Misfit Dislocations in Heterojunctions

Advanced

- Calculating the critical thickness of a layer with lattice constant a_1 on top of a substrate with lattice constant a_2 can become rather involved, if all components contributing to the elastic energy are taken into account.
  - In particular, you may want to consider the anisotropy of the situation, the effect of a finite thickness of the top layer, the real geometry with respect to the dislocations (their line energy depends on this and that, and they may be split into partial dislocations).
  - Then, after arriving at a formula, you may chose to make all kinds of approximations.
  - In the backbone part of the script we had a simple formula (taken from a paper of the very well known scientist Sir Peter **Hirsch**) which you can find in the link (together with some comments):

$$d_{crit} = \; = \frac{b}{8 \cdot \pi \cdot f \cdot (1 + \nu)} \cdot \ln \frac{e \cdot d_{crit}}{r_0}$$

  - With b = **Burgers vector** of the dislocations; usually somewhat smaller than a lattice constant, f = misfit parameter = $(a_1 - a_2)/a_1$, ν = Poisson ration ≈ **0,4**, **e** = really **e** = base of natural logarithms r_0 = inner core radius of the dislocation; again in the order of lattice constant.
- Lets look at some other approaches
  - A formula taking into account most everything going back to J. W. **Matthews** and A.E. **Blakeslee** (**1974**) , who pioneered this field of research, is

$$d_{crit} = \frac{b \cdot (1 - \nu) \cdot \cos^2\Theta}{8 \cdot \pi \cdot (1 + \nu) \cdot f \cdot \cos\lambda} \cdot \left(\ln \left(\frac{d_{crit}}{b} \right) + 1 \right)$$

  - with Θ = angle between the dislocation line and its Burgers vector, λ = angle between the slip direction and that line in the interface plane that is normal to the line of intersection between the slip plane and the interface.
  - For simple systems ($\Theta = 90^o$ and $\lambda = 0^o$), we have

$$d_{crit} = \frac{b}{8 \cdot \pi \cdot f \cdot (1 + \nu)} \cdot \left(\ln \left(\frac{d_{crit}}{r_0} \right) + 1 \right)$$

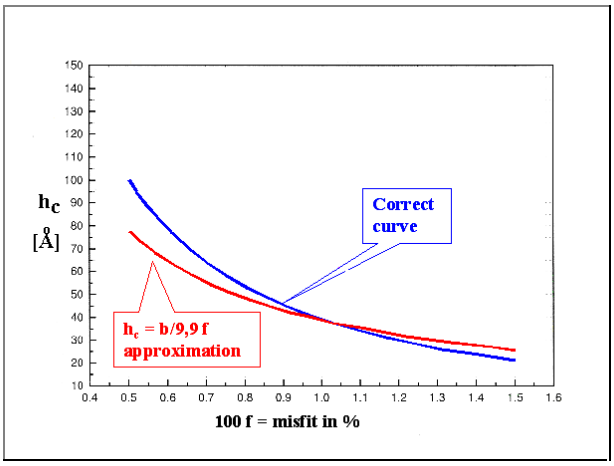
  - And that is Sir Peters equation if you insert **ln(e)** for the **1** in the **ln** term.
- While Sir Peter used the simple approximation

$$d_{crit} \approx \frac{b}{6f}$$

  - the comparison with the (computer-generated) correct functional dependence suggests

$$d_{crit} \approx \frac{b}{9f}$$

  - which is a bit different!
- A plot of the full formula and the approximation looks like this:



- Similar curves are contained in the books of Mayer and Lau or Tu, Mayer and Feldmann; they supposedly use the same equation but show *rather different results*.
  - Well, somewhere should be a mistake (maybe I made one?). In any case, it nicely demonstrates the point made in the backbone section: Do not blindly believe a theory. In case of doubt, try it out.