Surface reconstructions under external magnetic fields

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Surface reconstruction is a subtle phenomenon where small energy changes can give rise to very different surface structures. In this article we consider the possibility that the reconstruction of a heteroepitaxial system will depend on the presence of external electric or magnetic fields. First, we propose a theoretical framework based on an Ising-like extension of the Frenkel-Kontorova model, which is analysed in detail in 1D using the transfer matrix formalism, determining a complex phase diagram. Many-body spin configurations can be represented as a continuous matrix product state with interesting properties. The feasibility of our model is validated using simple \textit{ab initio} calculations with density functional theory (DFT), which allow us to search actual materials where this complex phenomenon can be obtained in the laboratory.

I. INTRODUCTION

Surface atoms can behave in a very different way from their bulk counterparts [1]. Their reduced coordination number usually manifests itself in a change in the effective lattice parameter, which induces stresses along the surface which can be relaxed through a surface reconstruction, i.e. a full change of symmetry of the surface layer, creating very interesting patterns. Naturally, these reconstructions are also usual in the case of heteroepitaxial systems, where the surface atoms belong to a different species. The differences in energy of the different surface configurations can be quite small, and kinetic effects can mask them in practice, although they are revealed when the system is annealed into their equilibrium configuration.

Predicting the reconstructed form of minimum energy for a homo- or heteroepitaxial system is a complex computational problem, even when the interactions between the film and bulk atoms are known [1, 2]. Standard approaches include \textit{ab initio} calculations, such as density functional theory (DFT). Yet, the large computational cost demanded by large scale DFT simulations suggests to complement them with effective statistical mechanics approaches, such as the Frenkel-Kontorova (FK) model. In its original formulation, the FK model represented the film atoms as point-like masses joined with springs, sitting on a rigid periodic potential energy representing the substrate. When the natural length of the springs and the substrate periodicity differ, the equilibrium configurations can become very rich [3, 4]. Many extensions of the FK model have been proposed, such as allowing for more realistic film potentials, tiny vertical displacements [5] or even quantum behavior of the film atoms [6]. Interestingly, FK can be effectively complemented with small-scale DFT calculations in order to fix the form of the interaction, resulting in accurate predictions both for the equilibrium and the kinetic effects [2, 7].

In this work we explore the possibility of obtaining different surface reconstructions when external fields, either electric or magnetic, are applied. Even if the energetic differences are tiny, external fields can change notably the electronic configuration, effectively preventing certain bonds or enhancing others, thus giving rise to subtle changes in the surface lattice parameters. Indeed, both bulk magnetoelastic lattice distortions [8, 9] and spin-phonon interactions [10, 11] have attracted considerable interest. Moreover, examples of magnetization mediated surface reconstructions have been reported [12, 13], and the complementary concept of magnetic reconstruction, where the surface spins present a different symmetry from the bulk, has also been discussed in the literature [14–17].

We will propose a theoretical framework, which we term \textit{Ising-Frenkel-Kontorova} (IFK) model, an extension of the FK model where the film atoms possess an Ising-like spin, that can point either up or down. When two neighboring film atoms have the same spin, their interaction is different from the case in which they have opposite spins. An external magnetic field, then, can polarize the spins, forcing them to adopt a parallel spin configuration and, therefore, to change their equilibrium configuration. We have characterized the phase diagram of the IFK model in 1D at finite temperature, using the transfer operator formalism. The results of the statistical mechanics approach are then validated using simple \textit{ab initio} calculations of a chain of hydrogen atoms, showing that the results qualitatively agree.

This article is organized as follows. In Sec. II we describe the Ising-Frenkel-Kontorova model in detail, along with numerical results about the phase diagram. The \textit{ab initio} calculations are carried out in Sec. III. The article ends with a presentation of our conclusions and our proposals for further work.

