



Research articles

On the conditions for ordered hexagonal mm2 Co₃PtXiao Lu^{a,b,*}, David E. Laughlin^{a,b,c,d}, Jian-Gang (Jimmy) Zhu^{a,b,e}^a Department of Electrical and Computer Engineering, Carnegie Mellon University, Pittsburgh, PA 15213, USA^b Data Storage Systems Center, Carnegie Mellon University, Pittsburgh, PA 15213, USA^c Department of Materials Science and Engineering, Carnegie Mellon University, Pittsburgh, PA, USA^d MSE Department, Carnegie Mellon University, Pittsburgh, PA, USA^e College of Engineering, Carnegie Mellon University, Pittsburgh, PA, USA

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ABSTRACT

A lattice-based Monte Carlo model is used to investigate the ordering conditions necessary to produce the ordered Co₃Pt phase (mm2). In this phase, Co and Co₅₀Pt₅₀ atomic layers alternate along the c-axis of the parent hexagonal structure. It is found that perpendicular ordering where the Co and Co₅₀Pt₅₀ layers alternates, is strongly correlated with in-plane ordering of the Co₅₀Pt₅₀ layers. In these layers the Co atoms and Pt atoms form alternating rows in parallel. Such atomic ordering within the plane is only facilitated by a deformation of the hexagonal lattice such that the ratio between the atomic spacing transverse to the row and along the row, b/a , becomes significantly smaller and the structure becomes orthorhombic. At adequate lattice spacings and b/a ratio, both in-plane ordering and perpendicular ordering occur simultaneously. In addition, the Co₅₀Pt₅₀ layers are also staggered alternately, forming a structure with the Imm2 space group. The ordered Co₃Pt with Imm2 symmetry is also found to be sensitive to changes in the Pt composition.

1. Introduction

The HCP derivative Co₃Pt phase in a form of ordered Co/Co₅₀Pt₅₀ superstructure has been predicted to have very high uniaxial magnetocrystalline anisotropy [1]. Pursuing this material, experimental studies of sputtered c-axis textured HCP derivative Co₃Pt thin films have found that measured perpendicular anisotropy showed direct correlation with the ratio between (0 0 0 1) and (0 0 0 2) peaks in x-ray diffraction (XRD) analysis [2–5]. However, despite of extensive experimental efforts [6–12], the ratio of the XRD peaks in these films remained relatively small, indicating the mixing of Pt in the layers that were supposed to be pure Co layers. Consequently, the experimentally achieved anisotropy constants are significantly below the theoretically predicted value of PMA $K_u = 2.8 \times 10^7$ erg/cm³ [1].

It is conceivable that the mm2 ordering along the c-axis, i.e. the formation of alternating pure Co atomic layers maybe well correlated to the in-plane ordering in the Co₅₀Pt₅₀ layers. However, there is little understanding of the conditions for the in-plane ordering of the 50/50 mixed layers. The focus of this work is to provide a fundamental understanding of the conditions in which the HCP derivative Co₃Pt structure with a perpendicular ordering of alternating Co/Co₅₀Pt₅₀ layers would form. We also wanted to see if there is a correlation of perpendicular ordering with the in-plane ordering of the Co₅₀Pt₅₀

layers. Our paper is organized as follows, Section 2 is a theoretical and fundamental analysis of the ordering of Co₃Pt and explains the simulation approach we used. Section III shows the result from the simulations and analyzes the fundamental conditions necessary to produce thin films of the ordered HCP Co₃Pt structure. The stability of the ordered HCP Co₃Pt in the vicinity of Co:Pt = 3:1 stoichiometry was also studied and is discussed in Section 3.

