Formation and phase transition of Co nanowires on vicinal Cu(111) surfaces

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Wires formation and lengths distribution

The length of wires generally depends on many parameters of the experiment. It was shown that distributions of wires' lengths have various number of peaks [1–3] (see Fig. 1). There are some explanations for it but they raise more questions than answers. It motivated us to conduct our own research.

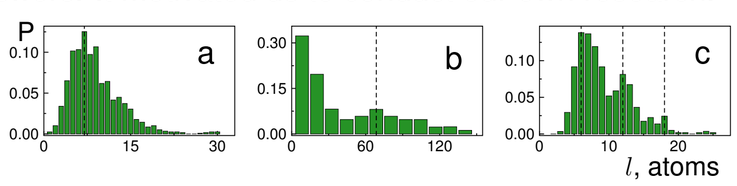


Figure 1: Three types of experimental distributions of atomic wire lengths. (a): Ag (0.04 ML) on Pt(997) at 400 K [1]. (b): Co (0.12 ML) on Cu(775) at 165 K [3]. (c): Ir (0.3 ML) on Ge(001) at 300 K and annealed at 650 K [2].

We performed large-scale kinetic Monte-Carlo simulations based on ab initio calculations.

It was shown that the interactions between Co adatoms depend on the distance from a surface step and also on the magnitude of the repulsive barrier which is connected to the surface step. It is larger for Co adatoms located at the upper surface terrace and smaller for those located at the lower surface terrace [4] (see Fig. 2). This difference is related to the charge redistribution at the step edge [5].

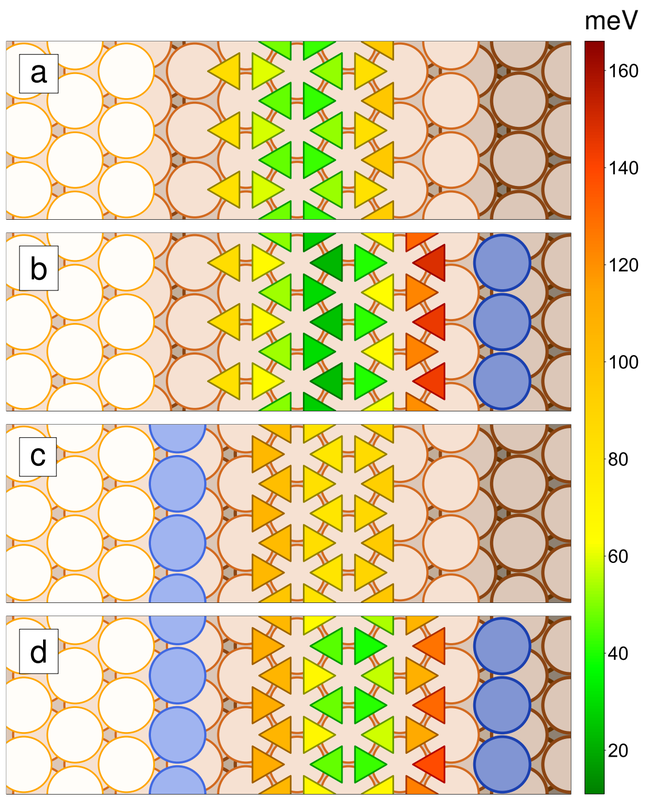


Figure 2: Map of potential energy for the Co adatom on Cu(775). ◁ denote fcc sites, ▷ — hcp sites.