II. THE ISING-FRENKEL-KONTOROVA MODEL

Let us consider a simple extension of the Frenkel-Kontorova model, that we have termed \textit{Ising-Frenkel-Kontorova} (IFK), which consists of adding an Ising spin variable, $+$ or $-$, to each film atom, representing its spin polarization along a certain \textit{easy axis}. We will only con-
Consider coherent films, where the number of film and substrate atoms are the same, and each film atom is always in correspondence with a substrate atom. Let \( r_i \) be the position of the \( i \)-th atom, and \( s_i \) be its spin polarization. The total Hamiltonian of the model for \( N - 1 \) atoms is:

\[
\mathcal{H} = \sum_{i=1}^{N-1} \left( V_s(r_i) + V_f(|r_i - r_{i+1}|, s_i s_{i+1}) - H s_i \right),
\]

where \( V_s(r_i) \) stands for the (periodic) substrate potential felt by each film atom, while \( V_f(d, s_i s_{i+1}) \) represents the atom-atom film interaction, which depends on their distance and their relative polarization: if the two spins are parallel, the interaction potential is \( V_f(d, +1) \), and if they are anti-parallel, it is \( V_f(d, -1) \). Moreover, \( H \) represents the external magnetic field along the chosen axis. Minimizing that Hamiltonian we obtain a semi-classical configuration: positions plus spin polarization of all atoms.

Notice that neighboring atoms can interact through two different potential energy functions: a ferro potential, \( V_F(d) = V_f(d, +1) \) or an anti-ferro one, \( V_{AF}(d) = V_f(d, -1) \). These two potentials can have different equilibrium distances, \( V_{0, AF}, a_F \) and \( a_{AF} \). Indeed, in some cases one of them (typically, the ferro potential) may not present a minimum at any distance. This will not constitute a problem in our approach.

Let us particularize for the case shown in Fig. 1, where we can see that \( V_F(d) \) does not present a minimum, while \( V_{AF}(d) \) does, and let us assume that \( a_{AF} \neq a_s \) (the lattice parameter of the substrate). Let us also assume that the lowest energy of the ferro potential exceeds the value for the anti-ferro case, as it is usually the case. In absence of an external field, there will be a misfit between the substrate and the film lattice parameters and, if the amplitude of the substrate potential is small enough, the film atoms will reconstruct. Yet, when an external magnetic field is applied, at a certain moment the ferromagnetic configuration will be preferred energetically. Then, the advantage of reconstruction is lost, and, if the film remains coherent it will wet the substrate, i.e. it will copy its structure.

We will choose the following expression for the three potential energy interactions:

\[
\begin{align*}
V_s(x) &= V_{s,0} \cos(2\pi x/a_s), \\
V_{AF}(d) &= V_{AF,0} (1 - \exp(-b_{AF}(d - a_{AF})))^2 - V_{AF,0}, \\
V_F(d) &= V_{F,0} \exp(-b_F d),
\end{align*}
\]

i.e. a sinusoidal form for the substrate potential, a Morse form for the AF film potential and an exponential decay for the F film potential, see Fig. 1 for an illustration.

A. Transfer operator approach

The physical properties of the system described by Hamiltonian Eq. (1) in equilibrium at temperature \( T = \beta^{-1} \) are determined by the partition function:

\[
Z = \sum_{\{r_i, s_i\}} \exp \left[ -\beta \mathcal{H}(\{r_i, s_i\}) \right].
\]

Since the system is one-dimensional, we can write this partition function as a trace over a product of transfer matrices. It is convenient to introduce new notation to simplify our expressions. Let \( x_i = \{r_i, s_i\} \) denote the multi-index which combines the position and the spin of the \( i \)-th atom. Then, the IFK Hamiltonian, Eq. (1) can be written as a sum of a one-body and a two-body terms

\[
\mathcal{H} = \sum_{i=1}^{N} \left( \mathcal{H}^{(1)}(x_i) + \mathcal{H}^{(2)}(x_i, x_{i+1}) \right),
\]

with \( \mathcal{H}^{(1)}(x_i) = V_s(r_i) - h s_i \) and \( \mathcal{H}^{(2)}(x_i, x_{i+1}) = V_f(|r_i - r_{i+1}|, s_i s_{i+1}) \). Let us consider \( x_i \) to be restricted to take only a value from a finite set with \( \ell \) elements. Then, we can define

\[
\begin{align*}
V_{x_i} &= \exp(-\beta \mathcal{H}^{(1)}(x_i)), \\
T_{x_i, x_{i+1}} &= \exp(-\beta \mathcal{H}^{(2)}(x_i, x_{i+1})), \\
M_{x_i, x_{i+1}} &= T_{x_i, x_{i+1}} V_{x_{i+1}},
\end{align*}
\]