2. Theory and simulation approach

To understand the condition for Co₃Pt with perpendicular Co/Co₅₀Pt₅₀ ordering, the in-plane (IP) ordering of Co₅₀Pt₅₀ layer should be firstly considered. Within the mixed Co₅₀Pt₅₀ layer, Co and Pt atoms which have different atomic sizes coexist and different atomic pairs, Co-Co, Co-Pt and Pt-Pt, are present. According to Vegard's law, different atomic pairs must relax at different atomic spacings. The relaxed distance of each pair is shown in Fig. 1b) in which the EAM potential [13,14] was used. This Figure shows that $a_{Co-Co} < a_{Co-Pt} < a_{Pt-Pt}$. Therefore, for the overall Co/Co₅₀Pt₅₀ structure to be stabilized, different atomic pairs in Co₅₀Pt₅₀ layer must be relaxed to certain extent so that the total energy of the Co/Co₅₀Pt₅₀ structure is the lowest compared to other possible structures. In other words, the atomic spacings in the basal plane of hexagonal structure need to deviate from

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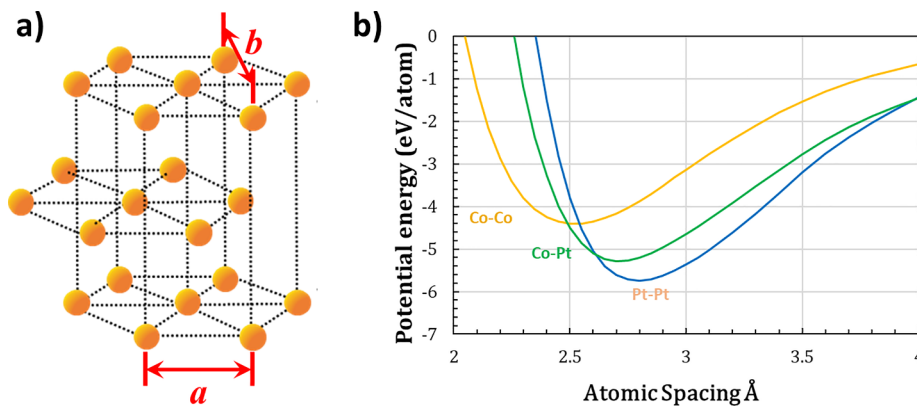


Fig. 1. Schematic crystal structure of: a) HCP structure with each site being randomly occupied; b) potential energy of Co-Co, Co-Pt and Pt-Pt atomic pairs [14].

the perfect HCP ratio ($b/a = \sqrt{3}$ in Fig. 1a) so that an in-plane structure which involves Co-Co, Co-Pt and Pt-Pt distances that minimize the energy can be stabilized. Therefore, whether the atomic-spacings are ideal for each of the atomic pair is fundamentally important for the relaxation of the in-plane and thus the entire structure. It is proposed that with a set of optimized atomic spacings, the total potential energy for the structure with desirable ordering can be the lowest compared to other orderings which can fundamentally enable the formation of the desired structure.

To search for such a set of optimized interatomic spacings, we used a simulation approach. There are different applicable methods such as molecular dynamics, DFT calculation, Monte Carlo and etc. As we are interested in the stable structure under different conditions, molecular dynamics will suffer from the fact that events like atomic jump and diffusion will require tremendous amount of simulation time to finish one event. On the other hand, DFT calculation can provide more accurate interatomic interactions considering the actual electron density and exchange interactions. However, the energy calculation for a similar box size will be expensive to achieve a set of statistical data. Therefore, we have chosen lattice-based Monte Carlo and used an empirical EAM potential for the energy calculation. To allow possible structures to form in a hexagonal-derivative lattice, an orthorhombic unit cell is employed. In each orthorhombic unit cell (u.c.), eight atoms are incorporated. With three lattice parameters of each u.c. being a , b and c ($a < b < c$), the positions of the atomic sites are: $(0, 0, 0)$, $(1/2, 1/2, 0)$, $(0, 1/3, 1/4)$, $(1/2, 5/6, 1/4)$, $(0, 0, 1/2)$, $(1/2, 1/2, 1/2)$, $(0, 1/3, 3/4)$ and $(1/2, 5/6, 3/4)$ respectively. The overall simulation system consists of $n \times n \times n$ of such orthorhombic unit cells with $n = 8$. At the system boundaries, periodic boundary conditions are applied. The Co and Pt atoms are distributed to the sites on this orthorhombic lattice with the atomic ratio of 3:1 to represent the Co_3Pt stoichiometry. It should be noted that the value of n is chosen as a compromise between the computational efficiency and the finite-size effect [15]. With n being too small, the interaction from a neighboring atom on a given atomic site would be unphysically overlaid, leading to an unreliable prediction. For calculations of potential energy, instead of pairwise models used in other computation works [16–18], we use a many-body EAM potential [13] developed by Zhou [14] to more accurately represent the many-body nature of binary metallic system. Hyperparameters for the potential functional are modified in this study to better represent the fundamental properties of Co and Pt such as lattice constants and elastic constants [19–21]. The potential energy is calculated using open-source LAMMPS software [22].

