

The Introduction of the Concept of Electronic Growth

“Electronic Growth” of Metallic Overlayers on Semiconductor Substrates

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- Zhang, Niu, and Shih, Phys. Rev. Lett. 80(24), 5381 (1998)

In the paper, Zhang, Niu, and Shih present a model which can explain the existence of 2 types of film stability:

Two types of film stability:

1. critical thickness: film is stable either above or below some specific thickness ($L \geq L_c$, or $L < L_c$)
the “critical” term in the case of Ag on GaAs has the opposite meaning compared to conventional film growth concept of critical thickness; in conventional meaning, a film always becomes unstable above a certain critical thickness, resulting in the formation of 3-D growth mode and/or development of defects, dislocations, for example
2. ‘magic thickness’: film is stable only at a particular thickness, but not above or below that value ($L = L_c$ but not $L < L_c$ or $L > L_c$)

There are several physical terms leading to the stability of the thin film in this new model:

1. quantum confinement
2. charge spilling
3. interface-induced Friedel oscillations

1. Quantum confinement:

QC leads to an effective repulsive force between the substrate/film interface and the film surface

QC depends on the thickness

→ tends to stabilize the flat film overlayer

The energy of this term is the confinement energy of the electrons or charge carriers.

2. Charge spilling:

Charge density imbalance between the film and the substrate leads to transfer of electronic charges from the film to the substrate, or vice-a-versa

→ leads to the formation of net opposite charge on both sides of the interface

→ leads to an effective attractive force between the film/substrate interface and the film surface

→ tends to destabilize the flat film surface

The energy of this term can be modeled as a capacitive energy.

3. Interface-induced Friedel Oscillations:

Oscillations in the electron wave functions as a function of film thickness leads to additional terms in the films energy

Definition of Friedel oscillations:

- decay of the density oscillations induced by a defect
- a long-standing problem in solid state physics
 - http://www.physik.uni-augsburg.de/theo2/Publications/Schmitteckert/P96_1/node3.html
- According to the above website, “This phenomenon, called Friedel or Ruderman-Kittel oscillations (depending on the context), is closely related to the singularity in the response function for wave-vectors close to $2k_F$.
- The induced electron density oscillations near a defect are expected to decay asymptotically like:

$$dn(x) \sim \cos(2k_F x + n_F) / x^\delta$$

- http://www.physik.uni-augsburg.de/theo2/Publications/Schmitteckert/P96_1/node3.html

- Friedel oscillations can be observed on metal surfaces using STM and are seen as the electron “waves” at a surface. There will also be Friedel oscillations in the z-direction (out-of-plane).

The energy of this term is more complex, having to do with the energy of the surface due to the match up of the thickness with the electron wave-function

Each of these terms adds into the total film’s free energy

Results of the Model:

From their model, Zhang et al. were able to confirm the behavior of Ag on GaAs

Note this system is Noble metal on medium gap semiconductor

From the model, they could also explain other well-known phenomena:

For alkali metals on semiconductors, only the first monolayer is known to be stable

Method of the theory:

Calculate the QC, charge spilling, and Friedel oscillations energies and add them together to form the total energy of the film as function of the film thickness

$$E_T(L)$$

Then evaluate the shape of the energy vs. film thickness curve

1. if curvature is positive → stability

$$d^2E_T(L) / dL^2 > 0$$

2. if curvature is negative → instability
in this case, the film can stabilize by forming a mixed phase of different film thicknesses

$$d^2E_T(L) / dL^2 < 0$$

Some results:

Ag on GaAs(110)

