Molecular Dynamics and Monte-Carlo simulations: study CoPt system

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Part I

1. Introduction

The CoPt System

2. TB-SMA Model

3. Monte-Carlo simulations (SMA)

4. Molecular Dynamics simulations

Part II

MC–Ising in thin films

Conclusion & Outlook

1. Introduction

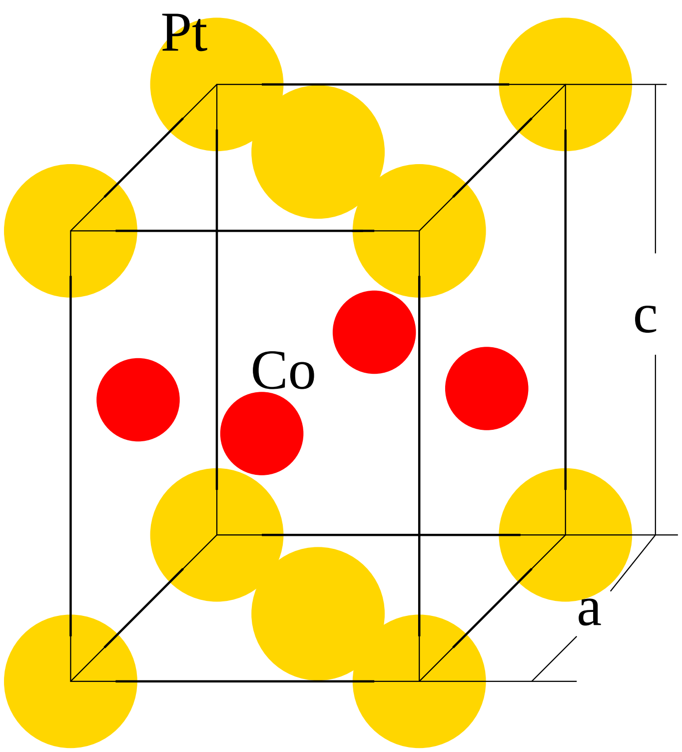
The CoPt system

- equiatomic CoPt:

• A_1 (c.f.c) disordered phase.

• $L1_0$ ordered phase $(a \neq c)$

⋆ shows a high magnetic anisotropy along the growth direction $\Longrightarrow$ magneto-optic recording interest



⋆ alloys of CoPt have a good corrosion resistance and High coercitive force.

2. TB-SMA Model

(Tight Binding - Second Moment Approximation)

$\longrightarrow$The energy of atom at site i:

$$E_i = E_i^b + E_i^r$$

$\imath$) E_i^b, the band term, is obtained by integrating the local density of states up to the Fermi level:

$$E_i^b = -\sqrt{\sum_{j, r_{ij} < r_c} \xi_{IJ}^2 \ \ exp(-2q_{IJ}(\frac{r_{ij}}{r_0^{IJ}} - 1))} \qquad (1)$$

$\imath\imath$) The repulsive term E_i^r is described by the sum of Born-Mayer ion-ion repulsive interactions:

$$E_i^r = \sum_{j, r_{ij} < r_c} A_{IJ} \ \ exp((-p_{IJ}(\frac{r_{ij}}{r_0^{IJ}} - 1))) \qquad (2)$$

r_{ij}: distance between atoms at sites i and j

ξ_{ij} effective hopping integral

{I,J}: Indexes for species {Co, Pt}

r_0^{II}: first-neighbor distance in metal I

r_0^{IJ}=(r_0^{II}+r_0^{JJ})/2

r_c cut off radius.

- (ξ_{IJ}, A_{IJ}, p_{IJ}, q_{IJ}) parameters of model.

$\longrightarrow$ Co-Co and Pt-Pt int. parameters: (ξ_{II},A_{II},p_{II},q_{II}) are determined by fitting the cohesive energy, lattice parameter and bulk modulus to the experimental values.

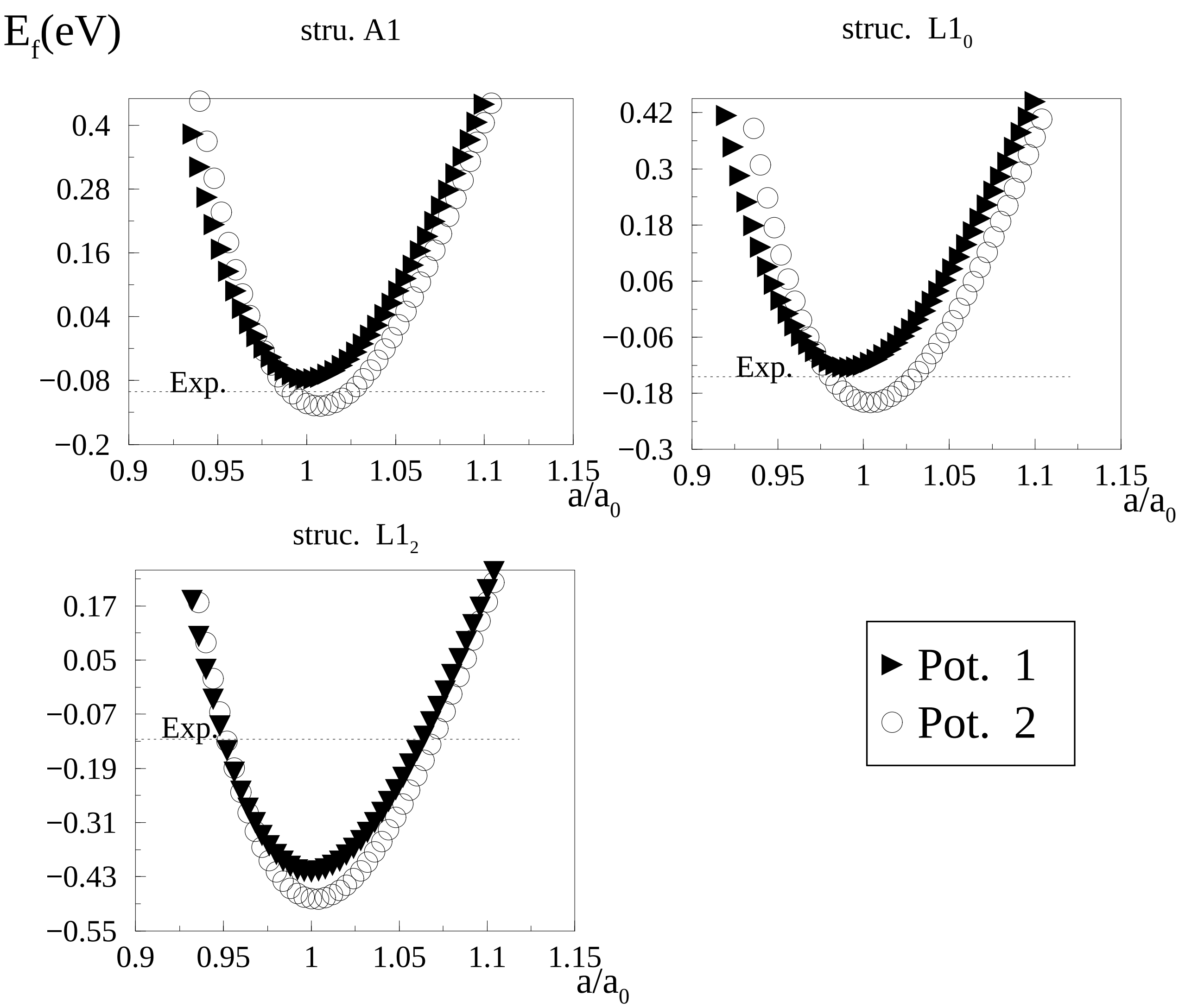
$\longrightarrow$ Co-Pt int. parameters:
Two ways to obtain the (ξ_{IJ},A_{IJ},p_{IJ},q_{IJ}):

$\imath$) fitting the formation energies of the $L1_0$ and A_1 of CoPt alloys, (**Pot. 1**) (our work).

