Magnetism and Structure of Oxide Chains of Binary Alloys of Co and Ni on Ir(100)

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The morphological evolution of chains during heteroepitaxial growth has recently been a topic of extensive experimental and theoretical [1, 2] studies in part due to its fundamental interest, but also because of possible applications to the formation of self-assembled nanostructures. The self-assembled growth is limited to certain choices of materials, but one can produce one-dimensional structures to high perfection and with high surface density. This opens the opportunity to employ spatially averaging methods to determine their properties.

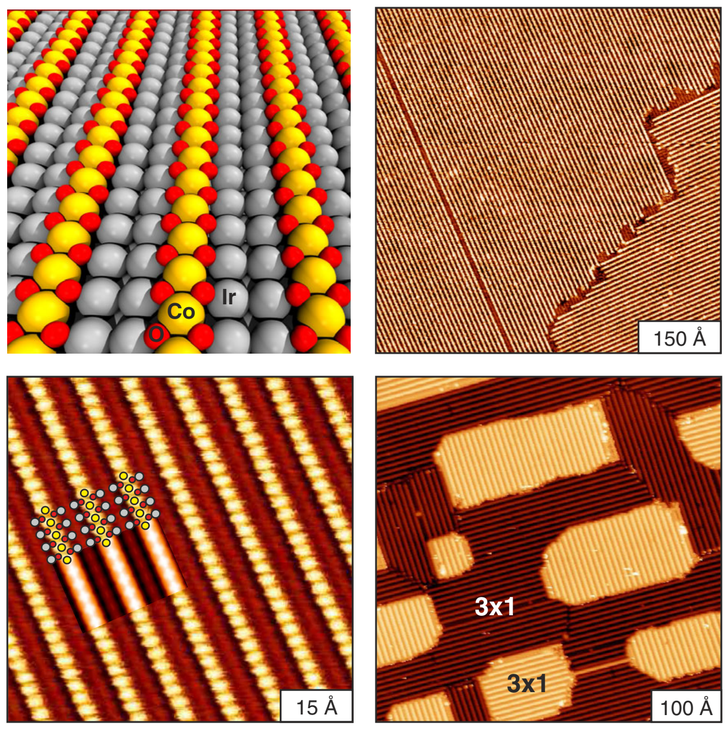

Figure 1: **(a)** Top view of the (3×1) CoO_2 structure. **(b)** Corresponding large scale STM image taken at room temperature [3]. **(c)** Resolved STM image showing monatomic chains in (3×1) periodicity [3]. **(d)** Large scale STM image of a preparation annealed only at 670 K. The (3×1) structure is still homogeneously formed but islands are observed that cover one-third of the surface area

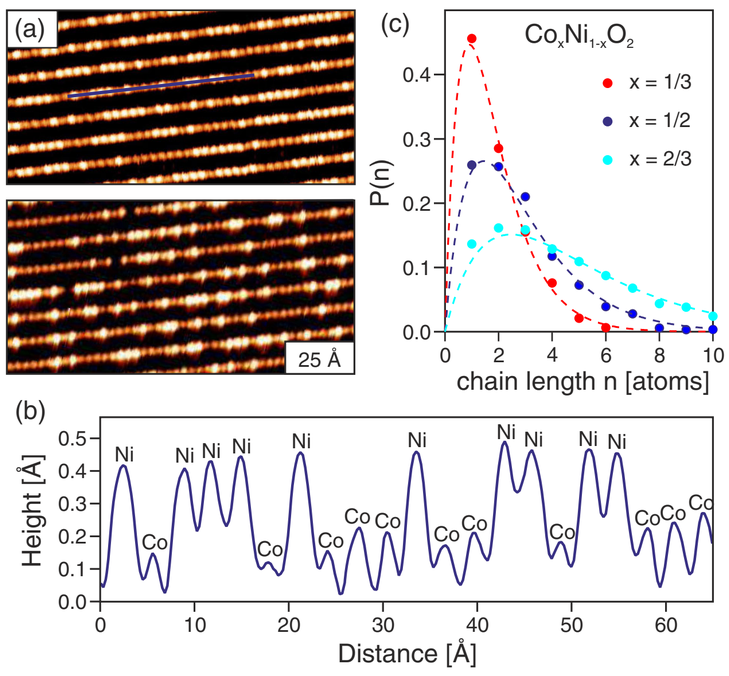

Figure 2: **(a)** Atomically resolved STM image of $Co_{0.5}Ni_{0.5}O_2$ (upper panel) and $Co_{0.67}Ni_{0.33}O_2$ chains (lower panel). **(b)** Line section along the line indicated in (a). The two species are easily identified. **(c)** Analysis of the probability $P(n)$ of an M atom to reside in a chain segment of length n as a function of different M content x of the alloy oxide. The experimental data (symbols) follow closely the expectation (lines) according to a random incorporation of the metal atoms

