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Trends and perspectives in solid-state wetting / Mouillage solide–solide : tendances et perspectives

One-dimensional Ge nanostructures on Si(001) and Si(1 1 10): Dominant role of surface energy

Structures unidimensionnelles de Ge sur Si(001) et Si(1 1 10) : rôle dominant de l'énergie de surface

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ABSTRACT

Ge/Si(001) is a prototypical system for investigating three-dimensional island self-assembly owed to the Stranski–Krastanow growth mode. More than twenty years of research have produced an impressive amount of results, together with various theoretical interpretations. It is commonly believed that lattice-mismatch strain relief is the major driving force leading to the formation of these islands. However, a set of recent results on Si(001) and vicinals point out that, under suitable conditions, this is not the case. Indeed, we here review experimental and theoretical results dealing with nanostructures mainly determined by surface-energy minimization. Results are intriguing, as they reveal the existence of magic sizes, show the presence of very peculiar morphologies, such as micron-long wires, and distinguish among attempts to facet the wetting-layer and true SK islands.

RÉSUMÉ

Le système Ge/Si(001) constitue un prototype pour l'étude de l'auto-assemblage des îlots tridimensionnels dans le cadre de la croissance Stranski–Krastanov. Plus de vingt ans de recherches on produit une quantité impressionnante de résultats, ainsi que des interprétations théoriques variées. Il est communément admis que la relaxation de la contrainte due au désaccord de maille est la force motrice dominante qui mène à la formation de ces îlots. Cependant, de nouveaux résultats sur Si(001) et sur des surfaces vicinales indiquent que, dans des conditions adaptées, ce n'est pas le cas. En effet, nous rapportons ici des résultats expérimentaux et théoriques décrivant des nanostructures qui sont essentiellement déterminées par la minimisation de l'énergie de surface. Ces résultats intriguent, car ils révèlent la présence de tailles magiques, et montrent la présence de morphologies très particulières, comme des fils de longueur micronique. De plus, elles mettent en évidence les différence entre les tentatives de facettage de la couche de mouillage et la formation de véritables îlots Stranski–Krastanov.

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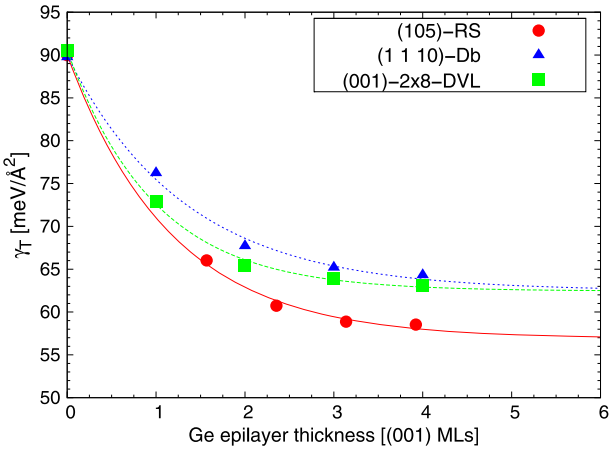

Fig. 1. From Ref. [27]. Trend of the surface energy density γ as a function of epilayer Ge thickness N for three different orientations. Color figure available on the web.

1. Introduction

More than twenty years have passed since the first seminal reports on three-dimensional (3D) Ge islands on Si(001) were published [1,2]. Massive research followed, as Ge/Si was soon recognized as a prototypical, simple-enough system following the Stranski–Krastanow (SK) growth mode. As such, its profound understanding could lead to the development of predictive models for other, technologically more appealing but more complex, heteroepitaxial lattice-mismatched systems such as III–V compounds (see, e.g., [3–7]). Reviews on Ge/Si (and, Ge_xSi_{1-x} alloys on Si(001), showing a similar behavior for high enough Ge concentration x) SK growth can be found in Refs. [8–13]. We now know that typical 3D islands tend to change morphology during growth, evolving from low height-to-base aspect ratios R to large R values as their volume increases (see also [14] and references therein). A multitude of islands shapes were indeed observed, starting from small mounds [15,16], leading to {105}-faceted pyramids ($R \sim 0.1$) and huts [1,17], to larger-volume (V) multifaceted domes ($R \sim 0.2$) [18,19], barns [15] ($R \sim 0.3$) and cupola islands ($R \sim 0.4$) [20] with increasing V. What typically defines an island of each family is the set of different exposed facets.

Some general features of Ge/Si SK growth are now well understood. As the first layer of Ge is deposited, a strong driving force determines perfect wetting, to saturate highly-energetic Si dangling bonds with the weaker Ge ones. As a result, the film surface energy γ_{WL} drops. If a second Ge layer is now added, the interface-effect due to the presence of the Si substrate below is still strong (owed both to electronic [21] and elastic [22] effects), so that the surface energy γ keeps on dropping. If N is the number of deposited layer, this effect in semiconductors is well described by an exponential decrease of the surface energy with N [23], convergence to the $N \to \infty$ limit being controlled by a system-specific *wetting factor*. To add on complexity, the WL typically changes its reconstruction with increasing N [21,24–26], without however affecting the general $\gamma_{WL}(N)$ behavior described above. Examples of the $\gamma_{WL}(N)$ dependence as obtained by ab initio calculations are given in Fig. 1 for the orientations of direct relevance for the problem discussed in Sections 4 and 5. It is clear that the driving force for wetting decreases with N, so that departure from a simple 2D WL configuration is increasingly facilitated with WL thickness, provided there is a driving force for doing so. Obviously, this additional driving force is provided by strain relaxation. A planar WL configuration determines biaxially compressed Ge (Ge lattice parameter being ∼4% larger than the Si one), only partially reacting through a tetragonal relaxation of the elastic energy. Formation of 3D structures introduces further degrees of freedom allowing for R-dependent lowering of the volumetric elastic energy density ρ_{is}, higher R values leading to lower ρ_{is} [12]. On the other hand, islands with high R values also determine an increased additional-surface exposure [12,14], scaling as $V^{2/3}$, so that the following simple interpretative scheme emerges. Provided that the WL is thick enough (above some ∼3 ML, but see discussion in [28]), 3D islands are formed. At small V, only low-R islands can be observed as evolution towards optimal (high-R) strain relaxation is hindered by surface-energy costs. As the volume increases, however, volumetric strain relaxation dominates and high-R structures are eventually formed. Although this simple description seems to yield a qualitative explanation of the experimental findings, a substantial upgrade of the theory is needed in order to account for a semi-quantitative description of the Ge/Si(001) behavior. A general discussion is presented in the next section, considering various additional effects which can significantly alter the simplified description presented in this Introduction. Then, in the remaining sections of the manuscript, we shall review recent theoretical and experimental results demonstrating that the very concept of islands being created as a result of strain relaxation frustrated by a flattening surface-energy driving force does not apply under peculiar conditions. This leads to a new class of Ge/Si nanostructures of major scientific interest, whose potential for applications has not been yet explored.