During the Monte Carlo simulations, atomic swaps take place to allow for energy minimization toward an equilibrium state. In particular, following the Metropolis algorithm [23], attempts are made to swap neighboring atoms if they are chemically different. The probability of each attempt is determined as in Eq. (1):

$$P = \min\left(\exp\left(-\frac{\Delta E}{k_B T}\right), 1.0\right) \quad (1)$$

where ΔE represents the change of total energy E in Eq. (1) induced by the atomic swap; k_B is the Boltzmann constant and T is the temperature. The temperature was fixed at 400 K to allow for sufficient thermal fluctuations so that MC system does not freeze in a local energy minimum. An attempt is accepted if $P > P_{\text{random}}$ (randomly generated probability) and rejected otherwise. In each Monte Carlo iteration, N_{Pt} attempts are made where N_{Pt} is the number of Pt atoms. After 5×10^4 iterations to achieve energetically steady state, two long-range order parameters are calculated (i.e. in-plane S_{IP} and out-of-plane S_{OP}). To account for the structural relaxation, we relax the c -dimension after each MC step. The ordering of the structure is then sampled during another 5×10^4 iterations. The detailed definition of S_{IP} and S_{OP} is included in Appendix A.

3. Results and discussion

3.1. Stability of the $mm2$ phase within perfect HCP structure

As aforementioned, in the experimental efforts, the maximum perpendicular order was found to be $S \approx 0.5$ when the underlayer being used were mainly HCP-based materials while the in-plane order was not

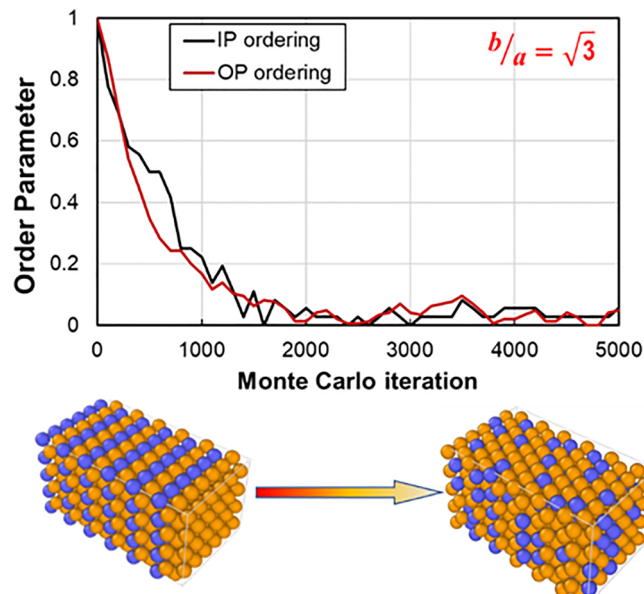


Fig. 2. Unstable $Pmm2$ Co_3Pt within an HCP Structure ($b/a = \sqrt{3}$).

