

Solution problem 6 , FYS4310

tgf

PROBLEM 6

Imagine that we force the unit cell of Ge to occupy the same volume as the unit cell of Si. The Ge is thus deformed elastically and we need to apply a stress (pressure) to maintain this.

a) Calculate the value of the deformation.

Hint: assume elastic deformation, characterize it by the strain in scalar form

$$\sigma = \frac{F}{A}, E = \frac{\sigma}{\epsilon}, \epsilon = \frac{\Delta l}{l}, \text{ where } \sigma: \text{stress}, \epsilon: \text{strain}, E: \text{Young's modulus}$$

b) Calculate the value of the stress.

> restart;

We need to look up some values. First the lattice parameters for Si and Ge

The lattice constant for Si is 5.43 Å, and the lattice constant for Ge is 5.66 Å

d_Si=0.543 nm d_Ge=0.566 nm

E_Ge=102.7 GPa

> lookups:={d_Si=0.543*1e-9*m,d_Ge=0.566*1e-9*m,E_Ge=102.7e9*N/m^2};

$$\text{lookups} := \left\{ d_{\text{Ge}} = 5.66 \cdot 10^{-10} \text{ m}, E_{\text{Ge}} = \frac{1.027 \cdot 10^{11} \text{ N}}{\text{m}^2}, d_{\text{Si}} = 5.43 \cdot 10^{-10} \text{ m} \right\}$$

a)

> "The deformation is";
subs(lookups,(d_Ge-d_Si)); 'OR'; subs(lookups,(d_Ge-d_Si)/d_Ge);
"The deformation is"

$$2.3 \cdot 10^{-11} \text{ m}$$

OR

$$0.04063604240$$

There is no strict definition of 'deformation', a measure for it is the elongation or the relative elongation. The latter is the strain

b)

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> sigma=E*epsilon;
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$$\sigma = E \epsilon$$

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> sigma=E_Ge*((d_Ge-d_Si)/d_Ge);
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$$\sigma = \frac{E_{\text{Ge}} (d_{\text{Ge}} - d_{\text{Si}})}{d_{\text{Ge}}}$$

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> subs(lookups, %);
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$$\sigma = \frac{4.173321555 \cdot 10^9 \text{ N}}{\text{m}^2}$$

The stress is 4.2 GP.

Compare that to the yield stress of Ge. "Apparent Elastic Limit = 89.6 MPa"

The numbers for this may vary in tables, It is of course dependant on temperature.

But the important thing is that the stress required is very large. So large that it is unlikely to force a pure Ge crystal inside a Si lattice and then take over its lattice parameters- there would be a tendency for this being favourable by direct bonding arguments at the interfaces, but the elastic energy would have been very big.

This is of relevance for epitaxial growth of Ge or GeSi on Si.