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# Effect of mesoscopic misfit on growth, morphology, electronic properties and magnetism of nanostructures at metallic surfaces

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**Abstract**

Stress and strain originating from mesoscopic misfit at interfaces can have diverse effects on the properties of surfaces and nanostructures thereon. We review the sources and consequences of mesoscopic misfit at metallic surfaces and elucidate various ways in which it affects growth, morphology, electronic properties and magnetism of thin films in early stages of epitaxy and epitaxial nanostructures.


*Keywords:* Mesoscopic; Misfit; Relaxations; Stress; Strain; Nanoscale

**Contents**



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## 1. Introducing mesoscopic misfit

Today, after more than a century of active research on the subject of stress and strain at surfaces, the notion that the latter play a crucial role in determining morphology and growth dynamics of both the surface itself and the nanostructures thereon seems almost trivial. To name just a few examples, we usually expect that the outermost atomic layers of a crystal cleaved along a high-symmetry crystal plane shall not retain the bulk interlayer spacing but be contracted due to the reduced coordination of surface atoms (schematically shown in Fig. 1(a)). The equilibrium bond length contraction that causes this also introduces an excess stress in-plane of the crystal surface. Both excessive tensile and compressive stresses can lead to a reconstruction of a surface (hinted in Fig. 1 (b)) as the latter strives to relieve some of the stress thus minimizing the surface energy. Contrary to flat surfaces, for finite-size nanoscale structures this in-plane stress is inherently uncompensated and leads to an in-plane deformation of the structure (Fig. 1(c)). While homo-epitaxial adsorption partially recovers the coordination of atoms at the surface–structure interface,[1] in hetero-epitaxial systems (having differing equilibrium values of lattice constants and surface stresses) complex and highly anisotropic strain fields in both substrate and epitaxial nanostructure are often observed (Fig. 1(d)).

It is nowadays customary to generalize under the name of "mesoscopic misfit" the deformations of the surface and the nanostructures thereon induced by a multitude of effects connected with the finite size of the system or the inherent mismatch of lattice constants of different materials it is composed of. With the present review we shall summarize and bring some order into the current understanding of how and when mesoscopic misfit arises in nanostructures at metallic surfaces and what implications it has for morphology, growth, electronic and magnetic properties of the system.

In the following, after a brief historical overview of the subject in Section 2 we shall outline the state-of-the-art understanding of the mesoscopic misfit in metallic systems (Section 3). We start with the most obvious consequence of the misfit – geometric relaxations in the system and their implications for morphology of homo- and hetero-epitaxial systems as predicted by theory (Sections 3.2 and 3.3). Supporting the theoretical predictions with ample experimental observations we discuss the elementary processes of adatom adsorption and diffusion that underlie the observed growth dynamics and morphologies of mesoscopic systems (Sections 3.4–3.6). Having established the fundamentals, we proceed to the discussion of the effects that misfit (and resulting strain relaxations in the system) can have on the system's electronic (Section 3.7) and magnetic (Section 3.8) properties.

While numerous indirect hints as to the omnipresence and importance of mesoscopic misfit exist, direct proofs of misfit-induced strain are scarce. That is why, in the last few sections of the review we summarize the existing direct evidence of such strain as provided by surface x-ray diffraction (Section 4), extended x-ray adsorption fine structure (Section 5) and stress measurement (Section 6) techniques.

The review is rounded up by a short summary.

## 2. Mesoscopic misfit – the history in brief

While our to-date understanding of the possible origins of mesoscopic misfit still cannot be deemed absolute, the idea itself that strain and stress of a surface play a fundamental role in defining the properties of the latter is more than a century old, dating back to the works of Gibbs [1,2]. Theoretically conceived and originally applicable on a macroscopic level to an interface between any two "phases" of matter, it is much older than the interest of the community in the atomic structure of the interfaces. In the early 20th century, during the boom of crystallography, when a crystalline material A was grown onto a crystal surface of material B (a process for which the term "epitaxy" was coined by Royer [3]) the stress at the interface of A and B was usually considered to come from the "natural misfit" alone (the difference in the lattice constants of A and B). At that time the only important implication of stress was its effect on morphology and growth behavior of epitaxial systems. The understanding that stress was an excess quality that the surface will strive to relieve in order to minimize its energy [4,5] called for a good predictive

[1] In fact, as shall be discussed in the following, even in the case of homo-epitaxy, the stress relief patterns are very much size dependent and lead to considerable deformations of both the ad-structure and the substrate. Here, however, for the sake of simplicity we present a naive picture in the spirit of continuum elasticity theory.