$\imath\imath$) fitting the experimental heats of dissolution of a Pt impurity in Co (and Co in Pt), (**Pot. 2**), C. Goyhenex, *et al.* Phys. Rev. **B 60** (1999) 2781.

2.1 Formation and dissolution energies

Formation energies of $L1_0$, $L1_2$ and A_1 structures



E (eV)	Pot.2	Pot.1	Exp
E_{fL10}	-0.2	-0.145	-0.145
$a/a_0(L1_0)$	1.002	0.999	
E_{A1}	-0.125	-0.076	-0.10
$a/a_0(A_1)$	1.007	1	
E_{fL12}	-0.47	-0.41	-0.12
$a/a_0(L1_2)$	1	1.001	
E_{sol}(Co in Pt)	-0.47	-0.55	-0.47
E_{sol}(Pt in Co)	-0.64	-0.33	-0.64

Formation energies and solution energies in CoPt

$\longrightarrow$The new parameters give a good description of formation energy in $L1_0$ structure which is the system we are interested in further growth studies.

	Par.	SMA		
Interaction	A (eV)	$\xi(eV)$	p	q
Pt-Pt	0.242	2,506	11.14	3.68
Co-Co	0,189	1,907	8.8	2.96
Pt-Co Pot.1	0.245	2.386	9.97	3.32
Pt-Co Pot.2	0.20039	2.1998	8.4092	2.7886

Parameters of inter-atomic interactions in SMA.

3. Monte-Carlo simulations–SMA

- The model being based on vacancy-atom jump mechanism
- Glauber-type of atomic jumps

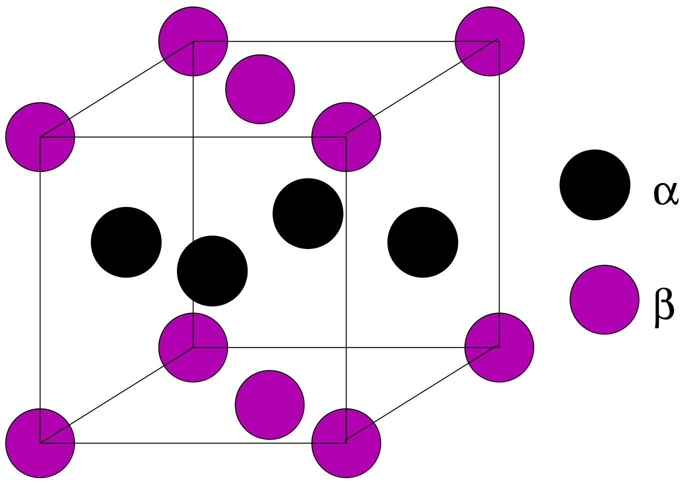
$$P(A \leftrightarrow Pt \ or \ Co) = \frac{exp(-\Delta E/k_B T)}{1 + exp(-\Delta E/k_B T)} exp(\epsilon_A/k_B T),$$

- $\epsilon_A = 0$ (No saddle point energies).
- The energy balance $\triangle$E of atom-vacancy exchange is evaluated using TB-SMA.

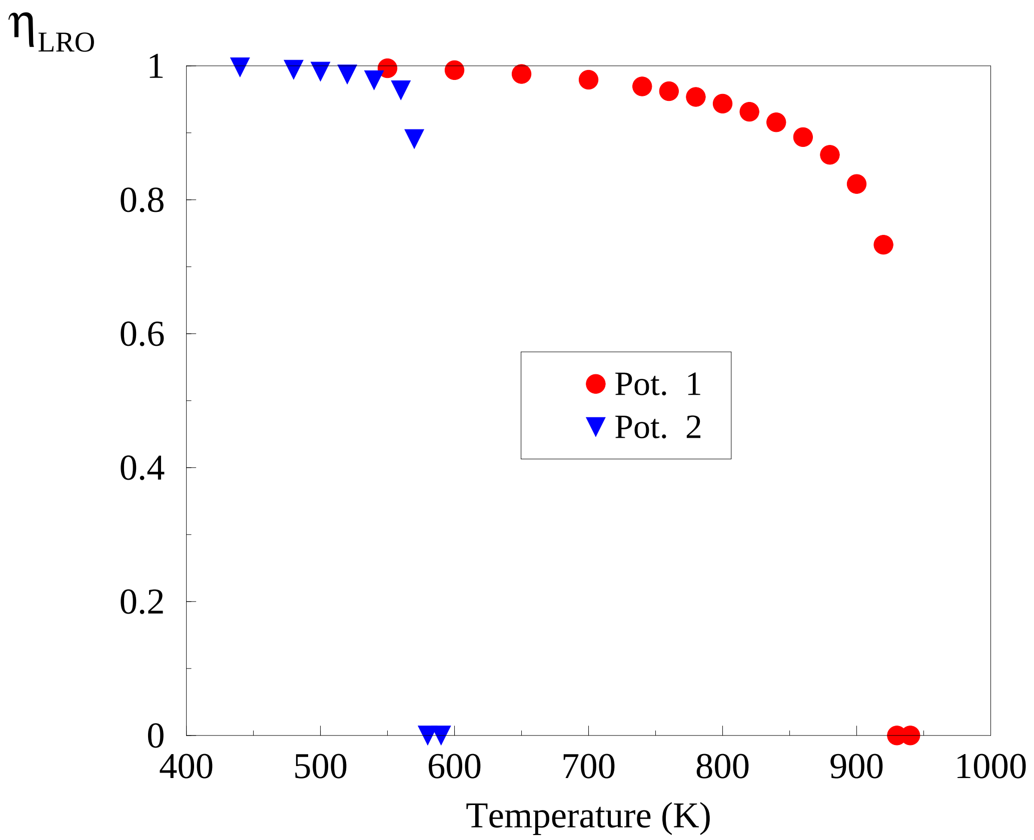
- Simulation box of 32×32×32 with periodic boudary conditions

- LRO parameter:

$$\eta = 2\frac{N_A^{\alpha} - N_A^{\beta}}{N}$$



• M.C. simulation of the equilibrium long-range order parameter: evolution with temperature.



	Pot. 2	Pot. 1	Experimental value
T_C	580 K	930 K	1110 K

$\longrightarrow$ The Pot.1 gives a good description of the order-disorder ($L1_0 \Rightarrow A1$) transition temperature in CoPt system.