To simulate the evolution of the system, we apply the two-dimensional kinetic Monte-Carlo (kMC) model, similar to [4]. Elementary stochastic processes in our model were calculated using the Arrhenius equation (1), and prefactors ν_0 for all events are set to 10^{12} Hz.

$$\nu = \nu_0 \exp\left(-\frac{E}{kT}\right), \qquad (1)$$

where E is a diffusion barrier, k is Boltzmann constant and T is temperature of substrate. To avoid unnecessary jumps of temperature, local temperature profile was mirrored along half of the terrace to match the temperature values on terrace boundaries.

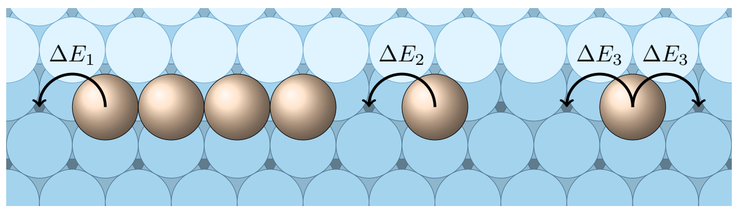

Figure 3: Main diffusion processes

Each numerical experiment consisted of several phases, which could differ by substrate temperature, adatoms deposition parameters, duration and so on. Substrate temperature could remain constant or change exponentially with time

$$T_{\text{exp}}(t) = T_2 - (T_2 - T_1)\exp\left(-\frac{t}{\tau}\right),$$

$$T_{\text{lin}}(t) = T_1 + (T_2 - T_1)\frac{t}{\Delta t},$$

where t is cooling time, T_1 and T_2 are initial and final temperatures, τ is the relaxation time of the cooling process [4] (see Fig. 7). Every unique set of parameters required several thousands of calculations, results of which were averaged and analyzed.

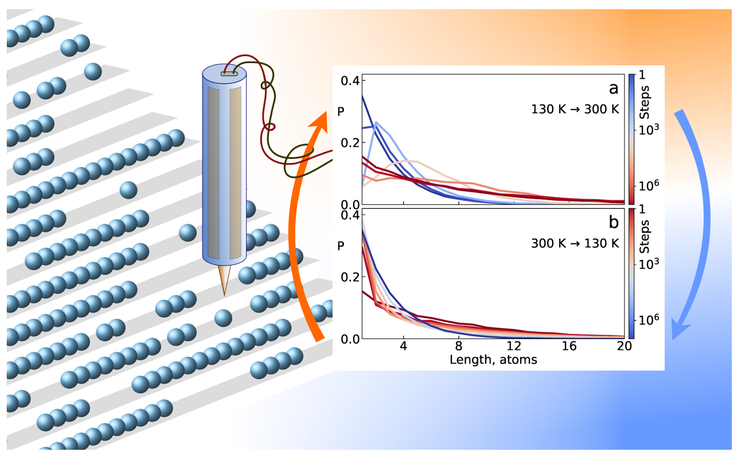

Figure 4: Distributions of chain lengths during **(a)** heating from 130 K to 300 K and **(b)** cooling from 300 K to 130 K with $\tau = 300$ s

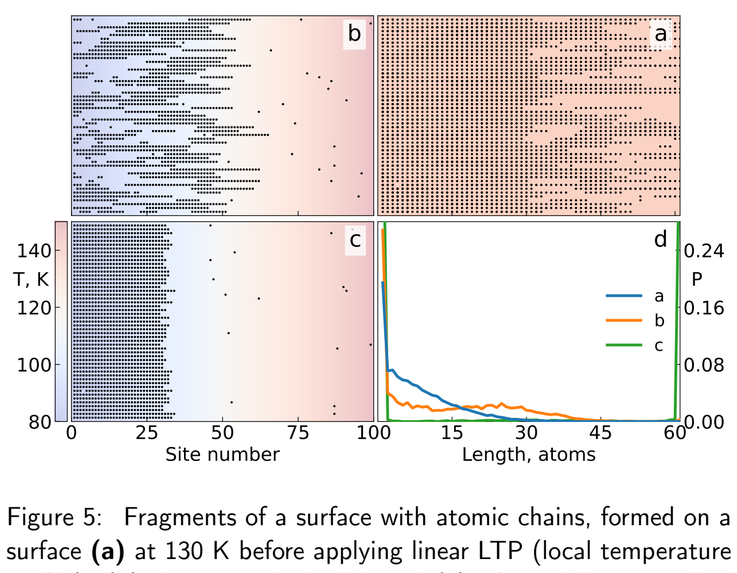

Figure 5: Fragments of a surface with atomic chains, formed on a surface **(a)** at 130 K before applying linear LTP (local temperature profile), **(b)** during applied LTP and **(c)** after LTP was applied (equilibrium state). LTP was changing from 80 K to 150 K. **(d)** Distributions of lengths of atomic chains formed on a surface with a linear LTP applied