leaving the dependence on the parameters (\( \beta, H \)) implied. Now, \( V \) is a vector with \( \ell \) components, \( T \) and \( M \) are matrices with dimension \( \ell \times \ell \). We can write now:
\[ Z = \sum_{\{x_i\}} V_{x_1} T_{x_1,x_2} V_{x_2} T_{x_2,x_3} V_{x_3} \cdots T_{x_{N-1},x_N} V_{x_N} \]
\[ = \sum_{\{x_i\}} V_{x_1} M_{x_1,x_2} M_{x_2,x_3} \cdots M_{x_{N-1},x_N} \]
\[ = \sum_{x_1,x_N} V_{x_1} (M)^{N-1}_{x_1,x_N} \]
\[ = V^T (M)^{N-1} S, \quad (6) \]

where \( S = (1, \ldots, 1)^T \). In the last two lines we have assumed that all \( M \) matrices are equal, which need not be the case. Notice that the evaluation of expression \( 0 \) for the partition function can be performed more accurately by diagonalizing matrix \( M \), and noticing that the highest eigenvalues are the most relevant for large sizes calculations.

If the system presents periodic boundaries, we have \( x_1 = x_N \) (with only \( N - 1 \) particles) and we obtain
\[ Z = \text{Tr} \left( V \odot M^{N-1} \right), \quad (7) \]

where \( \odot \) stands for the row Hadamard product (not the usual vector-matrix product).

Expectation values are obtained by inserting appropriate operators in the matrix product. Let us consider \( \ell \) component vectors \( R_{x_i} \) and \( S_{x_i} \), which measure the expectation value of the position and spin of the \( i \)-th atom: \( R_{x_i} = r_i, S_{x_i} = s_i \). Then,
\[ \langle r_i \rangle = \frac{1}{Z} \sum_{\{x_i\}} V_{x_1} M_{x_1,x_2} \cdots R_{x_i} M_{x_i,x_{i+1}} \cdots M_{x_{N-1},x_N} \]
\[ \langle s_i \rangle = \frac{1}{Z} \sum_{\{x_i\}} V_{x_1} M_{x_1,x_2} \cdots S_{x_i} M_{x_i,x_{i+1}} \cdots M_{x_{N-1},x_N}, \quad (8) \]

Two-point correlators are found in a similar way, inserting two operators, e. g. \( R_{x_i} S_{x_j} \).

### B. Numerical Results

The formalism presented in the previous section can be extended easily to continuous values of \( r_i \). Yet, for practical calculations, it is convenient to consider a suitable discretization. A straightforward strategy would be to consider a length \( L \) sufficiently large to hold the full chain of atoms, and to discretize it in small values \( \Delta x \), studying the limit \( \Delta x \to 0 \). Taking spin into account, this would give a matrix size \( \ell = 2L/\Delta x \). In practice, this leads to working with large matrices.

In this work we will only consider coherent films, with the same density as the substrate, and with only one film atom per unit cell. Thus, each \( r_i \in [0,a] \), with \( i = 1, \ldots, \ell \), and the discretization step need only be taken as \( \Delta x = a/\ell \). Thus, the dimensions of the matrices will always be \( 2\ell \times 2\ell \).

As substrate and film potentials we have chosen those in expressions \( 2 \), with the following parameters: \( a_s = 1 \) Å, \( V_{s,0} = 2 \) eV, \( V_{F,0} = 4 \) eV, \( b_F = 2 \) Å\(^{-1} \), \( V_{AF,0} = 5 \) eV, \( b_{AF} = 6 \) Å\(^{-1} \), \( a_{AF} = 0.6 \) Å. We have computed exactly the partition function for an open chain with \( N = 20 \) atoms, obtaining the expected value of the total magnetization through
\[ m = -\frac{1}{\beta} \frac{\partial \log Z}{\partial H}. \quad (9) \]

The expected position and magnetization of all atoms can also be calculated, using Eq. \( 5 \).

Fig. 2 shows two configurations for the atoms at low temperature, \( T = 0.2 \), and \( H = 0 \) and \( H = 5 \). We can see that, for \( H = 0 \) the system dimerizes, i.e. presents an elementary reconstruction, doubling its unit cell.

The total magnetization curve, \( m(H) \), is shown in Fig. 3 for several temperatures, \( T = 0.2, T = 1 \) and \( T = 10 \). We can see that, for high temperatures, the system is completely paramagnetic, with a nearly constant magnetic susceptibility. For low temperatures, \( T = 0.2 \), we see a sharp increase in the magnetization for finite values of \( H_c \approx \pm 2 \), which would correspond to a transition paramagnetic-ferromagnetic. The curve is still very round because the number of particles is still very low, \( N = 20 \). The critical temperature must be in the range from \( T = 1 \) to \( T = 0.2 \).