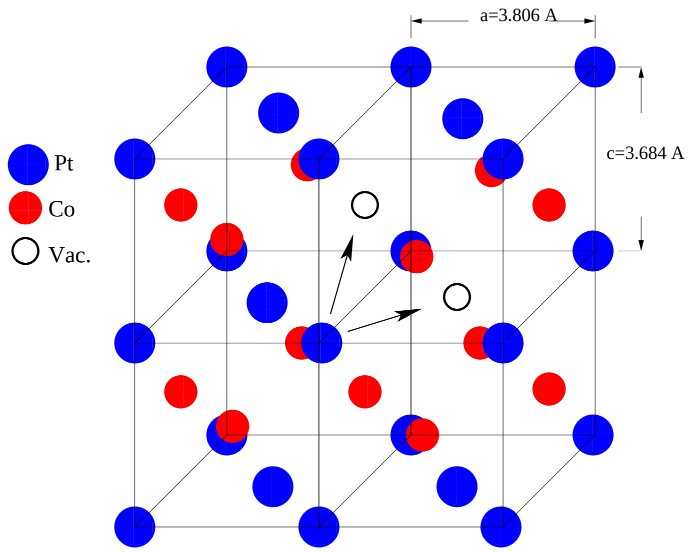
4. TB-QMD-SMA

(Tight Binding Quenched Molecular Dynamics Second Moment Approximation)

→Force acting on the atom at site i:

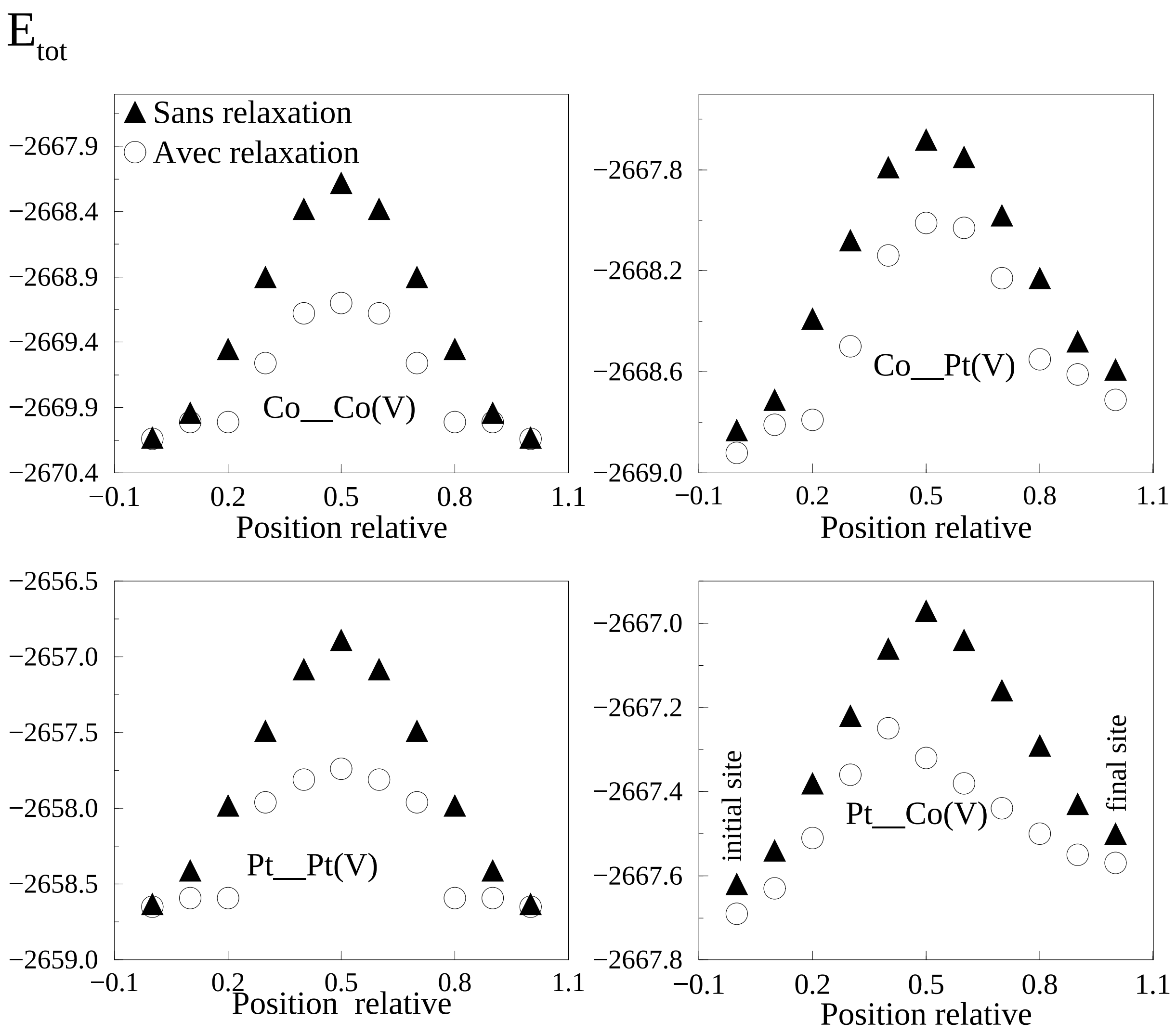
→ $\mathrm{F}_i^\alpha = -\frac{dE_{tot}}{dr_i^\alpha}$

with $E_{tot} = \sum_i E_i^b + E_i^r$



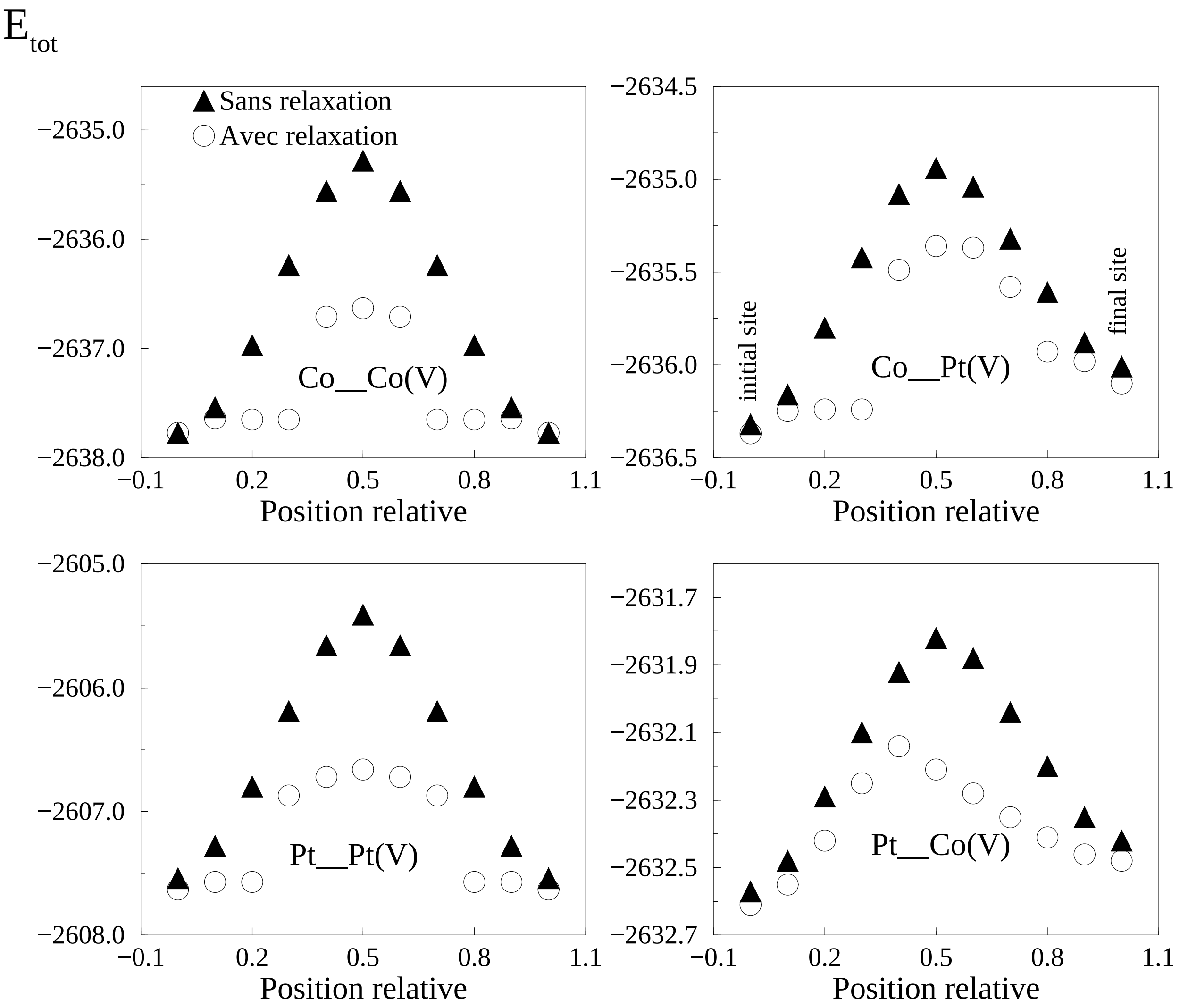
→ The various superstructures are optimized via the relaxation algorithm.

