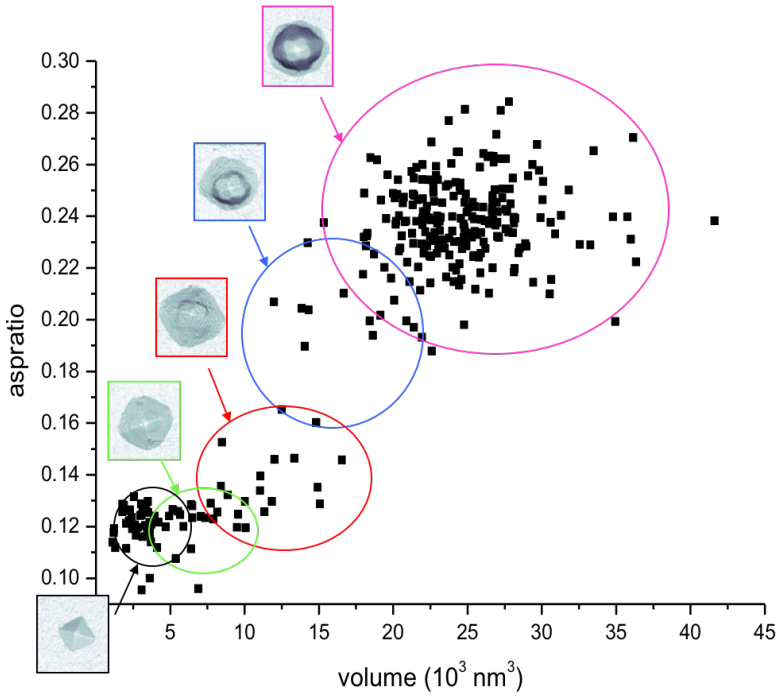
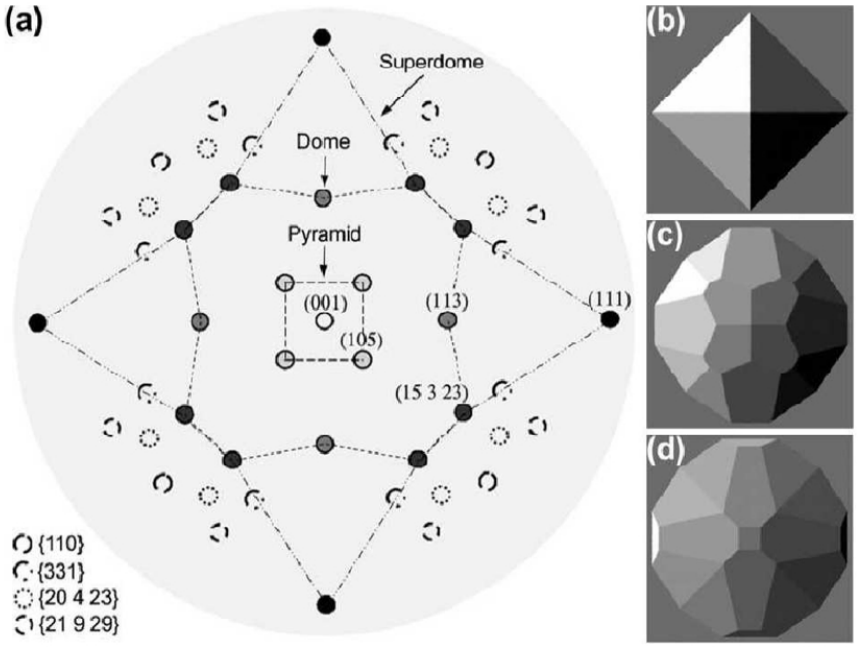
Homework **Epitaxial evolution of germanium on silicon substrate**

The aim of this exercise is to look at the phenomenon of epitaxial growth with a concrete example: nucleation and evolution of epitaxial islands of Ge on the Si {100} surfaces. *Reminder: the lattice parameter of Si is* 5.43 Å*, while Ge has* 5.66 Å.
The following plot shows the relation between the shape (precisely, the aspect ratio) of the nucleating island and its volume: "simple" shapes appear at smaller volume.



The following figure, instead, is a calculated "stereographic map" around the (001) surface showing the position of the facets of bulk Ge. The facets making up a (b) pyramid, (c) dome and (d) barn islands are represented on the map by connecting facets indices with long–dashed, short–dashed and dotted–dashed lines, respectively.