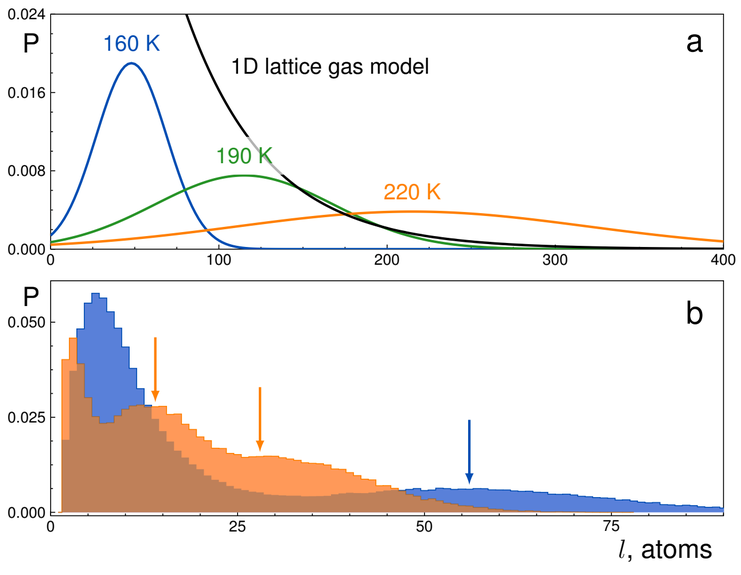


Figure 3: (a): Distributions of atomic wire lengths for three different temperatures, annealed at 300 K. Solid black line shows fitting the data in the framework of 1D lattice gas model. (b): The surface has terraces with two (blue) or three (orange) characteristic widths. The peaks marked with the arrows appear in the distribution due to the presence of wider terraces.

These results give an explanation to the fact that the formation of nanostructures at temperatures ≈100 K occurs at the lower part of the step, whereas at room temperature, they are formed at the upper part of it [5].

We compared the results of our simulations with the experiment (see Fig. 3). By varying width of the terraces we obtained multimodal distributions closely resembling experimental ones. Antiripening effect, however, does not affect our distributions.

Furthermore, we found the Co wire to act as a "nano traffic light" for adatoms rushing along the terrace (see Fig. 2). It will increase the interaction energy between the adatom and the surface in the middle of the lower terrace and decrease it in the middle of the upper one.

Additionally, we have shown that 1D island size distribution depends significantly on the time of the experiment [6]. Our model predicts that during annealing or cooling, the transition from one state of thermodynamical equilibrium to another occurs through a non-equilibrium state (see Fig. 4). This transition consists of Ostwald ripening and decay of 1D islands.

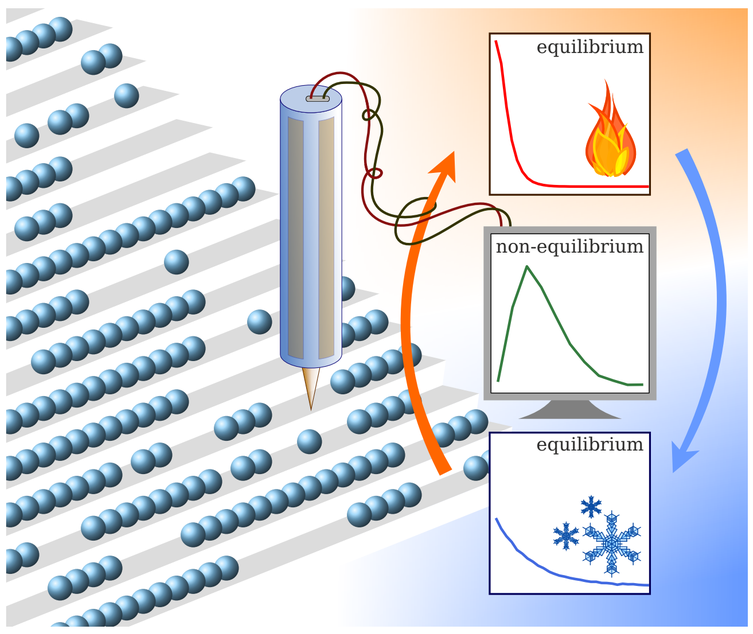


Figure 4: Schematic drawing showing how the distribution of wires' lengths changes during annealing or cooling.

Therefore, experiment shows only the non-equilibrium part of the process, which renders interpreting its data using 1D lattice gas model incorrect [7] (see Fig. 3 (a)).

Phase transition

In paper [8] low-temperature STM observations of a dimerization instability of a Co atomic-wire system self-assembled on a vicinal Cu(111) substrate were presented. Also a discrepancy between experimental and theoretical values of the binding energy for atomic wires on a metal surface [3] acted as a motivation for this research.

We have found two ferromagnetic states of Co wires [9]. In the first state the Co wire consists of dimers, while in the second state the distance between atoms in Co wire is equal (see Fig. 5).

