Effect of local atomic relaxations on the elastic properties of a disordered metallic alloy

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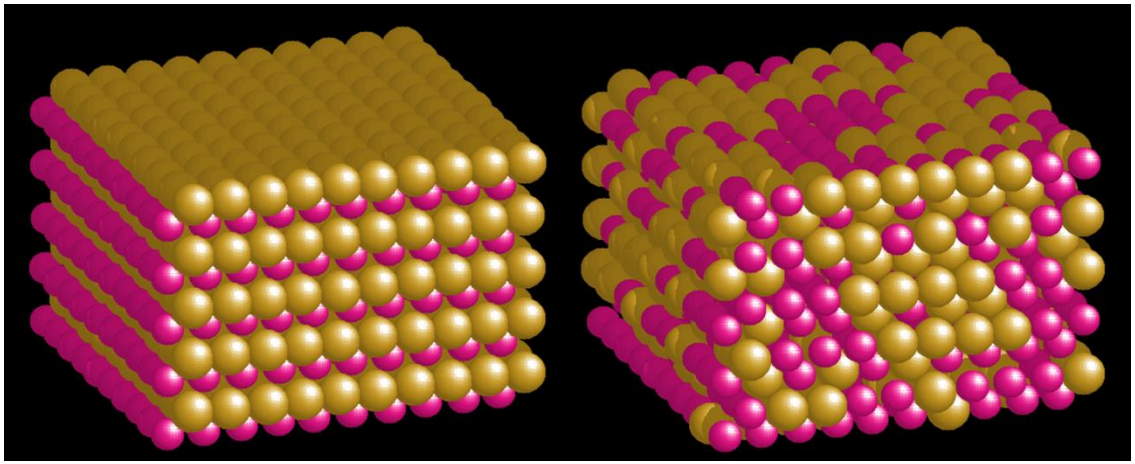

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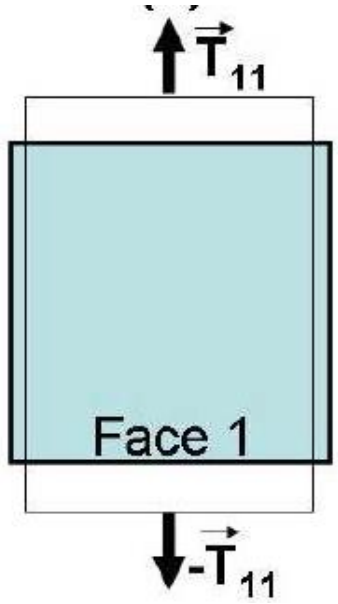
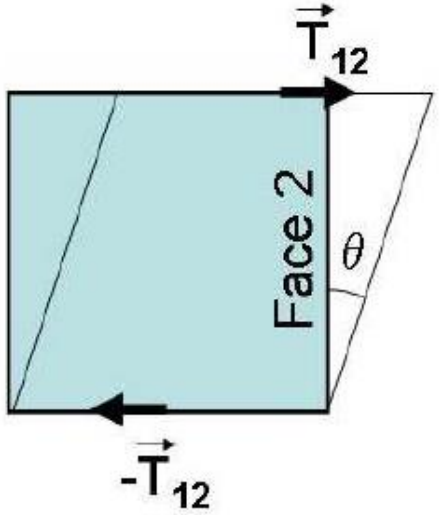
Elasticity for a material
Linear laws between stress and strain in the regime of Hooke's law



elongation

$$\sigma_L = E\ \varepsilon_L$$



shear

$$\tau = G\ \gamma$$

σ = tensile stress : T/A (force per unit area)
E = Young modulus
ε = relative elongation (strain)

τ = shear stress : T/A (force per unit area)
G= shear modulus
γ = tan θ (shear strain)

Generalization (tensors)

$[\sigma] = [C]\,[\varepsilon]$ → C_{ij} = elastic constants

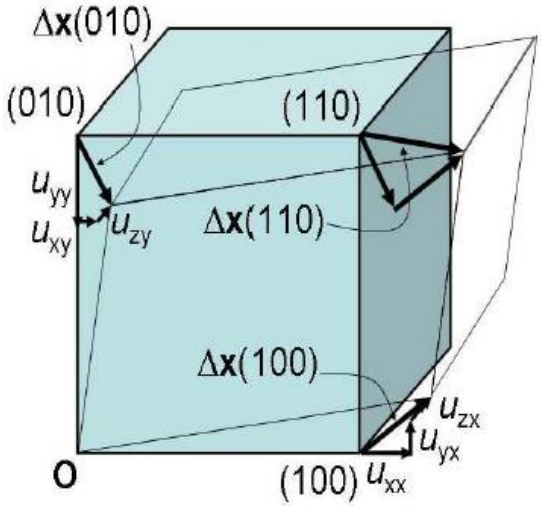
Cubic material

$$C = \begin{pmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{44} \end{pmatrix}$$