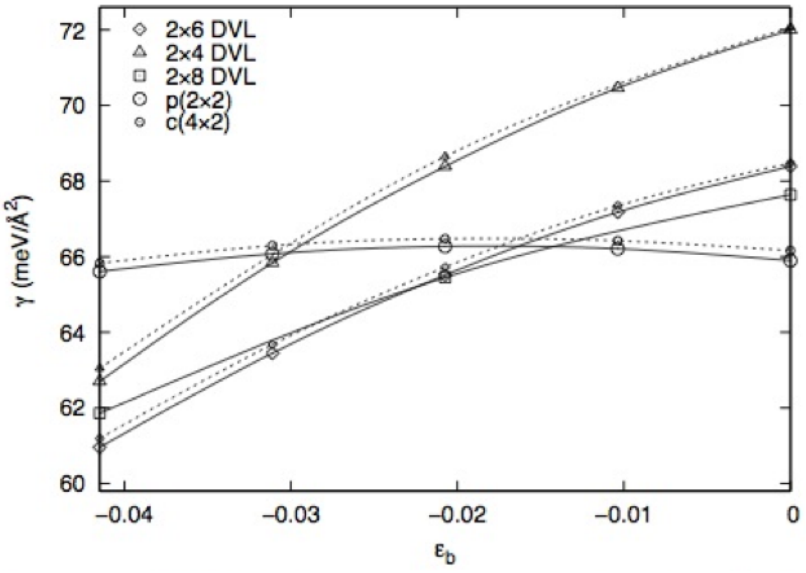


There are two opposing contributions that explain the morphological evolution of these islands:

1. Lower elastic energy in volume
2. Different surface energies and area of facets

The first factor is related to the relaxation of elastic energy by a transfer of the load to the Si substrate and it is larger for higher aspect ratios. On the other hand, higher aspect ratios mean greater exposed surface and steeper facets have often larger surface energies.

To understand why some facets are more favoured than others in the presence of strain, look at the following plot: it shows different Ge (001) reconstructions and the corresponding surface energy with respect to biaxial strain (i.e. strain introduced in two perpendicular directions along the surface).



Cont.

(a) Can you explain why surface energies show different behaviour with respect to different reconstructions?

(b) Consider the Si substrate with N Ge layers deposited on top of it. If another layer is added (i.e. having a total of $N + 1$ layers), what is the energy difference between these two "configurations"? *Hints: you can think of the addition of one Ge layer as an increase of the thickness of the wetting layer of Ge without changing the surface reconstruction.*

(c) Determine the energy difference between the configuration "N layer Ge plus an island" and "$N + 1$ Ge layers".

(d) Using the formula obtained in (c), are you able to explain also the morphological evolution of the islands? *Hints: in other words, why are pyramids, then domes and eventually barns forming?*

Cont.

Homework's solution

(a) Surface energy of reconstructed surface is always sensitive to the presence of strain. For example, if a surface reconstruction pairs dangling bonds with a bond length slightly greater that the equilibrium one, the corresponding surface energy will decrease if a compressive strain is applied, because the bond length is now much more similar to the preferred one.

(b) Adding one layer of Ge atoms means inserting another middle layer of strained Ge while keeping the same surface reconstruction. So, if we call ρ^t the volumetric density of elastic energy of strained Ge, we have that the energy difference between the two configurations is

$$\Delta E = V \times \rho^t.$$

(c) Now we need simply to add the energy terms related to the formation of an island. We have one volume energy term, namely

$$E_V^{\text{is}} = V \times \rho^{\text{is}},$$

where V is the same as in the case of adding another layer because we are depositing the same amount of material. ρ^{is} is the energy per unit volume of the island and we know that this is always lower that the energy density of a layer.
On the other hand, the island has also two surface energy terms:

$$E_S^{\text{is}} = A\gamma_{\text{is}} - B\gamma_{\text{WL}},$$

where A is the surface of the exposed facets of the island (and γ_{is} is the corresponding surface energy) and B is the area of the underlying layer which is covered by the island (with a surface energy of γ_{WL}). Putting everything together, we have

$$\Delta E = V(\rho^{\text{is}} - \rho^t) + A\gamma_{\text{is}} - B\gamma_{\text{WL}}.$$

(d) This is quite simple if we recall that the higher the aspect ratio, the larger will be the relaxation of the elastic energy accumulated during the deposition. So, since elastic energy density of domes is always smaller than the one of pyramids (and bigger than that of barns), first are expected pyramids, then at larger volumes domes and eventually barns.

The End.