4.1.a Saddle point energies with Pot.1



⟶Without relaxation, the saddle point energies are larger.

4.1.b Saddle point energies with Pot. 2



Par. Set 1 Atom jump	Without relaxation	E_f-E_i	With relaxation	E_f-E_i
Co⟶Co(V)	1.74 eV	0 eV	1.04 eV	0 eV
Co⟶Pt(V)	1.15 eV	0.245 eV	0.80 eV	0.10eV
Pt⟶Co(V)	1.735 eV	0 eV	0.91 eV	0 eV
Pt⟶Pt(V)	0.58 eV	0.12 eV	0.30 eV	0.15 eV

Saddle point energies with Pot. 1

Par. Set 2 Atom jump	Without relaxation	E_f-E_i	With relaxation	E_f-E_i
Co⟶Co(V)	2.48 eV	0 eV	1.47 eV	0 eV
Co⟶Pt(V)	1.539 eV	0.318 eV	0.87 eV	0.27eV
Pt⟶Co(V)	2.12 eV	0 eV	0.97 eV	0 eV
Pt⟶Pt(V)	0.66 eV	0.144 eV	0.33 eV	0.13 eV

Saddle point energies with Pot. 2

⟶The Pot. 2 yield greater saddle point energies.

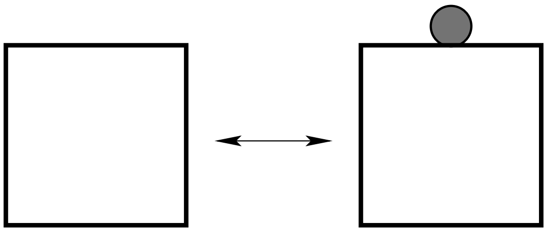
4.2 Adsorption energies of Co and Pt on CoPt(001)

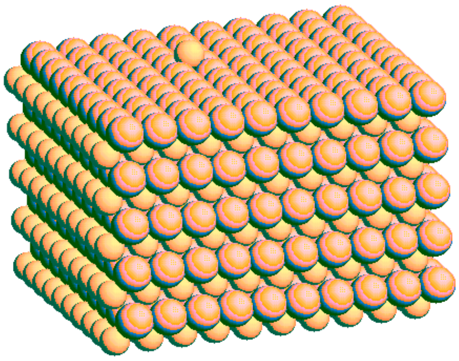
$$\mathrm{E}_{ads}A^{B} = \mathrm{E}_{tot}\ (\mathrm{A} + \mathrm{B}\ ) - \mathrm{E}_{tot}(\mathrm{A})$$

Where:

B atom deposited on A

A Matrix (alloy CoPt)





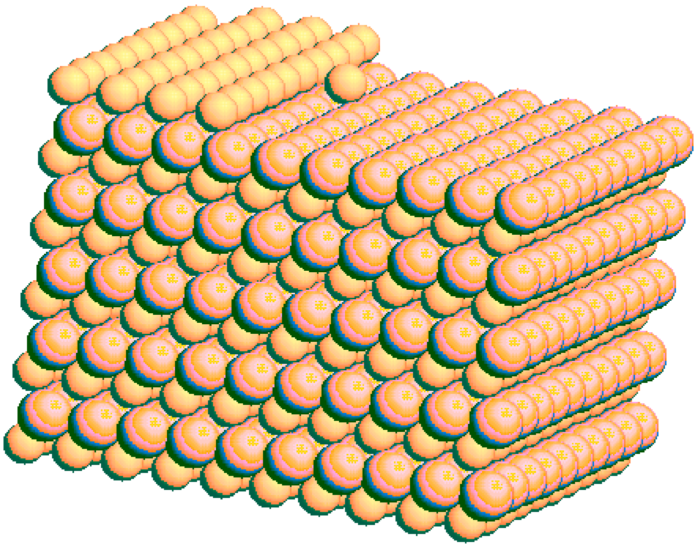
Atom deposited on CoPt(100) alloy.

$\mathrm{E}_{abs}(\mathrm{Pt})$	$\mathrm{E}_{abs}(\mathrm{Co})$
-4.9951 eV/at	-4.4649 eV/at

4.3 Energies of a stair of Co, Pt deposited on CoPt(001)

$$E_{ads}A^{\theta} = \frac{E_{tot}(A+\theta) - E_{tot}(A)}{\theta}$$

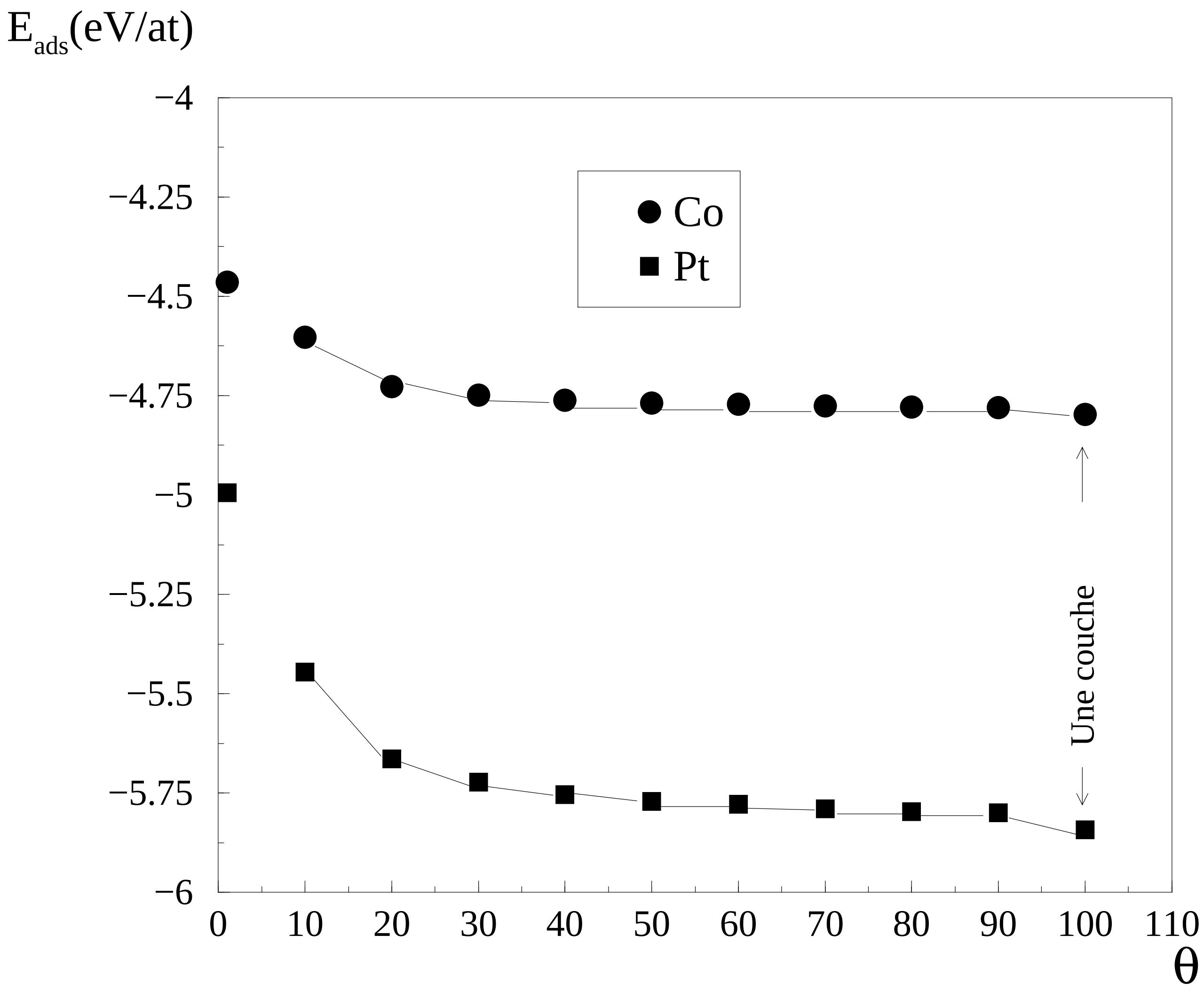
Where: $\theta =$ N$_{Pt\ or\ Co}$ atom deposited on A