Yet, the atomic and spin configurations for low temperatures can be rather complex, as we can see in Fig. 4. The top panel of this figure shows the average magnetization of each atom, using expressions \( 4 \) for different values of the external magnetic field, \( H \). For \( H \sim 0 \), the average magnetization is close to zero, increasing in amplitude near the borders, but keeping an approximate anti-ferromagnetic pattern. The outer spins, nonetheless, are parallel to the external magnetic field, thus explaining the increase in the average magnetization, but holding a frustrated structure in the interior, because the number of atoms is even. The magnetization pattern, as we can see, is complex for intermediate values of the magnetic field, becoming fully ferromagnetic only for very large values of \( H \).
of the chain, due to the fact that the rightmost extreme prefers to be polarized along the direction of the external field. For $H \sim 2$, the whole pattern attenuates substantially, and for large magnetic fields we can see that the film wets the substrate, copying its structure.

C. Matrix Product States from the IFK Model

According to Eq. (9), the probability for any spin configuration can be written in the following way:

$$P(s_1, \cdots, s_N) = \sum_{\{r_i\}} A^{s_1}_{r_1} B^{s_1,s_2}_{r_1,r_2} A^{s_2}_{r_2} B^{s_2,s_3}_{r_2,r_3} \cdots A^{s_N}_{r_N}. \quad (10)$$

We can interpret Eq. (10) as a variant of a matrix product state [20], with two differences: (1) we alternate matrices which depend on a single spin value, and matrices that depend on the product of two consecutive spin values; (2) the bond dimension is represented by a continuous variable. The first difference is not rather relevant, but the second deserves further study. Physically, the bond dimension of a MPS represents the information that we need to keep from the visited part of the chain in order to determine the probability for the unvisited part. Thus, in our case this information is represented by a continuous variable, allowing for a richer behavior.

III. AB INITIO CALCULATIONS

In this section we show proof-of-principle ab initio calculations performed with DFT, showing that the general mechanism provided in this article can work in real materials. We have chosen the simplest atom and have built a chain of $N = 8$, hydrogen atoms with periodic boundary conditions, fixing the total length, $L = a_x N$, where $a_x$ is assumed to be the substrate lattice parameter. Crucially, the total spin of the chain is fixed to three values: zero magnetization, maximum magnetization and half magnetization, which corresponds to a total spin of $S_z = 0$, $2h$ and $4h$. This way, we are able to characterize the behavior of the interaction in absence of external magnetic field (zero magn.), for a moderate magnetic field (half magn.) and for a strong magnetic field (full magn.). The substrate potential is absent from our calculations, except through the imposed substrate lattice parameter.

Electronic calculations were performed using code SIESTA [21]. The exchange and correlation potential was described using the Perdew, Burke, and Ernzerhof (PBE) functional [22]. This functional was already used in previous works on H$_2$ adsorption on single and double aluminium clusters doped with vanadium or rhodium [23][24]. The core interactions were accounted for by means of norm conserving scalar relativistic pseudopotentials [25] in their fully nonlocal form [26], generated from the atomic valence configuration 1s$^2$ for H. The core

Figure 3. Magnetization curves $m(H)$ for the IFK model using the parameters discussed in the text, for several temperatures, $T = 0.2$, $T = 1$ and $T = 10$.

Figure 4. Top: average magnetization of each atom in the open chain with $N = 20$, for $T = 0.2$ and different values of the magnetic field. Bottom: average position within the unit cell of the substrate of the film atoms, for the same values of the magnetic field.

The bottom panel of Fig. 4 shows the position of each atom within the unit cell of the substrate, with $x = 0.5$ denoting its center, always assuming $T = 0.2$ and the same values of the external magnetic field. For $H \sim 0$, we see the alternating pattern corresponding to the dimerized reconstruction that we could see in Fig. 2. The alternating pattern attenuates near the center as the magnetic field increases, and for $H \sim 1.5$ we can observe a change of the deformation phase in the right extreme of the chain.
radii for the s orbital of H is 1.25 Å. For the calculated H₂ molecule we obtain a binding energy $E_b = 4.29$ eV, and a bond-length $d = 0.79$ Å, compared to the measured values of 4.48 eV and 0.74 Å.

The matrix elements of the self-consistent potential were evaluated by integrating in an uniform grid. The grid fineness is controlled by the energy cutoff of the plane waves that can be represented in it without aliasing (150 Ry in this work).