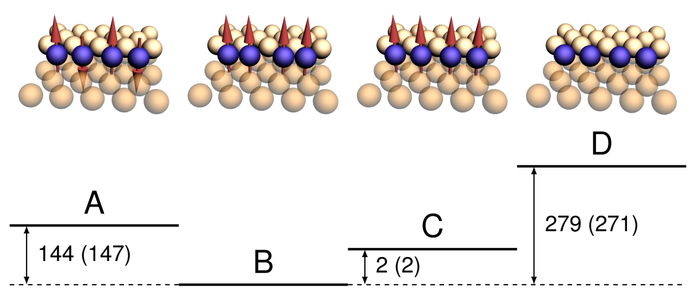
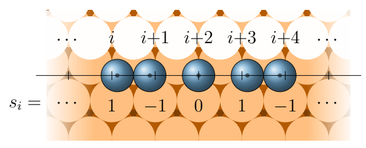


Figure 5: (A) antiferromagnetic, (B) dimerized ferromagnetic, (C) ferromagnetic, and (D) zero-spin configurations of Co nanowire deposited on stepped Cu(111) surface, together with the energy levels (in meV/atom) for B-type (A-type) step.

Using Monte Carlo simulations we demonstrated the structure phase transition in a Co wire (see Fig. 6). The state of Co atomic wire can be characterized by order parameter η, which is defined in our model as:



$$\eta = \frac{2}{N}\left|\sum_{i=1}^{N/2} s_{2i}\right|$$

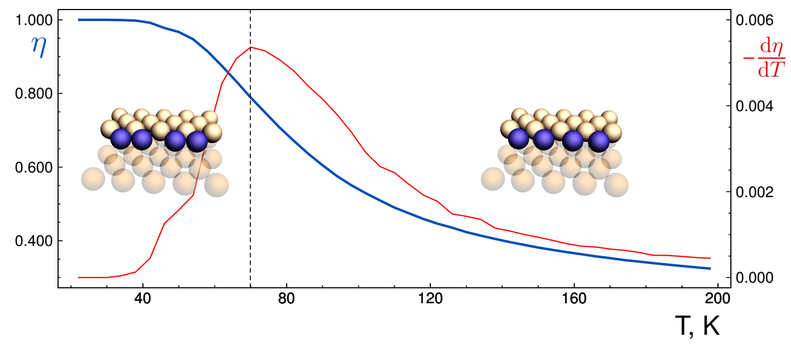


Figure 6: Temperature dependences of order parameter η averaged over 2000 numerical experiments and its derivative $\mathrm{d}\eta/\mathrm{d}T$. The length of the Co wire is 32 atoms; ΔE = 16 meV.

Moreover, the phase transition temperature was determined and the size-effect was studied [10].

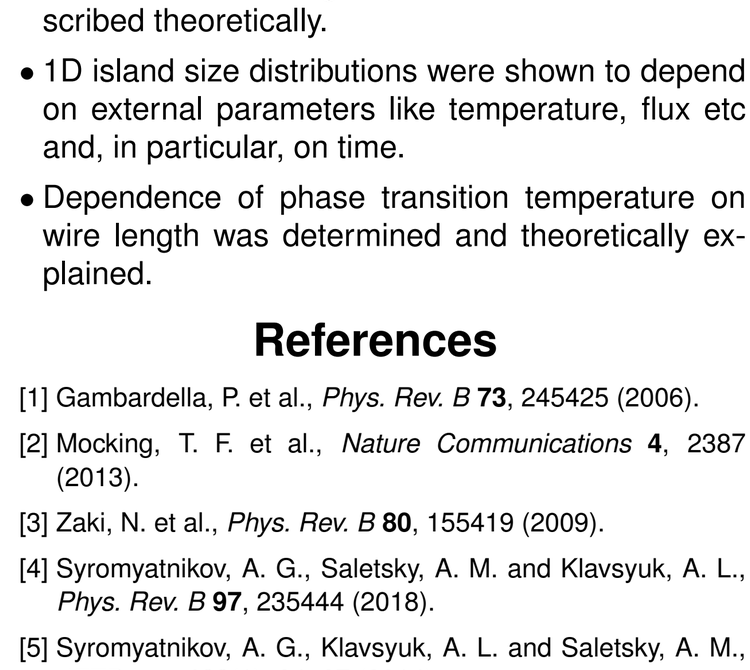


Figure 7: Dependence of the phase-transition temperature on 1 / ln N, where N is the wire length. ΔE = 16 meV.

Summary

- Tendency to form nanowires on lower terrace instead of the upper one was explained.
- Multimodal wirelengths' distributions were described theoretically.
- 1D island size distributions were shown to depend on external parameters like temperature, flux etc and, in particular, on time.
- Dependence of phase transition temperature on wire length was determined and theoretically explained.

References

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