Stair of Co atoms on L$1_0 CoPt$(001).

Stair dimension	for Co	for Pt
$\theta = 10$	-4.6024	-5.4456
$\theta = 20$	-4.7266	-5.6633
$\theta = 30$	-4.7489	-5.7232
$\theta = 40$	-4.7610	-5.7535
$\theta = 50$	-4.8281	-5.7713
$\theta = 60$	-4.7720	-5.7820
$\theta = 70$	-4.7760	-5.790
$\theta = 80$	-4.7780	-5.7965
$\theta = 90$	-4.7800	-5.800
layer	-4.7970	-5.842

Adsorption energies E_{ads}(eV/at.) of different stairs deposited on CoPt(001) alloy.



E_{ads} dependence with stair dimension.

$E^{Pt}_{ads} > E^{Co}_{ads}$

$E_{ads} \searrow \longrightarrow$ width of stair $\Rightarrow$ the largers staires are stable.

Part II
MC-Ising in thin films

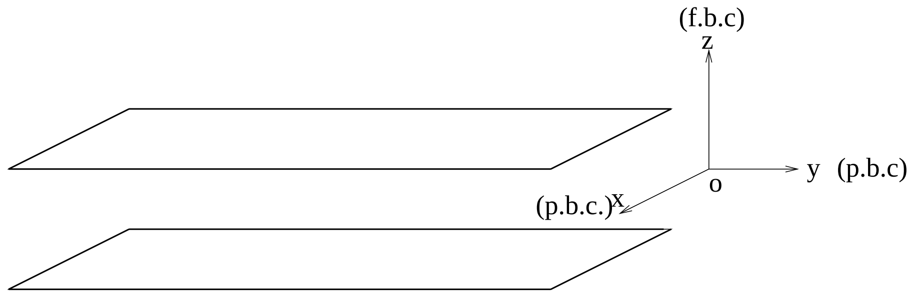
• Previous work on $L1_0$ bulck (Kerrache *et al.*) Comput. Mater. Sc. 17 (2000)
• present work on $L1_0$ thin films with 64×64 cells on (xoy) and oz variable

• Vacancy-atom jump mechanism
• Glauber-type probability.

• Saddle point energies $\epsilon_A = \epsilon_B = 0$.

• The energy balance is evaluated using an Ising Hamiltonien.

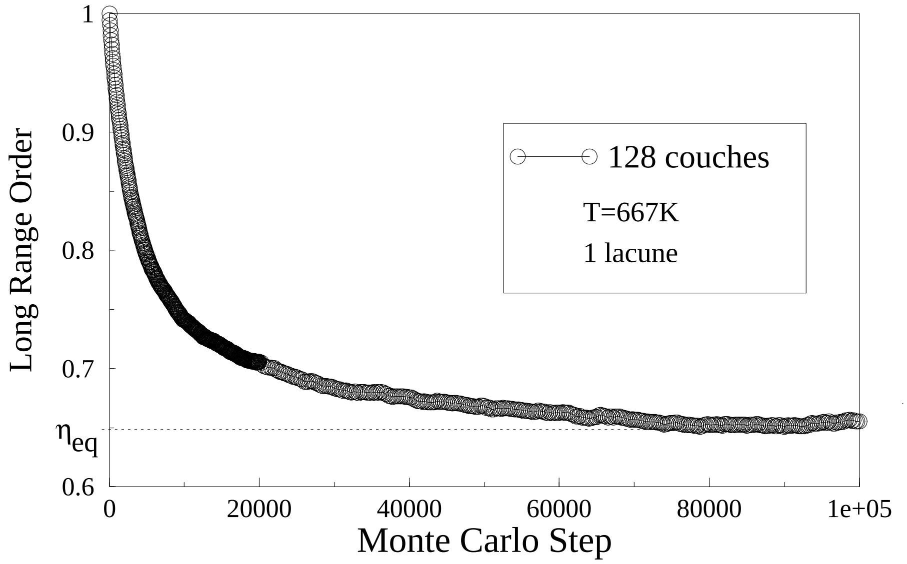
• Interactions up to 2nd nearest neighbour atoms