measured. It was proposed in a theoretical study that the Pmm2 symmetry with a smallest orthorhombic unit cell is a possible structure for Co_3Pt with Co/ $\text{Co}_{50}\text{Pt}_{50}$ ordering [1]. However, a hexagonal underlayer would provide a hexagonal lattice for the deposited materials in which the atomic spacing in the basal plane are identical in different directions. Whether such orthorhombic Pmm2 should form within a hexagonal lattice remains unclear. In other words, we want to know whether Pmm2 is stable when $b/a = \sqrt{3}$ which is the case in experimental efforts. To understand this, we performed a MC simulation in which a fully ordered Pmm2 structure was initialized. Atoms swap can take place and the probability is determined by Eq. (1). The lattice was fixed with $b/a = \sqrt{3}$ ($a = 2.61 \text{ \AA}$ [1]) representing the hexagonal lattice from the HCP underlayer materials. The Monte Carlo procedure was conducted. Both order parameters, S_{IP} and S_{OP} , are recorded and plotted vs MC steps in Fig. 2 which shows them to diminish quickly within 2000 MC iterations. This simple test simulation clearly shows that within a perfect HCP structure, Pmm2 is unstable. In the basal plane of a

hexagonal lattice, neighboring atoms are forcibly kept at the same distance. The alignment of Pt (or Co) rows in Pmm2 structure is not energetically favored in such a hexagonal structure. Therefore, the order-disorder transition could involve swaps between Pt and Co neighbors to relax one of Co-Co, Co-Pt or Pt-Pt to reduce the energy. As the structure of Pt rows is destabilized, the perpendicular ordering of Co/ $\text{Co}_{50}\text{Pt}_{50}$ /Co is disrupted and the whole structure becomes disordered.

Therefore, the instability of Pmm2 Co_3Pt in an HCP confined structure makes it challenging to prepare ordered Pmm2 Co_3Pt using an hcp underlayer. Next, we want to investigate whether the ordered Co_3Pt with $\text{Co}_{50}\text{Pt}_{50}$ structure can form; if so, what would be the atomic order and what is the fundamental condition.

