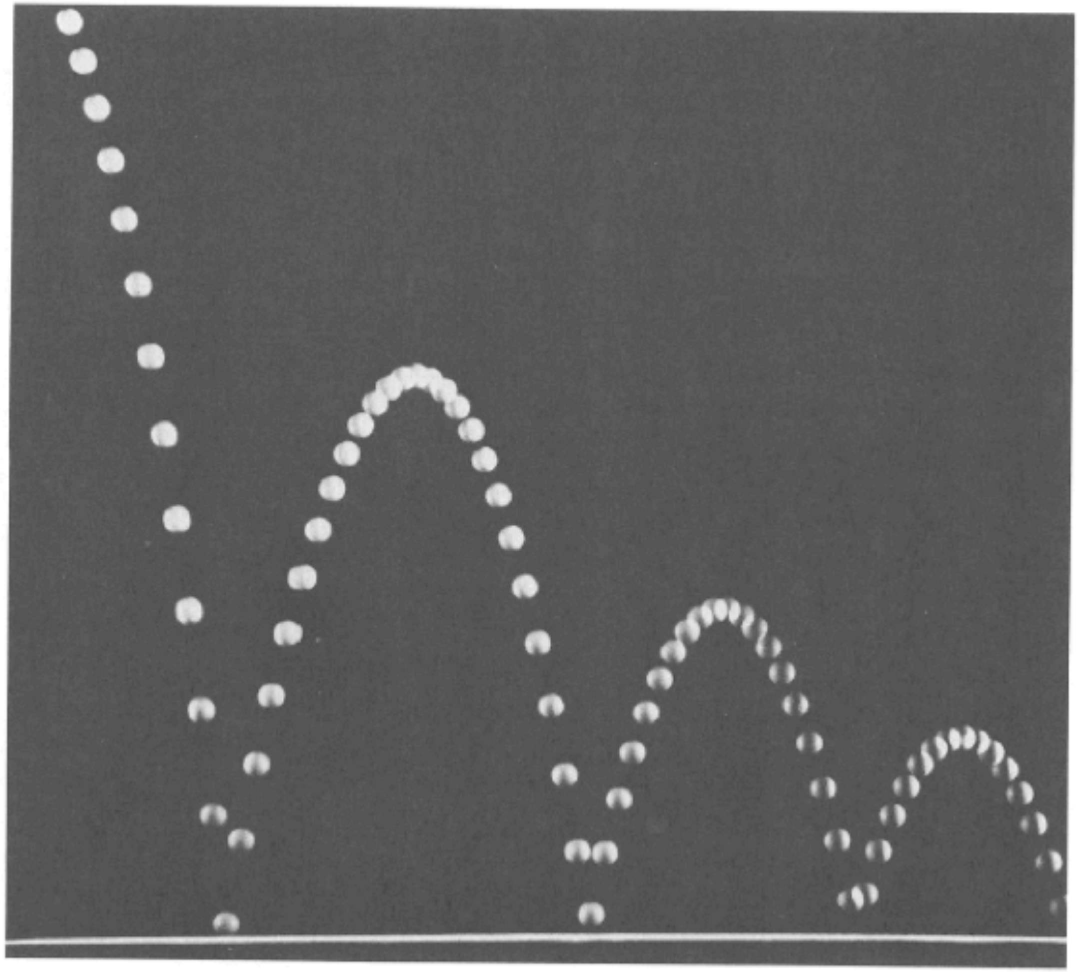
Katıların Elastik Özellikleri:
Elastik sabitleri, Young, Shear Modülleri..

13.2 Elasticity

Elasticity is a fundamental property of materials. Springs of all kinds are examples of elastic bodies. Let us consider the characteristics of a spring. We find that a spring will respond to distorting force and then return to its original shape after the distorting force is removed. Any material or body can be deformed by an applied force. If it returns to its original shape after the force is removed, it is said to be elastic. Most substances are elastic to some degree. In a technical sense a substance with a high elasticity is one that requires a large force to produce a distortion-for example, a steel sphere.

A multiple flash photograph of a bouncing ball. Many physics principles can be studied in this picture—projectile motion, transformation of energy, changes of momentum, elastic properties of material, among others. How would the picture be altered if the ball and surface that it strikes were perfectly elastic? (Picture from *PSSC Physics*, D.C. Heath and Company, Lexington, Mass., 1965.)