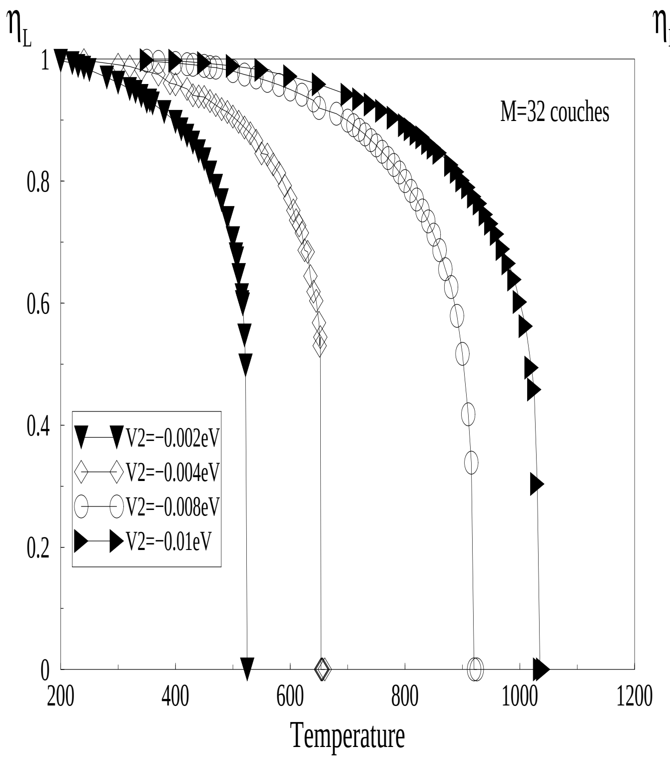


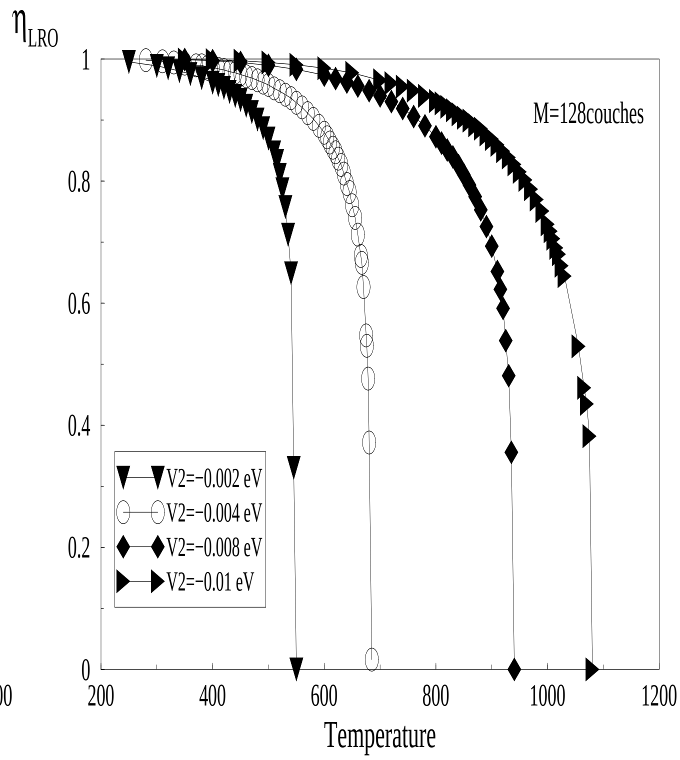
• The pair interactions with the following relations V_{AV}=V_{BV}=0 and V_{AA}=V_{BB}=-V_{AB}.

1 Order-Disorder Kinetics

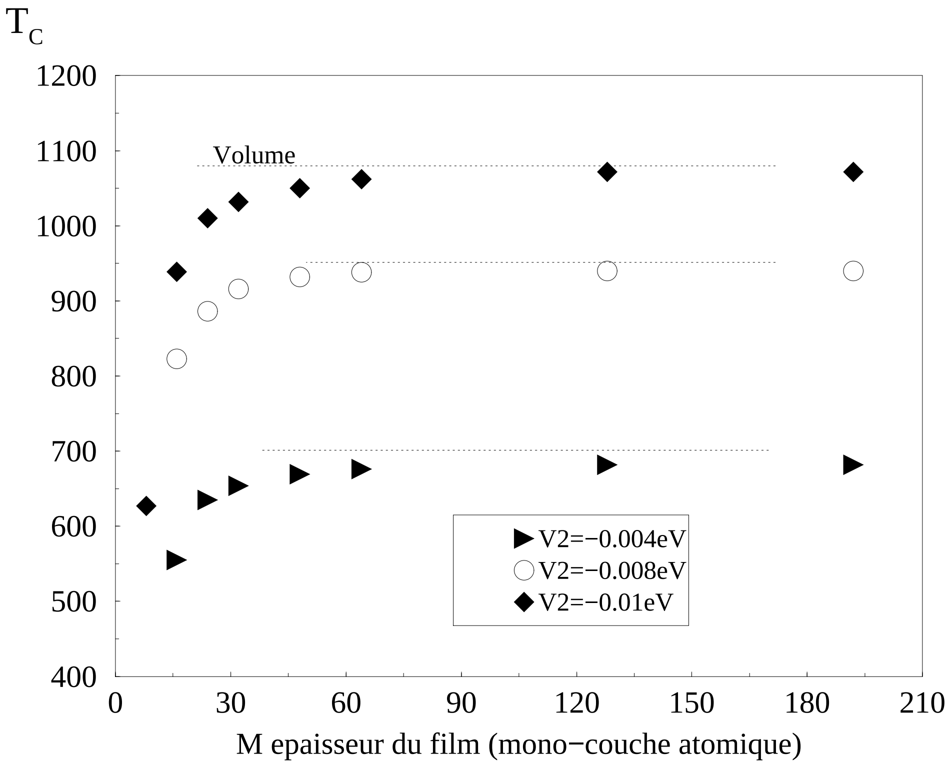
$$\eta(t) = \eta_{eq} + A_1 exp(-t/\tau_l)$$







2 Dependence of T$_c$ with the films thicknesses.

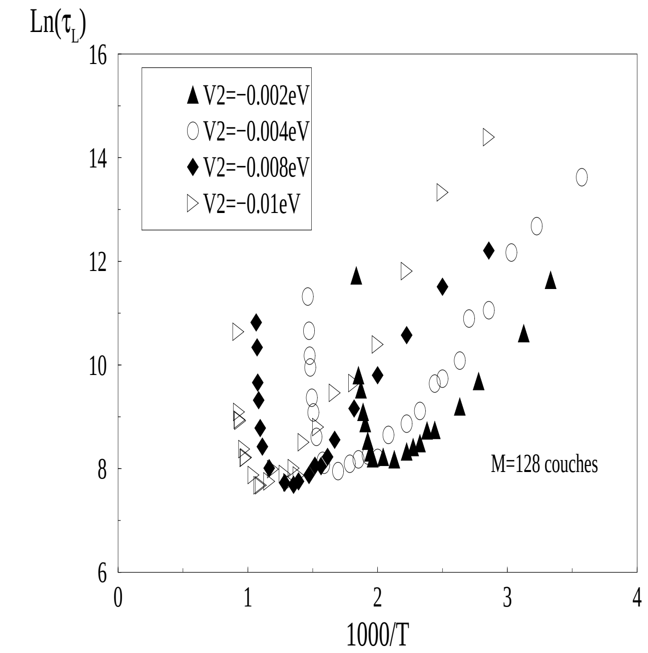


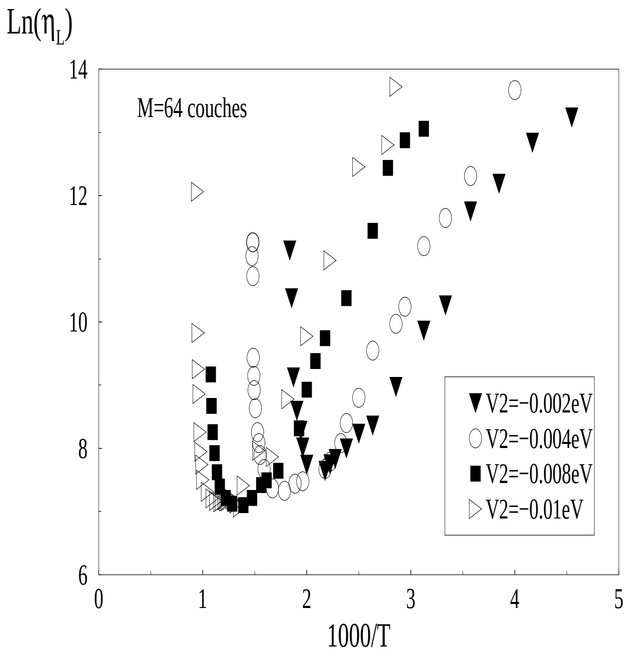
$\longrightarrow$Tc$\nearrow$ with the films thicknesses, for the M $\leq$ 65 monocouches.