3.2. Effect of atomic spacing with different b/a

As proposed earlier, the lattice which defines the interatomic

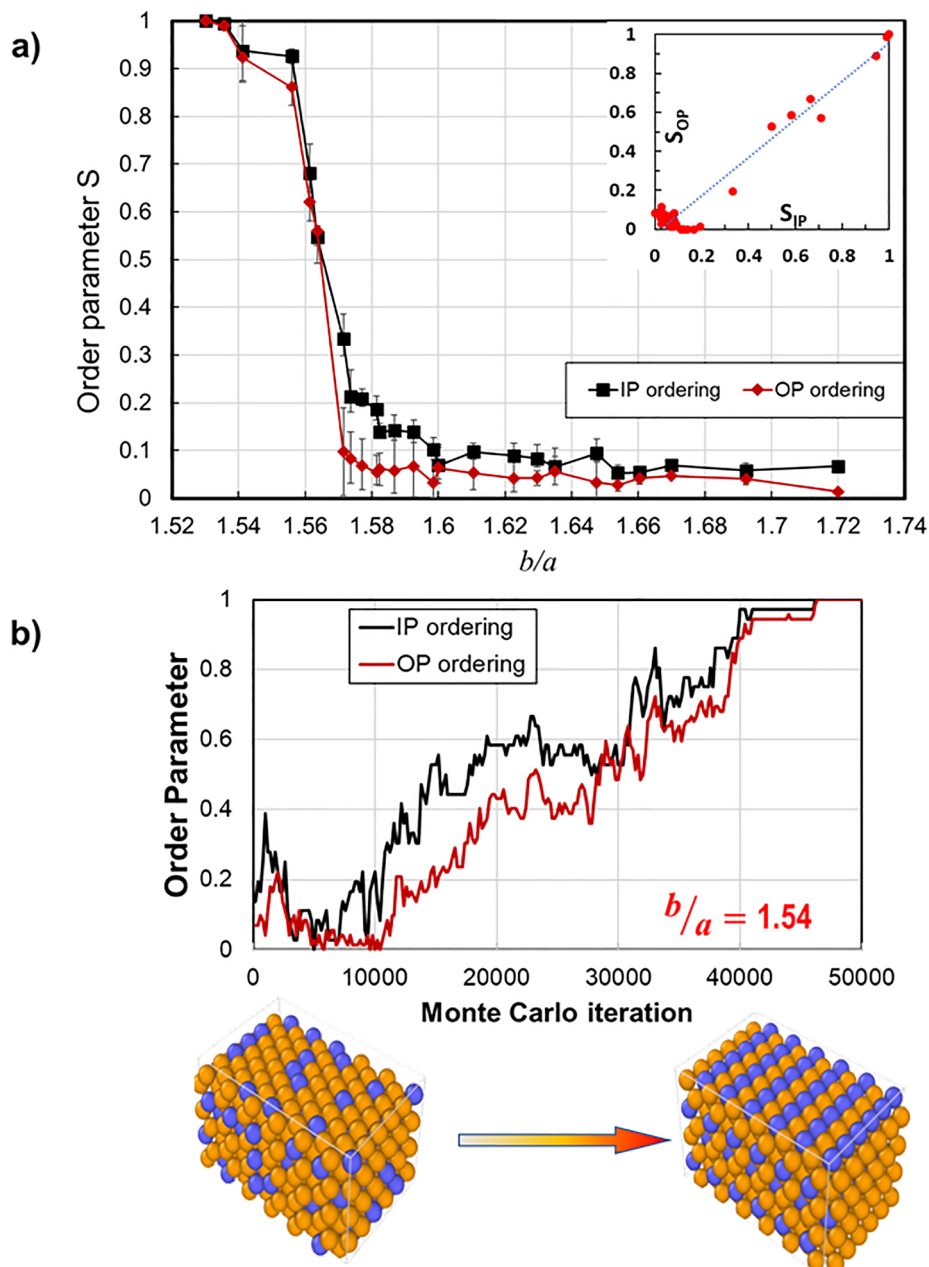


Fig. 3. In-plane and out-of-plane order parameters of the strained Co_3Pt after Monte Carlo process with different b/a ratios. The inset figure shows the correlation between In-plane and Out-of-plane ordering b) process of mm2 Co_3Pt formation.

spacings between all atoms plays a key role in the structural formation. To account for the atomic difference between Co and Pt and to investigate the effect of atomic spacings, we change the lattice parameter b and a in the range $b/a = 1.52\text{--}1.72$ ($a = 2.55\text{--}2.8\text{ \AA}$ and $b = 4.3\text{ \AA}$) in the orthorhombic unit cell. Different from the simulation in Fig. 2, a completely disordered Co_3Pt alloy is initialized within the orthorhombic lattice. Fig. 3a) shows the OP and IP ordering of the final crystal structures at different b/a ratios. The first observation of this curve is that OP and IP ordering change simultaneously across the scanned b/a range. Such correlation between the two order parameters is more obviously shown in the inset of Fig. 3a) where OP is plotted against IP ordering: when structure is fully or partially ordered ($S > 0.3$), the relation between OP and IP is almost linear, indicating a strong correlation; when the system is in disordered state ($S < 0.3$), the linear correlation does not exist. This strong correlation indicates that if the structure is ordered either in-plane or perpendicularly, the overall ordered structure can form. Therefore, the formation condition for superlattice Co_3Pt should closely relate to the condition where either in-plane or perpendicular ordering forms.

Another important fact is that that ordered structure can only form when b/a is sufficiently reduced. In a wide range of b/a ($= 1.6\text{--}1.72$), neither in-plane nor perpendicular ordering is observed. In-plane ordered structures are first shown to partially form when b/a is reduced to < 1.6 as S_{IP} increases to ~ 0.2 . At this stage, S_{OP} does not essentially increase but its variance becomes large, indicating the locally ordered perpendicular structure. As b/a is further reduced, both S_{IP} and S_{OP} increased significantly within a short range of b/a ($= 1.54\text{--}1.58$) and saturate simultaneously at the fully ordered value of $S = 1.0$. We determined the threshold value of ordering to be 1.57 as the order parameter is greater than 0.5 when $b/a < 1.57$. This threshold value is much smaller than the value in an HCP structure with $b/a = \sqrt{3}$. At this stage, the hexagonal lattice is reduced to an orthorhombic lattice in which interatomic distances depends on directions in the basal plane, different from the direction-independent situation in hexagonal lattice. Therefore, in an orthorhombic lattice with ‘proper’ interatomic spacing accounting for the difference of Co-Co, Co-Pt and Pt-Pt, the formation of superlattice Co_3Pt is enabled. As we relax the c dimension of the structure, we have observed that the c/a ratio for an ordered mm2 structure differs from a disordered structure. $c/a = 1.0$ was initialized for each MC simulation but we measure that $c/a \sim 0.96$ for the ordered mm2 structure whereas for disordered structure, $c/a \sim 0.99$. The reason is that along c dimension, Pt-Pt bond which has largest atomic spacing is minimized in ordered structure so that the c/a is reduced. For ordered structure, Pt-Pt bonds can exist along all directions, c/a is remained as the same in a perfect HCP structure.