13.3 Hooke's Law

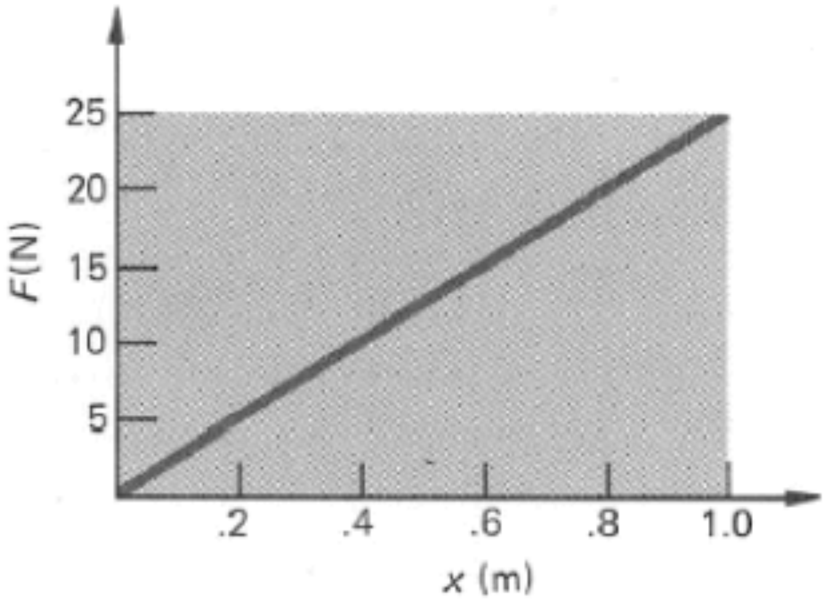


FIGURE 13.2
Hooke's law, $F = kx$, governs the stress-strain relationship within the elastic limits.

In 1676 in his study of the effects of tensile forces, Robert Hooke formulated and stated the law that is still used to define elastic properties of a body. He observed that the increase in length of a stretched body is proportional to applied force F as shown in the experiment above Figure 13.1.

$$F = kx \qquad (13.3)$$

Where x is the length increase (m), and k is a proportionality constant or *spring constant* (N/m). This equation is shown graphically in Figure 13.2. Note that k is the slope of the line.