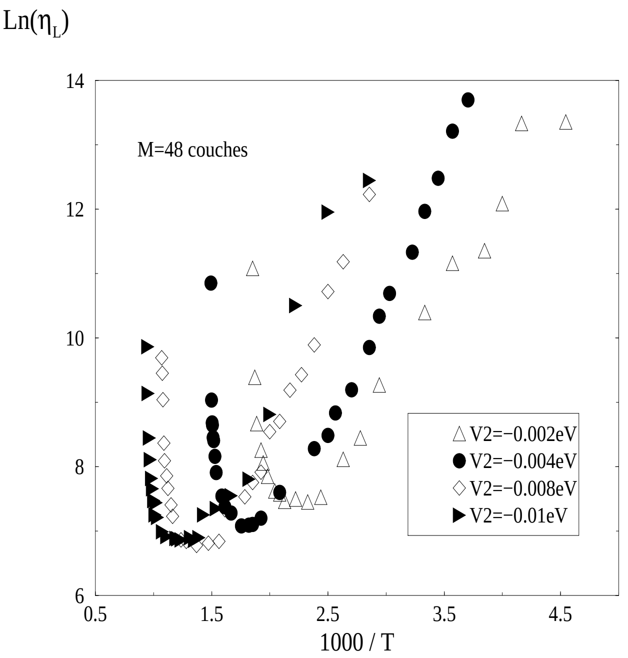
$\longrightarrow$Tc $\simeq$ constant for M$\geq$ 65 monocouches $\Rightarrow$ bulk properties.

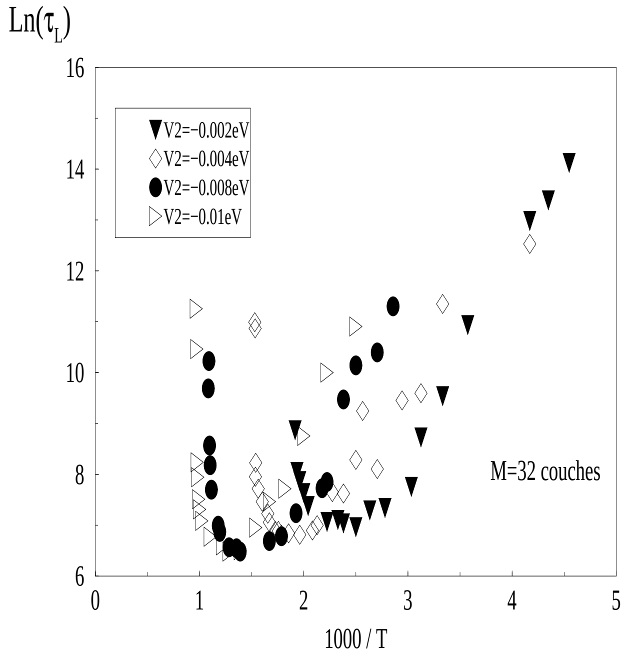
3. Kinetics.