Next, we investigated the detailed formation process at an optimal ratio of $b/a = 1.54$. The OP and IP order parameters were monitored, and they are plotted against MC steps as in Fig. 3b). The structure experiences a transition from an initially disordered alloy, to a partially ordered structure with $S_{IP} \sim 0.6$ $S_{OP} \sim 0.4$ at the intermediate stage and finally to a fully ordered structure with $S_{IP}, S_{OP} = 1.0$. During this transition, S_{IP} is larger than S_{OP} indicating that the formation of in-plane ordering occurs ahead of the formation of perpendicular ordering. The atomic configuration shows that alternating rows of Pt and Co atoms form locally at the intermediate stage. These local Pt rows form because the larger Pt-Pt pairs can be stabilized along the extended a axis. Along the compressed b axis, Co-Pt pairs which have shorter relaxation length can also be stabilized so that Pt and Co rows alternates along b direction. The remainders of the Pt atoms that do not form in a row structure will tend to ‘move’ (by MC swaps) to this locally ordered region and form new rows so that the ordered structure continues to grow after the intermediate stage. In this way, the locally formed atomic row structure act as a growth seed and alternating Pt/Co row structure can continue to grow from the locally ordered in-plane structures. In addition, layers that are adjacent to the layer containing Pt/Co rows become deficient in Pt content, inducing the alternating distribution of Pt atoms in adjacent

layer. Therefore, in the final stage, since all the Pt atoms form rows along the elongated a direction in every other atomic plane, the perpendicular superlattice ordering is formed as well.

Interestingly, the final ordered structure from the simulation in Fig. 3b) exhibits a difference in the $\text{Co}_{50}\text{Pt}_{50}$ plane compared to Pmm2 proposed in ref. [1] while the perpendicular Co/ $\text{Co}_{50}\text{Pt}_{50}$ /Co ordering remains the same. We refer this structure as Imm2 because Pt atoms occupy the vertices and the center of the unit cell and collectively form a body centered orthorhombic Bravais lattice.

To explain the formation of Imm2 instead of Pmm2 [1], the energy of Pmm2 and Imm2 structures within a range of $b/a = 1.54\text{--}1.57$ was calculated. Imm2 consistently has a lower energy compared to Pmm2 with an energy difference of ~ 0.01 eV/atom, meaning Imm2 is energetically more stable. In Imm2, Pt rows are shifted by one atomic position along b axis in every other A(A') planes shown in Fig. 4. Hence in Imm2, the distance of out-of-plane Pt rows is larger, and atoms form a denser structure compared to Pmm2. This denser atomic configuration is favored with the mm2 symmetry in an orthorhombic lattice. As the MC procedure is sensitive to energy difference, Imm2 structure is observed in our simulation study.

Therefore, with the results in Fig. 3, it becomes clear that a significantly deformed hexagonal lattice, or an orthorhombic lattice with small enough $b/a < 1.54$, enables the formation of fully ordered Pmm2 superlattice structure. Such deformation favors the in-plane ordering of mm2 in which Pt/Co rows can be stabilized along the elongated a axis as atomic spacings are optimal for Co-Co, Co-Pt and Pt-Pt. With the formation of in-plane ordering, the perpendicular superstructure ordering can be realized. The ordering condition for Imm2 is thus equivalent to the ordering condition of in-plane structure of alternating Pt/Co atomic rows.

3.3. Effect of Pt concentration

During an actual experimental deposition process, the stoichiometry might not be maintained at the deposited film surface due to the difference of atomic arrival rates between Pt and Co. A study to understand the effect of Pt concentration was carried out to understand the sensitivity of Imm2 ordering vs stoichiometry when b/a is kept optimal.