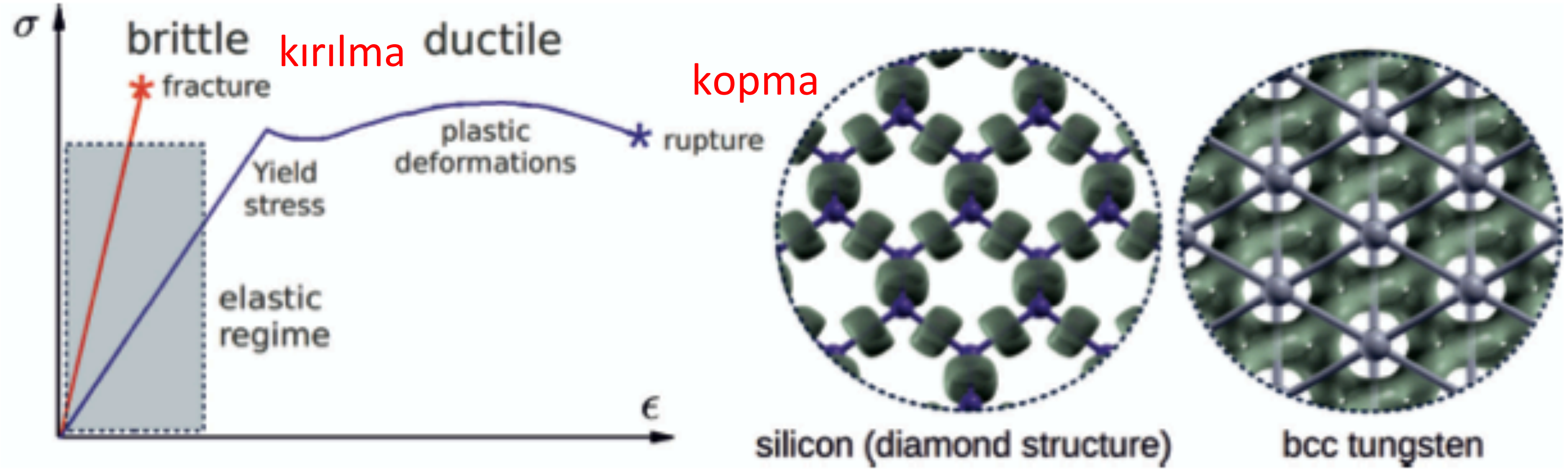


Fig. 6.1 The left panel shows schematic stress–strain curves for brittle and ductile solids. The elastic regime corresponds to the portion of the diagram where the strain is proportional to the stress. The ball-and-stick models on the right show the valence electron density distribution in silicon (brittle) and tungsten (ductile). Si atoms form covalent bonds and the charge is localized between nearest-neighbour atoms. W atoms form metallic bonds and the charge is spread all over the crystal. In both cases the density isovalue corresponds to 0.3 electrons/Å^3.

Örnekler:

Brittle : Al_2O_3, yarıiletken silikon

Ductile: Platin, bakır, tungsten

$$Y = \sigma / \varepsilon$$

Young’s Modulus

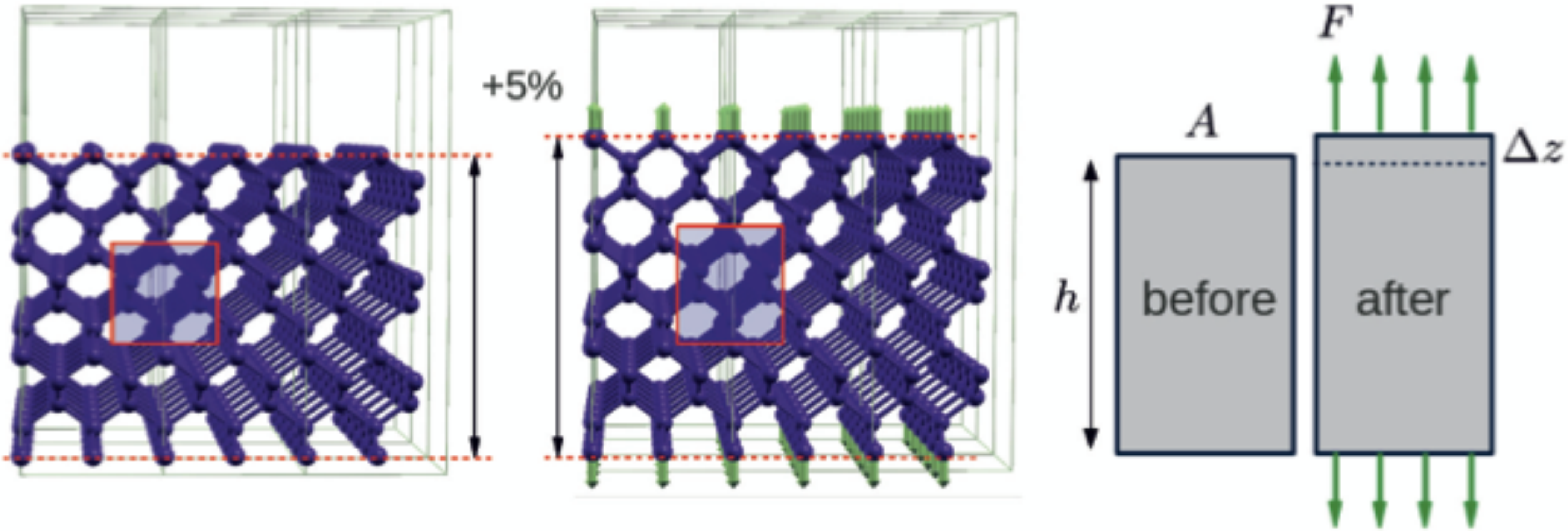
stress
(germe)

strain
(gerilme)

$$\nu = -\frac{\epsilon_x}{\epsilon_z} = -\frac{\epsilon_y}{\epsilon_z}$$

Poisson's Ratio

- Brittle fracture and plastic deformations are very complex phenomena which are related to the presence of dislocations and grain boundaries.