$$Ln(\tau_l) = Ln(\tau_0) + E_M/kT$$

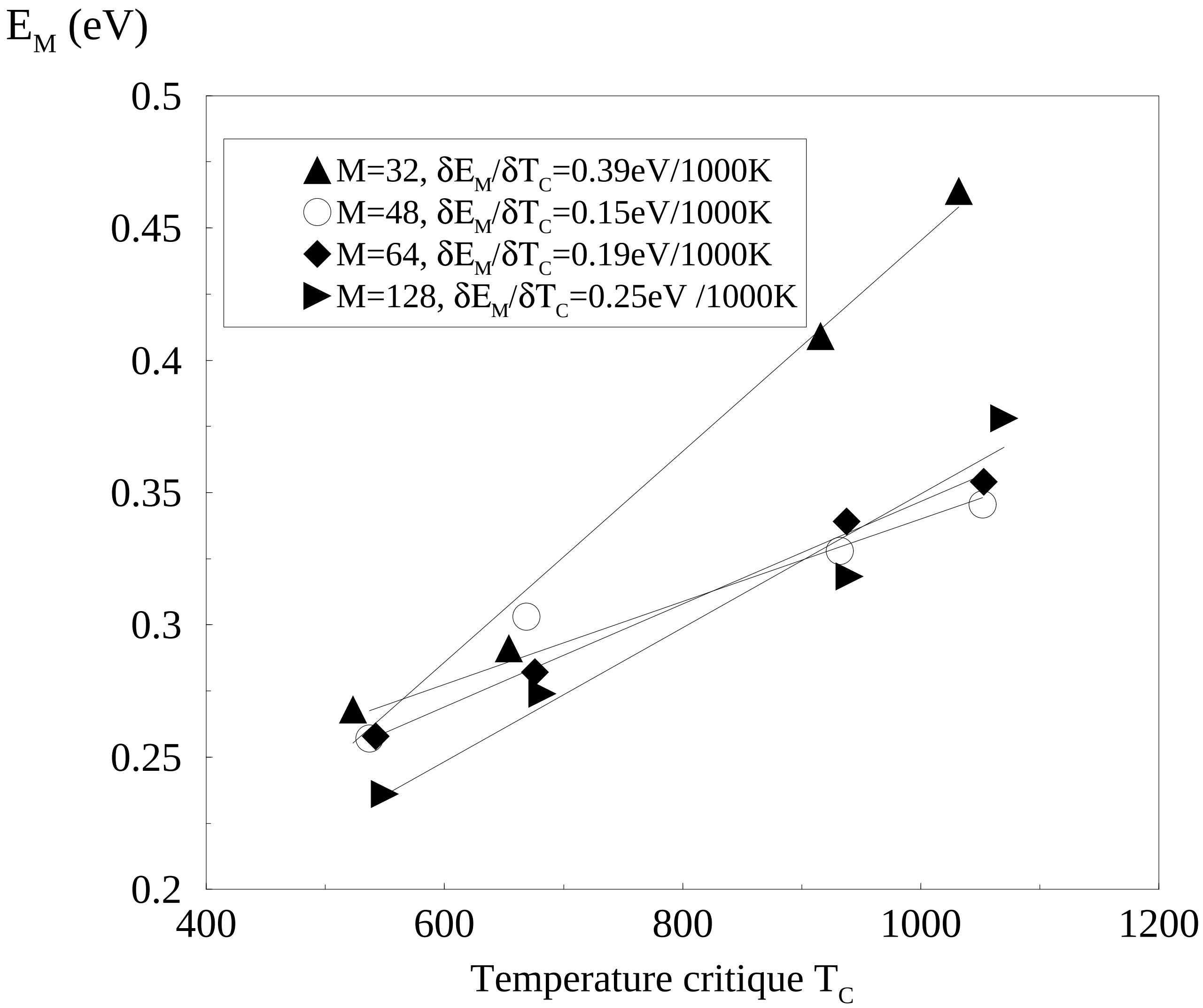






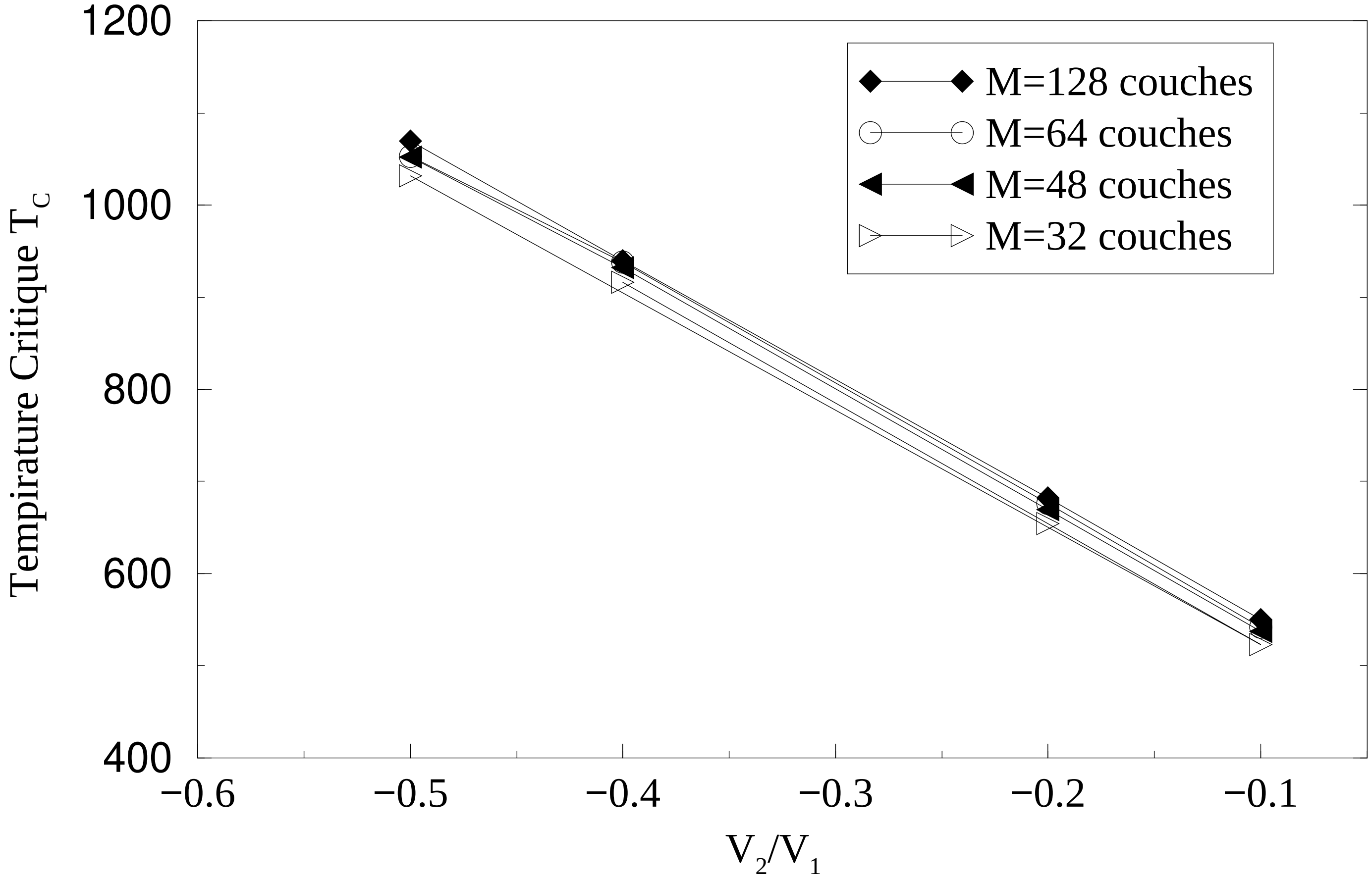


4. Correlation between the migration energies and Tc

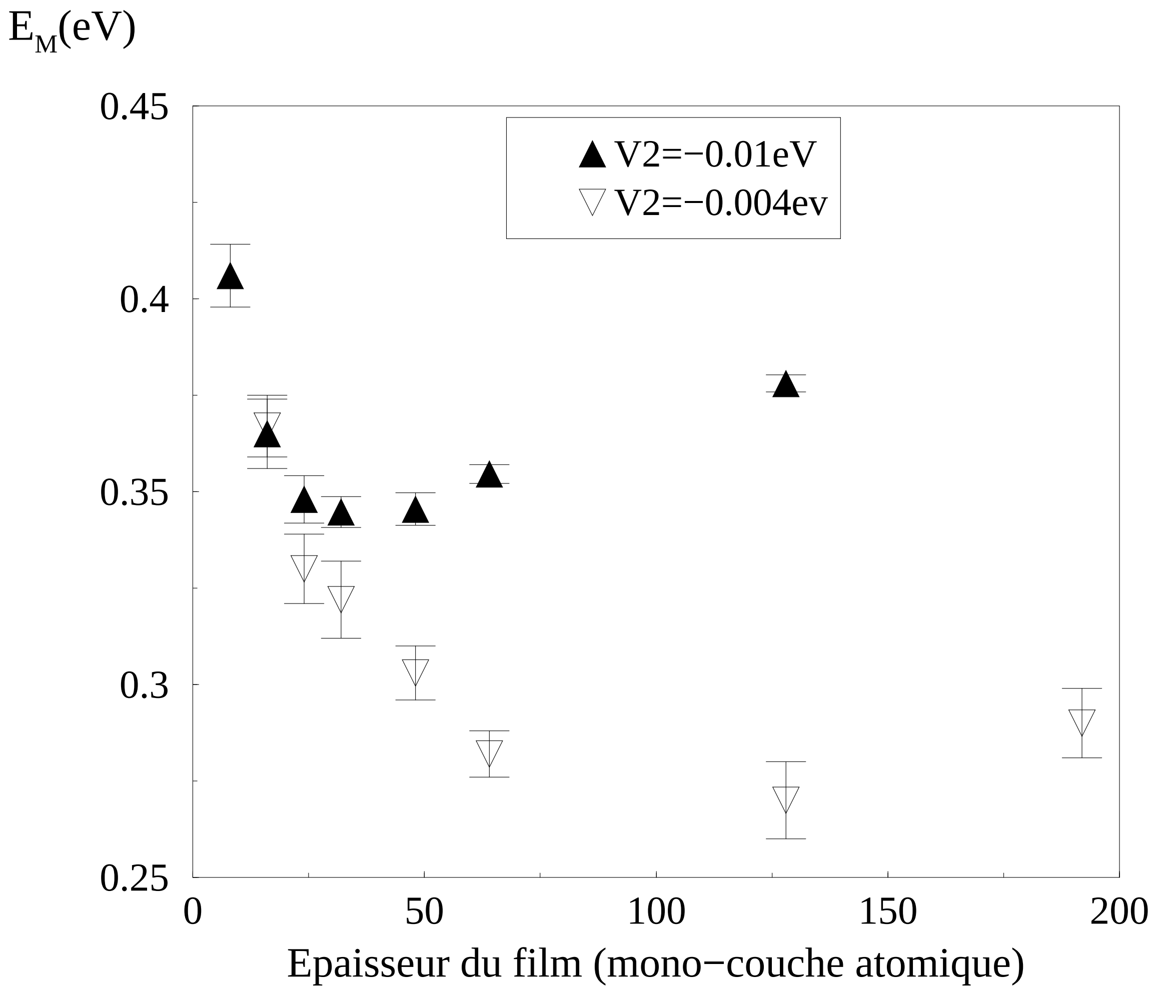


- M $\searrow$ $\Rightarrow$ Fluctuations $\nearrow$ E_m difficult to evaluate.

5. Variation of T_c with pairs interaction energies.



6. Dependence of E_m with the films thicknesses.



- M $\longrightarrow 0 \Rightarrow E_M \simeq$ value of 2D surface, Kerrache *and al.* Comput. Mater. Sc. 17 (2000).

- M $\longrightarrow 64 \Rightarrow E_M \simeq$ value of bulk, Kerrache *and al.* Defect Diffusion Forum, 194-199(2001)447-452.

Conclusion

•The new parameters (Pot.1) describe well the particular case of the $L1_0$ structure, and we will use then to simulate the growth of CoPt thin films.

• Our model MC-SMA with Pot. 1 give a good description of order-disorder ($L1_0 \Rightarrow A1$) transition temperature in CoPt system.

• We have obtained properties of bulck with thickness > 64 mono layers.

• In limite of much smaler thicknesses our E_M agrees very well with Kerrache *and al.* results obtained for 2D lattice.

Outlook

•Evaluation of realistic migration energies in CoPt bulk alloy.

•*Surface*: evaluation of order-disorder transition temperature at the surface (MC-SMA) and the saddle point energies of different atomic jumps (on the surface, along a step, up a step....).

•*Growth*: morphological, atomic and chemical re-arrangements in the first stages of the deposition of Co and Pt on CoPt, (TB-QMD).