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Size and shape dependent order–disorder phase transition of Co–Pt nanowires

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ABSTRACT

Monte Carlo simulation of the order–disorder transition revealed that the transition temperature of Co–Pt nanowires increases with wire diameter, approaching the bulk value if the size is large enough. The transition temperature is affected by the shape of cross-section, though the shape effect is less significant than the size effect. It is showed that the rise of transition temperature in nanowires is largely due to the decrease of surface area compared with nanoparticles. The phase separation and tetragonalization are discussed by introducing mixing parameter and asphericity parameter. It is also found that the order–disorder transition starts from the surface and then to the core, indicating that the order–disorder transition of nanowires is a surface-dominant phenomenon, governed by the atomic under coordination.

1. Introduction

The Co–Pt nanomagnets with a size below 10 nm, which could be applied in next-generation ultrahigh-density magnetic storage media [1–4], have been widely studied in recent years especially on their order–disorder transition phenomenon [5–12]. Co–Pt nanoparticles (NPs) might perform perfectly in magnetic storage materials due to the mixing 3*d* and 5*d* orbits [7], while the order–disorder transition is strongly related to their electronic structure. To investigate the transition mechanism, atomistic simulation method, such as Monte Carlo method, has already been adopted to reveal the possible mechanism of transformations at atomic level [7–12].

The order–disorder transition of Co–Pt NPs is regarded as a surface-dominant process [13], where in comparison with bulk materials, the size effect plays an important role in the variation of properties. Miyazaki et al. [9], Rossi et al. [14] and Chepulskii [19] found the significant size and shape effects in Co–Pt NPs, and Alloyeau et al. [7] indicated that the dimension could affect the order–disorder transition temperature, while the nanowires and the nanofilms have different transition temperature from the NPs even in identical size. For the nanosolids of smaller size, there might be more special transformations, which are the highlights in recent studies [14–18]. The order–disorder transition in Co–Pt nanosystems have been studied widely by using Monte Carlo method [5–12,14–16]. Generally, the Ising-type models on rigid lattices are often addressed to study the order–disorder transition. However, the off-lattice strategies should be applied instead of lattice model because of the significant tetragonalizaion ratio in the $L1_0$ system [14].

In our previous work, we developed a model based on Bond-Energy model [13] to account for the Size and shape dependent order–disorder transition temperature of Co–Pt nanosolids. Our model suggested that the transition temperature of both NPs and nanowires (NWs) decreases with the reduction of size, while the results on Co–Pt NPs were consistent with recent experiments [7]. However, there are no available data for Co–Pt NWs, while NWs are regarded as one-dimension nanomaterials exhibiting the properties of both NPs and bulk materials. Therefore, it is necessary to study the order–disorder transition of Co–Pt NPs to understand this phenomenon completely at nanoscale.

In this work, we aim at studying the order–disorder transition of Co–Pt NWs by using Monte Carlo method and with the sizes from 1.86 nm to 9.3 nm. Three cross-section shapes are considered, i.e. tetragonal, hexagonal and circular shapes. The computational methods are described in Section 2, and the results on the size and shape dependent order–disorder transition of Co–Pt NWs are presented in Section 3, with further discussion concerning the mechanism of order–disorder transition. Conclusions are given in Section 4.

2. Methods

The initial Co–Pt NWs are prepared from the order and disorder bulk Co–Pt solids, with three shapes of cylindrical NWs (C-NWs) (Fig. 1 (a)) and prism-like NWs with hexagonal cross-section

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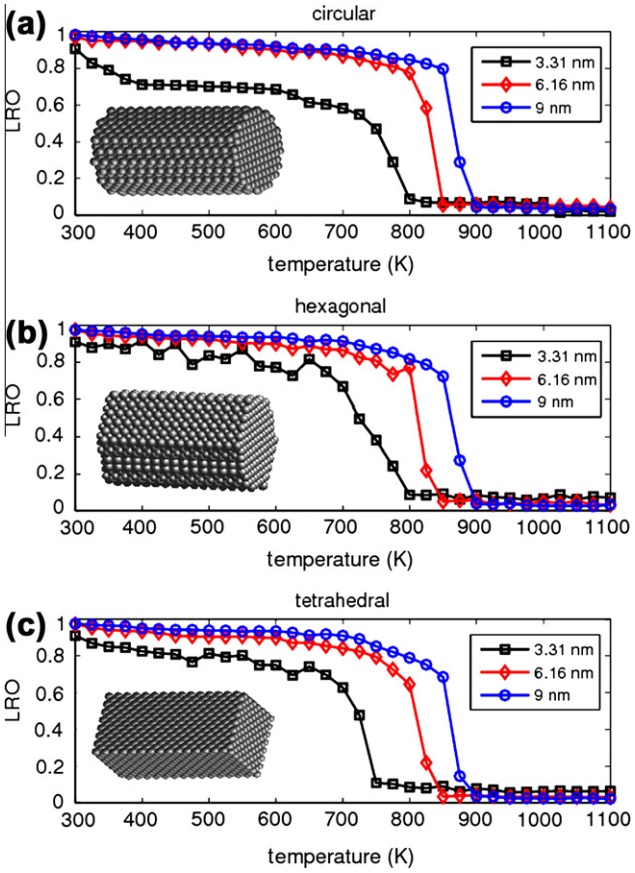