ΔU, of the total potential energy as the work of the external forces:

$$\Delta U = \int_h^{h+\Delta z} F(z)dz$$

where F is the sum of the external forces acting on the atoms of the topmost layer, which are displaced from height h to h + Δz. The bottom layer is fixed, hence the work done by the external forces there is zero. Since by definition the applied stress corresponds to the external force per unit area, σ = F/A, and the displacement of the top layer can be expressed in terms of the strain, ε = Δz/h, we can rewrite eqn as follows:

$$\Delta U = \Omega \int_0^{\epsilon} \sigma \, d\epsilon$$

with Ω = Ah the volume of one periodic repeat unit of the slab. The last step is to observe that we are in the elastic regime and therefore by definition the stress is proportional to the strain. By introducing the elastic constant, C, such that we obtain:

$$\sigma = C\,\epsilon,$$

$$\frac{\Delta U}{\Omega} = \frac{1}{2} C\,\epsilon^2.$$

Therefore a simple derivative yields the stress in terms of the total energy: $$\sigma = \frac{1}{\Omega}\frac{\partial U}{\partial \epsilon}$$

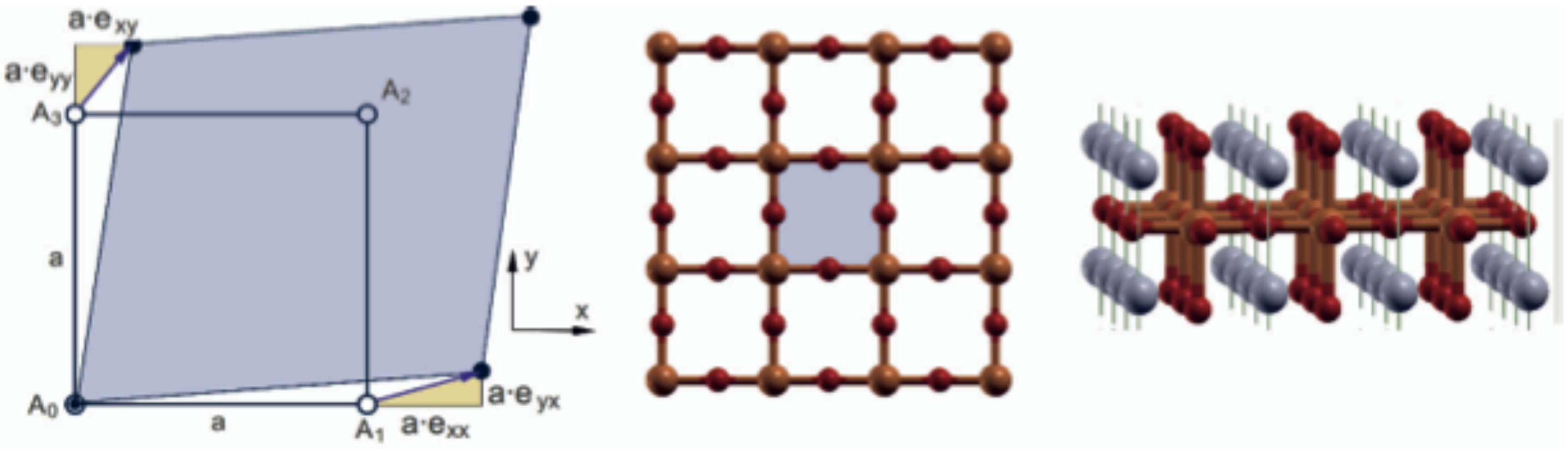


Fig. 6.3 Elastic deformation of a two-dimensional square lattice. The panel on the left shows the displacements of atoms A_0–A_3 according to the deformation $e_{\alpha\beta}$ of eqn 6.7. The components e_{xx} and e_{yy} of the deformation are referred to as 'normal strain' and are associated with dilations of the solid. The components e_{xy} and e_{yx} are referred to as 'shear strain' as they involve the sliding of the two opposite faces of the square. The displacements are highly exaggerated in the figure for clarity, but in reality they are very small: of the order of $0.01a$. An example of a two-dimensional square lattice is the basal CuO_2 plane of the copper oxide La_2CuO_4, where Cu atoms lie at the vertices of a square and the O atoms lie in the middle of its sides (light blue area in the middle panel). In the crystallographic unit cell the CuO_2 planes are stacked on top of each other and are separated by LaO layers (right panel). Copper oxides such as La_2CuO_4 have been investigated in great detail since they exhibit high-temperature superconductivity upon *p*-type doping (Pickett, 1989).