Flexible lineal combinations of numerical pseudo-atomic orbitals (PAO) are used as the basis set, allowing for multiple-ζ and polarization orbitals. To limit the range of PAOs, they were slightly excited by a common energy shift (0.005 Ry in this work) and truncated at the resulting radial node, leading to a maximum cutoff radii of 6.05 au (s) for H. The H chain structure remains fixed during the calculations, while the electronic part is relaxed.

We have made two numerical experiments on a chain of 8 atoms of H in a line. In the first one, we computed the total energy of the chain as a function of the substrate lattice spacing, assuming that the film chain copies the substrate, for zero, half and full magnetization. The results are represented in the top panel of Fig. 5. There we observe a behavior similar to the one shown in our illustration figure for the film potentials, Fig. 1. Indeed, we can see that, in the absence of an external magnetic field the system will choose the zero magnetization configuration, and the energy presents a minimum around a value $a_s = 1$ Å. As the magnetic field increases, the magnetic contribution to the total energy will eventually favor the upper curves, corresponding to higher total spin.

For the next numerical experiment, we have assumed that $a_s = 1.2$ Å and imposed a dimerization on the atom positions, according to the rule:

$$r_n = n a_s + (-1)^n \delta. \quad (11)$$

By varying the dimerization parameter $\delta$ we get the results shown in the bottom panel of Fig. 5 with the energies displaced vertically for better comparison. As we can see, in the case of zero magnetization, the energy presents a minimum at a dimerization parameter $\delta \approx 0.21$ Å, thus confirming our conjecture: the film will reconstruct in this case, if the substrate potential is not too strong. On the other hand, for the half and full magnetization schemes, we can see that the energy tends to a minimum for zero dimerization, showing that, at least, this reconstruction scheme does not reduce the total energy. Thus, we are allowed to conjecture, based on the presented data, that the present system will show different structures for zero and for high magnetic field.

Of course, these calculations are only a proof-of-principle, using the simplest atoms and the simplest possible geometries. Further calculations, using more realistic materials, are still needed in order to make experimental proposals to observe the predicted reconstruction effects.

**IV. CONCLUSIONS AND FURTHER WORK**

We have put forward the following question: can surfaces reconstruct differently in presence of external magnetic (or perhaps electric) fields? After our calculations, we can conjecture that this can indeed be the case. We have performed illustrative ab initio calculations using DFT, showing that this possibility exists even for the simplest atom, hydrogen.

Furthermore, we have proposed a statistical mechanical model, which is an Ising-like extension of the Frenkel-Kontorova model, that we have termed Ising-Frenkel-Kontorova (IFK), in which film atoms interact differently when their spin variables are the same or opposite. We have extracted physical consequences in the 1D case, using reasonable forms for the film potentials and a mere sinusoidal form for the interaction with the substrate, showing a rich behavior with a likely phase transition at a finite value of the temperature.
Our idea bears some similarity colossal magnetoresistance (CMR), where a metallic ferro configuration coexists with an insulating antiferro one, due to quench disorder. An external magnetic field will favor the ferro configuration, thus allowing to reach the percolation threshold and decreasing the resistance dramatically.

It is likely that, as we increase the magnetic field, the antiferromagnetic configuration will not become directly unstable, but metastable. In other terms: the transition may be of first order. This implies that, as one cycles over a range of magnetic fields, we will obtain a hysteresis cycle.

Moreover, considering the different energy scales associated to the motion of spins and nuclei, the Born-Oppenheimer approximation might be employed to integrate out the spatial degrees of freedom and to find an effective Ising model for the spins, very probably presenting effective long-range interactions. The reason for this conjecture is simple: entropic reasons prevent Ising-like models from developing a phase transition in 1D. Thus, long-range effective interactions are the only way to solve this apparent paradox. The matrix product state (MPS) representation of the state, described in the text, can be used as a starting point in order to characterize this effective spin interaction.

Throughout the article we have used magnetic field to force the change in reconstruction. In principle, electric fields can also be used, in the case of film atoms or molecules with a permanent electric dipole.

In order to proceed with this line of research, there are two complementary routes: (a) develop further the statistical mechanics of the IFK, in 1D and 2D; (b) choose more suitable materials, combining DFT and statistical mechanics tools in order to select those which will present a critical magnetic field within the experimental range. After these materials have been chosen and characterized, the next natural step would be to make a concrete experimental proposal.

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