Fig. 1. Size and temperature dependent order parameters of cylindrical and prism-like Co–Pt nanowires. (a) Cylindrical. (b) Prism-like structure with hexagonal cross-section. (c) Prism-like structure with tetragonal cross-section.

(H-NWs) (Fig. 1 (b)) and with tetrahedral cross-section (T-NWs) (Fig. 1 (c)). The size of NW is defined by its cross-section, more specifically, by the diameter of the circle with the same area as its cross-section. The size ranges from 1.86 nm to 9.3 nm. If Co and Pt atoms are randomly distributed on each position of FCC lattice, the NW is disordered; if Co and Pt atoms can only be placed in specified sub-lattice of L10, the alloy is ordered.

The second-moment approximation (SMA) to the density of states in the tight-binding theory provides an analytic expression for the attractive band energy through the square root of an additive term [6,7,20–22]. The TB-SMA potential function which has been applied to simulate the order–disorder transition [6–8,20] is used in the present simulation. The total energy E_{total} of N atoms is defined as:

$$E_{\text{total}} = \sum_{i=1}^{N} (E_R^i + E_B^i) \tag{1}$$

where

$$E_R^i = \sum_{i \neq j, r_{ij} < r_{\alpha\beta}^{cut}} A_{ij} \exp\left[-p_{ij}\left(\frac{r_{ij}}{r_0} - 1\right)\right] \tag{2}$$

$$E_B^i = -\left\{ \sum_{i \neq j, r_{ij} < r_{\alpha\beta}^{cut}} \xi_{ij}^2 \exp\left[-2q_{ij}\left(\frac{r_{ij}}{r_0} - 1\right)\right] \right\}^{1/2} \tag{3}$$

In the above two formulae, A_{ij}, p_{ij}, ξ_{ij} and q_{ij} are the potential parameters; r_0 and $r_{\alpha\beta}^{cut}$ are the nearest distance and cut distance, respectively. In order to obtain reasonable results, the cutoff radius is chosen large enough to reduce error. The parameters for Co–Pt system are shown in Table 1 [7–8,14].

Table 1
Potential parameters for tight-binding potentials of the Co–Pt system.

	A_{ij} (eV)	ξ_{ij} (eV)	p_{ij}	q_{ij}	r_0 (A°)
Co–Co	0.189	1.907	8.80	2.96	2.50
Co–Pt	0.245	2.386	9.97	3.32	2.63
Pt–Pt	0.242	2.506	11.14	2.68	2.76

Order–disorder transition is recorded by using the long-range order parameter (LRO), which is defined as [23]

$$LRO = \frac{n_A}{n}\left(\frac{p_A - c_A}{1 - c_A}\right) + \frac{n_B}{n}\left(\frac{p_B - c_B}{1 - c_B}\right) \tag{4}$$

where n_A, n_B and n are the numbers of sub-lattices occupied by A (or B) atoms and the total number of sub-lattices; p_A and p_B are the occupation probabilities of sub-lattice A and B, while c_A and c_B are their respective concentrations. In $L1_0$ structure, LRO is given by

$$LRO_{L10} = P_A + P_B - 1 \tag{5}$$

The Monte Carlo simulation is performed in canonical ensemble (NVT). For the bimetallic NWs, two types of trials are included during simulation. (1) A small expansion is chosen in each step, which corresponds to relaxation and vibration. During the trial, the state with be accepted following the Metropolis strategy, and it takes long time to reach stable. This procedure is necessary before the acceptance/rejection process concerning the tetragonalization during order–disorder transition. This is also highlighted in Rossi's research [14]. (2) When exchanging two randomly chosen atoms, the new configuration is accepted according to the standard Metropolis algorithm with probability as:

$$P_{new} = Min\left[1, \exp\left(-\frac{\Delta E}{kT}\right)\right] \tag{6}$$

where k is the Boltzmann constant, and ΔE is the energy difference between the new and the old configurations. If $\Delta E < 0$, the trial is accepted; if $\Delta E \geqslant 0$, the trial is accepted according to the Boltzmann probability. After a large number of trials (more than 10^6 Monte Carlo cycles depending on the size of NWs), the Co–Pt NWs will approach stable states, which were tested by carrying out 10^5 more trials. The temperature in simulation ranges from 300 K to 1100 K.