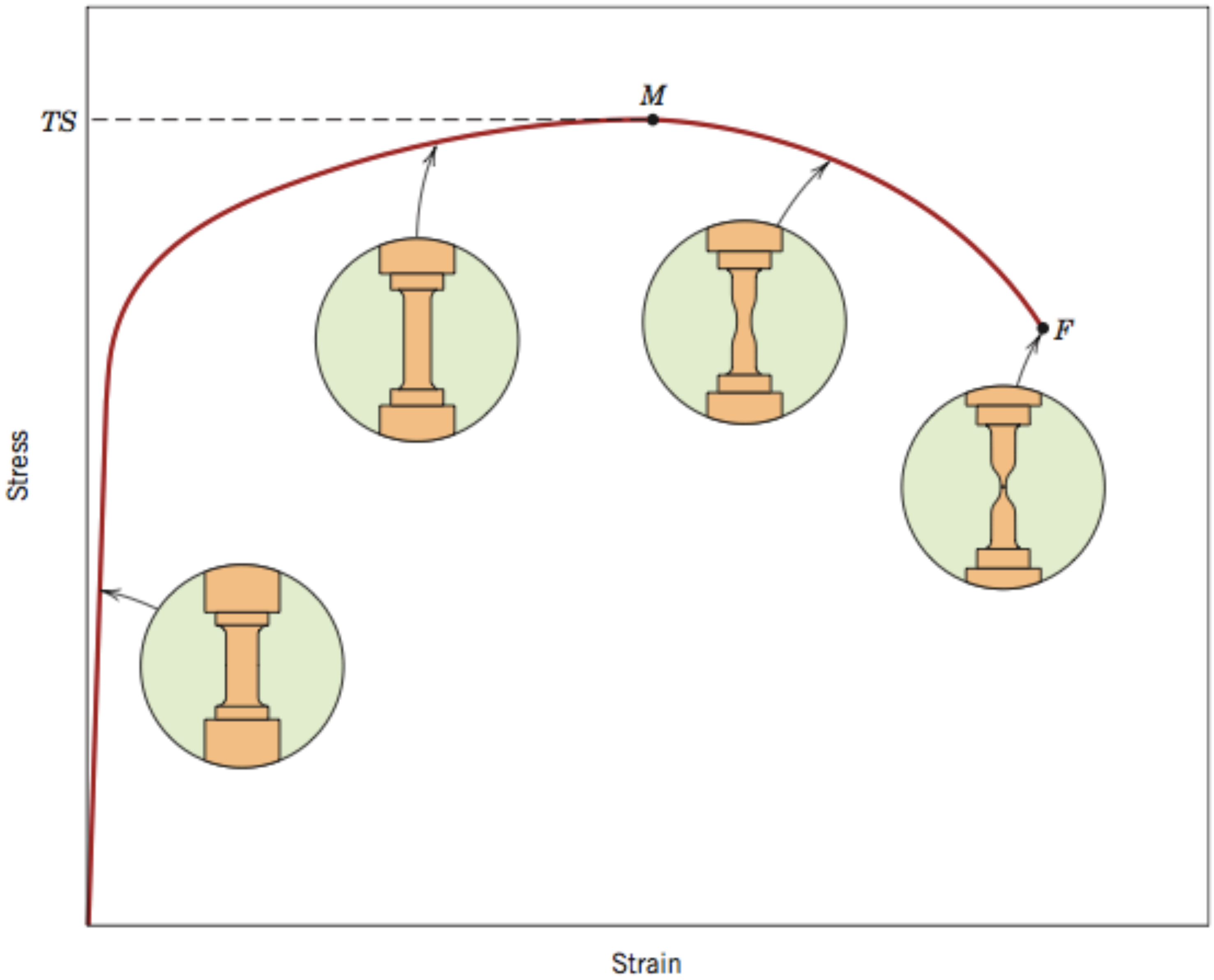


Figure 6.11 Typical engineering stress–strain behavior to fracture, point *F*. The tensile strength *TS* is indicated at point *M*. The circular insets represent the geometry of the deformed specimen at various points along the curve.

Voigt notation, strain tensor

$$\epsilon_{\alpha\beta} = \begin{pmatrix} \epsilon_{xx} & \epsilon_{xy} & \epsilon_{xz} \\ & \epsilon_{yy} & \epsilon_{yz} \\ & & \epsilon_{zz} \end{pmatrix} \rightarrow \epsilon_i = \begin{pmatrix} \epsilon_1 & \epsilon_6 & \epsilon_5 \\ & \epsilon_2 & \epsilon_4 \\ & & \epsilon_3 \end{pmatrix}$$

Hooke's Law in Voigt notation:

$$\sigma_i = C_{ij}\,\epsilon_j$$