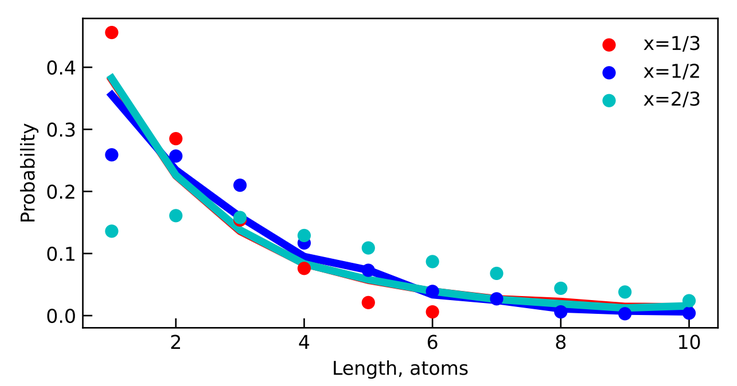

Figure 6: Experimental (dots) and calculated (lines) distributions of lengths of $Co_xNi_{1-x}O_2$ nanowires on Ir(100) surface.

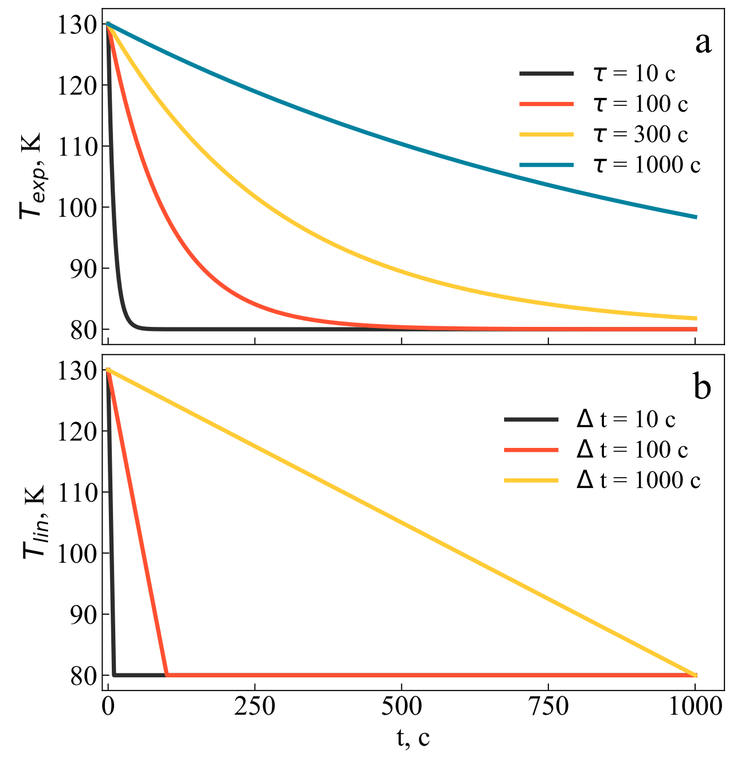

Figure 7: Dependence of temperature on time with different τ

Conclusion

The study of the evolution of atomic chains during heating and cooling by the kinetic Monte Carlo method showed that the transition from one equilibrium state to another during heating and cooling occurs in different ways. It was found that the system quickly reaches thermodynamic equilibrium during the experiment at temperatures above the critical temperature. However, below the critical temperature the system remains in a nonequilibrium state because the mobility of atoms is significantly reduced. In addition, the effect of local temperature prole was investigated. We found that well ordered long chains are formed if there is a temperature gradient of the sample near the critical temperature. Furthermore, we found that alloy oxide chains can also be produced from a mixture of two transition-metal species. Because of the different magnetic properties of the CoNi chains, this opens the possibility of forming complex magnetic structures where ferromagnetic segments are separated by nonmagnetic segments. We are confident that the results of our simulations will be useful in industry for creating atomic wires with a given length.

Acknowledgements

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