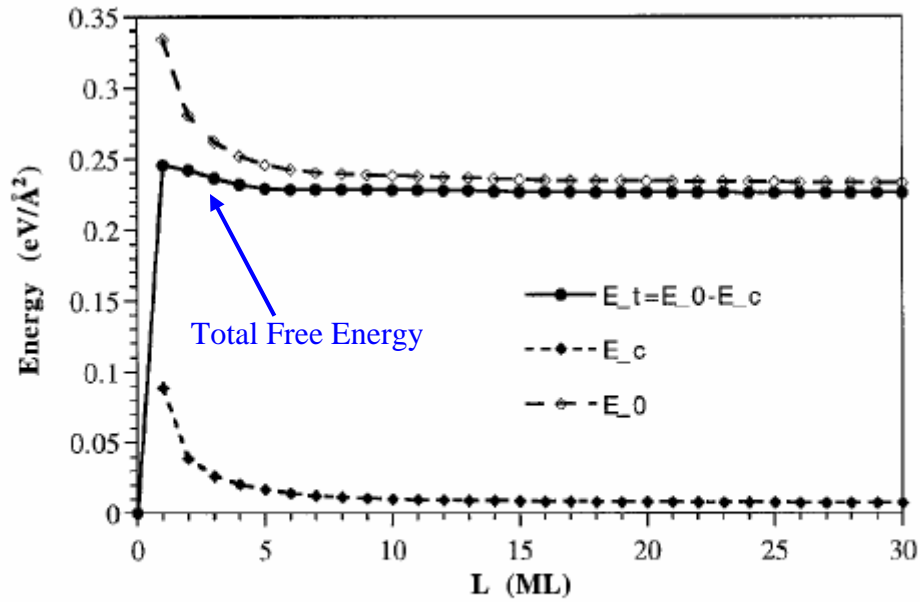


FIG. 1. Film thickness dependence of the film energies for Ag on GaAs(110). The dip at $L = 5$ ML defines the critical thickness for flat film growth.

- Zhang, Niu, and Shih, Phys. Rev. Lett. 80(24), 5381 (1998)

As can be seen, the curvature is positive below about 5 ML and then it becomes negative (stability) above about 5 ML.

Theory predicted 5ML as the critical thickness for Ag/GaAs

Experiment reported 7ML

→ quite good agreement

The same authors also showed that their model worked well to explain a variety of other metals on GaAs(110)

Other Metals on GaAs(110)

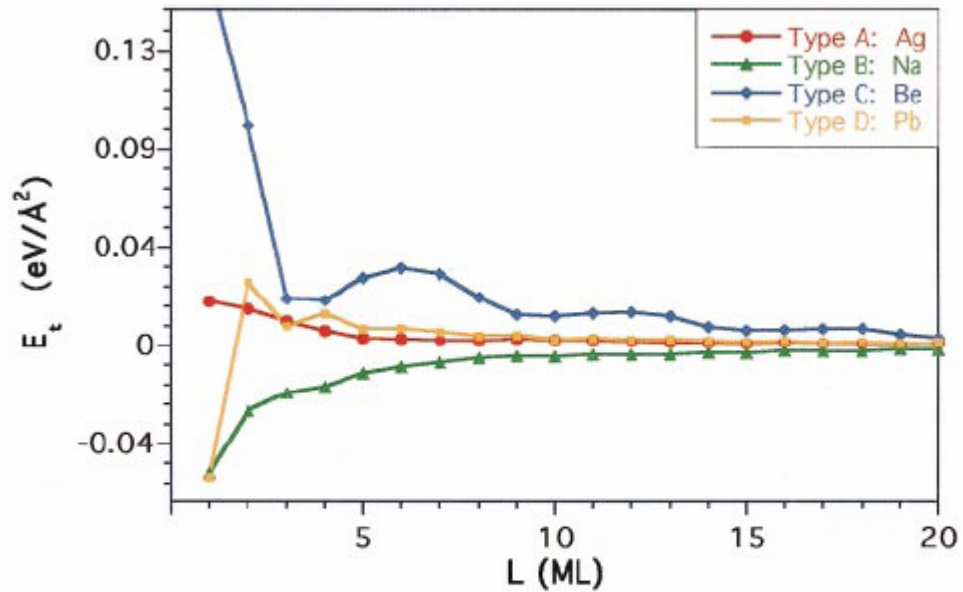


FIG. 2(color). Comparison of four representative types of film stability for different metals on GaAs, as defined in the text. Notice that an element-specific constant term has been substrated from each curve to make the total energy equal to zero at large film thickness.

- Zhang, Niu, and Shih, Phys. Rev. Lett. 80(24), 5381 (1998)

Overall, the electronic growth model set a new concept in surface growth which has since been explored in lots of detail in many systems, experimentally and theoretically.

A few examples of additional papers on this topic:

1. Title: **Role of the metal/semiconductor interface in quantum size effects: Pb/Si(111)**

Author(s): [Yeh V](#), [Berbil-Bautista L](#), [Wang CZ](#), [Ho KM](#), [Tringides MC](#)

Source: PHYSICAL REVIEW LETTERS 85 (24): 5158-5161 DEC 11 2000

2. Title: **Theory of quantum size effects in thin Pb(111) films**

Author(s): [Wei CM](#), [Chou MY](#)

Source: PHYSICAL REVIEW B 66 (23): Art. No. 233408 DEC 15 2002

3. Title: **Size model of Pb islands grown on Si(111)**

Author(s): [Wang GZ](#), [Webb JF](#), [Li S](#), [Zi J](#)

Source: PHYSICAL REVIEW B 68 (15): Art. No. 155406 OCT 15 2003

4. Title: **Effects of the substrate on quantum well states: A first-principles study for Ag/Fe(100)**

Author(s): [Wei CM](#), [Chou MY](#)

Source: PHYSICAL REVIEW B 68 (12): Art. No. 125406 SEP 15 2003