Fig. 5 shows that the Imm2 ordering could be preserved with both S_{IP} and S_{OP} being > 0.85 only in the close vicinity to 3:1 stoichiometry

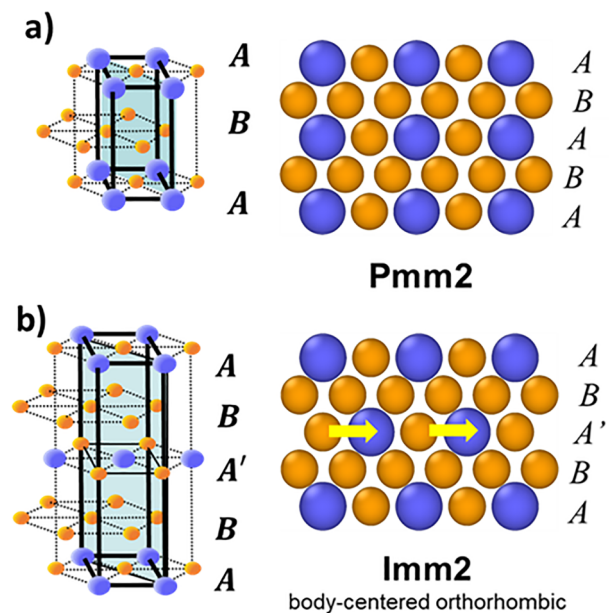


Fig. 4. Schematics of a) Pmm2 Co_3Pt and b) Imm2 Co_3Pt . The Pt rows in every other A(A') plane in Imm2 changed their positions.

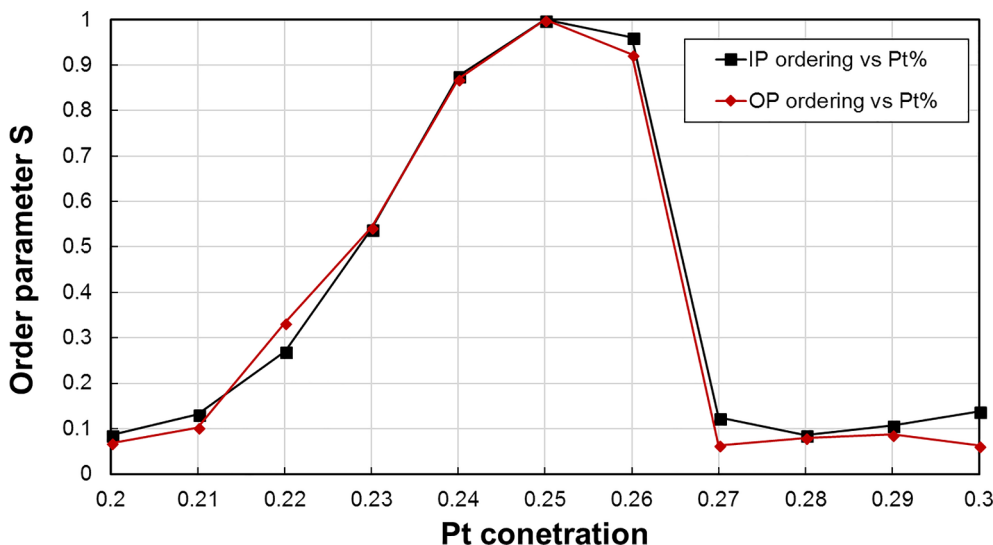


Fig. 5. In-plane and out-of-plane ordering parameter of $\text{Co}_{1-x}\text{Pt}_x$ after the Monte Carlo process with optimal $b/a = 1.54$ ($a = 2.8 \text{ \AA}$, $b = 4.3 \text{ \AA}$) with $x = 0.2-0.3$.