Change in internal energy for small deformations

$$E(V, \{\epsilon_k\}) = E_0 + V_0 \left(\sum_{i=1}^{6} \sigma_i \epsilon_i + \frac{1}{2} \sum_{i,j=1}^{6} C_{ij} \epsilon_i \epsilon_j \right)$$

$$C_{ij} = \frac{1}{V_0} \left[\frac{\partial^2 E}{\partial \epsilon_i \partial \epsilon_j} \right]_{\{\epsilon_k\}=0}$$

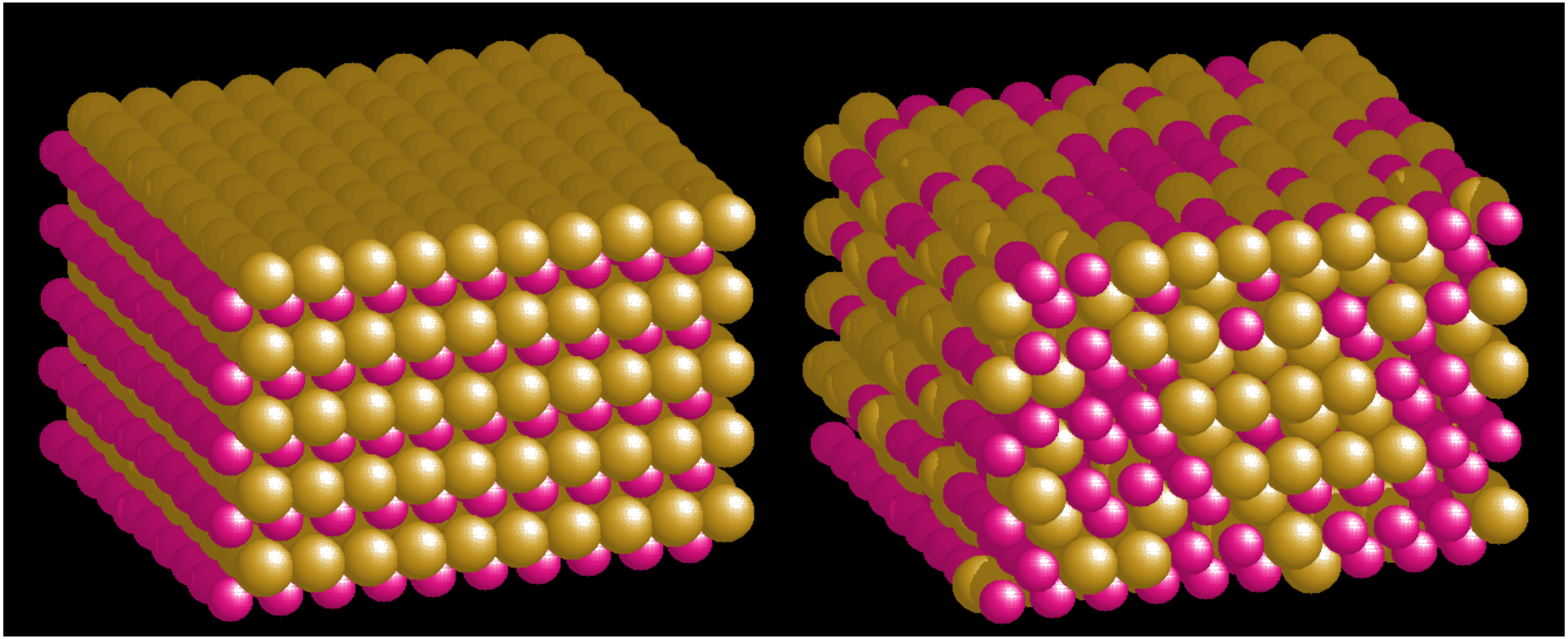


Energy from :Tight binding in the second moment approximation

$$E_i = A \sum_j e^{-p\left(\frac{r_{ij}}{r_0}-1\right)} - \sqrt{\xi^2 \sum_j e^{-2q\left(\frac{r_{ij}}{r_0}-1\right)}}$$

ordered alloy

disordered alloy



Training:

Write a program to create a disordered alloy (Monte –Carlo type)

Calculate the total energy within the frame of the second moment approximation

Deform the sample according to chosen strain, recalculate the total energy

Deduce the elastic constants: C_{11}, C_{12} and C_{44}

Make the same while allowing the atoms to relax around the rigid lattice position