($x = 0.24-0.26$). However, the addition and depletion of Pt affects the Imm2 ordering differently which is shown by the asymmetric ordering curve vs Pt concentration. In the situation with insufficient Pt (20%–24%), the Imm2 ordering increases gradually as Pt concentration increases. The reason is that for 20% Pt case, the neighbors of Pt are more likely to be Co atoms. As Pt is added, Pt-Pt pairs can be formed locally ratio along a direction due to the reduced b/a . Therefore, the in-plane ordering of Pt rows is gradually formed as more Pt is added and so is the out-of-plane ordering. As Pt concentration reaches 25%, atomic configuration becomes the most ordered as locally, every other row is saturated with Pt atoms in every other plane. However, as more Pt is added, S_{IP} and S_{OP} drastically drop to less than 0.2. Locally stabilize Pt rows can be disrupted because additional Pt-Pt will form along directions other than the elongated a direction. We observed that Pt rows will form in every third row in every plane. So both in-plane and out-of-plane ordering is disrupted instantaneously, shown by the drastic drop in Fig. 5. Therefore, without in-plane ordered alternating Pt/Co rows, the perpendicular ordering is unachievable as OP is determined by the in-plane ordering under deformed HCP lattice. Thus, Imm2 phase shows high sensitivity to the change of composition. For experimental considerations, accurate control of the deposited film of such Co_3Pt material with 3:1 stoichiometry would be necessary.

4. Conclusions

In summary, using a lattice-based Monte Carlo model with EAM

Appendix A. Definition of a unified ordering parameters for Pmm2 and Imm2

As two possible structures, Pmm2 and Imm2 exist in this study, it is necessary to define a set of unified order parameters for both structures. Two long range order parameters were defined as in Eq. (A), i.e. the in-plane (IP) order parameter S_{IP} and the out-of-plane (OP) order parameter S_{OP} referring to ref. [22] for the observed Imm2 structure.

$$S_{IP} = \frac{S_{IP}^A + S_{IP}^{A'}}{2} = \frac{1}{4} \left(\frac{|f_1^A - f_2^A|}{x_{Pt}} + \frac{|f_1^{A'} - f_2^{A'}|}{x_{Pt}} \right) \quad (\text{A.1})$$

$$S_{OP} = \frac{1}{2} \left(\frac{f^A + f^{A'} - f^B}{x_{Pt}} \right) \quad (\text{A.2})$$

where plane A , A' , B , and site 1 and 2 are defined in ref. [22]; S_{IP}^A or $S_{IP}^{A'}$ stands for the IP order parameter in the A or A' plane; f_1^A , $f_1^{A'}$, f_2^A or $f_2^{A'}$ denotes the fraction of site 1 or 2 on mixed plane A or A' being occupied by Pt atoms; x_{Pt} denotes the concentration of Pt atoms; S_{OP} stands for the OP order parameter; f^A , $f^{A'}$ or f^B denotes the fraction of sites in plane A , A' or B being occupied by Pt atoms. Hence, both S_{IP} , $S_{OP} = 1.0$ will represent a perfectly ordered Imm2 structure while S_{IP} , $S_{OP} = 0.0$ will represent a completely disordered structure with Co and Pt being randomly distributed. S_{IP} would be suitable for both Imm2 and Pmm2 with the absolute value sign.

interatomic potentials, the conditions for ordered Co_3Pt has been studied. We found that the perpendicular ordering in which Co and $\text{Co}_{50}\text{Pt}_{50}$ atomic layers alternate along the c -axis of a hcp structure is strongly correlated with the in-plane ordering of the $\text{Co}_{50}\text{Pt}_{50}$ layers. The correlated in-plane and perpendicular ordering occur together when a certain level of deformation of the hexagonal lattice, $b/a \sim 1.54$, is reached. In addition, the $\text{Co}_{50}\text{Pt}_{50}$ layers are also staggered laterally which leads to the minimization of the perpendicular lattice spacing, forming a structure with the Imm2 space group. The ordering at the obtained lattice condition is also found to be sensitive to the composition stoichiometry. The above results indicate that in practice, perpendicularly ordered Co_3Pt thin film could be obtained by epitaxial growth on an underlayer with adequate lattice dimension and geometry.

Conflict of interest

There is no conflict of interest between authors.

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Appendix B. Supplementary data

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.jmmm.2019.165570>.

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