3. Results and discussion

In order to study the size and shape effects on the order–disorder transformation of Co–Pt NWs, we construct NWs of different sizes in each shape. Periodic boundary condition is applied along Z-direction (the NWs are assumed to be in Z-direction). Three specified sizes, 3.31 nm, 6.16 nm and 9 nm, are experimented to show the size effects. Accordingly, in order to compare the size effects with those in NPs, we also simulate the transition procedure of these three sizes by removing the periodic boundary. Fig. 1 shows the order parameters of cylindrical and prism-like Co–Pt NWs depending on temperature and size. It is found that the order parameters of both shapes firstly approximate to ideal ordered state (the value is 1) at low temperature, and then drop to a low value (close to 0) in a certain range of temperature, which means that an order–disorder transition occurs during this temperature range. The results also indicate that the transition temperature increases with the rise of size. Furthermore, the transition temperature of circular section is the lowest whereas that of tetragonal section is the highest. The results suggest shape effect on transition temperature. However, the shape effect is less significant than the

size effect. For instance, the present simulated transition temperatures are 726 K (3.31 nm), 839 K (6.16 nm), and 851 K (9 nm) for C-NWs, 712 K (3.31 nm), 821 K (6.16 nm), and 840 K (9 nm) for H-NWs, and 695 K (3.31 nm), 805 K (6.16 nm), and 834 K (9 nm) for T-NWs. Among the three types of cross-section, the prism-like NWs has a larger specific surface area than the cylindrical ones. In the two kinds of prism-like NWs, the specific surface area of tetragonal NWs is larger than that of hexagonal NWs. From the simulation results, for the same size, the tetragonal NWs have the lowest transition temperature, while the cylindrical NWs have the largest transition temperature. This phenomenon clearly demonstrates the surface effect of order–disorder transition in NWs. We discuss this effect by introducing the energy of simulating system, and track the potential energy during the order–disorder procedures. Fig. 2 gives the energy variation of Co–Pt NWs with the increase of temperature. Energy is almost linear with lower temperature (the tiny fluctuations are related to random atom exchange at an extremely low probability), and then increases suddenly, but becomes smooth again at high temperature. The sudden energy changes just correspond to the order–disorder transition, which is also related to the sudden decrease of bond parameter. Furthermore, the energy variations during the transition of smaller NWs are lower than those of large ones, which is consistent with others' work [20]. The reasons can be explained from the strategy of Monte Carlo method. Initially, there could be rare atom exchange because the exchanges depend on the Boltzmann factor $Exp(-\Delta E/kT)$, which provides insight into the foremost low energy procedure in the real NWs. However, the probability of atomic immigration increases with the rise of temperature. If temperature increases to the transition region, the immigration probability of atoms increases, and the calculated potential energy will change rapidly as a result, which is also consistent with the sudden energy fluctuation in real system. With the continual increase in temperature, the atom immigration reaches an equilibrium, which indicates the formation of new disordered structure and the stabilization of energy state in ordered NWs.

The simulated order–disorder transition temperature of Co–Pt NWs is given in Fig. 3, and our previous theoretical results are represented by solid line for comparison. The transition temperature of prism-like NWs is lower than that of cylindrical ones with the same cross-section area. The prism-like NWs have larger atomic surface to volume ratio than that of cylindrical ones, indicating that the surface effect will be more significant for the prism-like NWs. The transition temperature difference between cylindrical and prism-like NWs increases with decreasing wire size, which suggests the shape effect is more obvious at a smaller size. In our previous work, we proposed a model based on Bond-Energy model [13] to account for the order–disorder transition of nanosolids. The NWs of Co–Pt NWs can be computed by $T_{NW} = (1-0.33/D) \times T_{Bulk}$, where T_{NW} and T_{Bulk} are the order–disorder transition temperatures of NWs and bulk; D is the diameter of NWs. From Fig. 3, it can be found that the present simulation results are consistent with the model predictions. Since NWs are low-dimension materials, they undergo the similar order–disorder transition as NPs, but have higher transition temperature due to dimension effect. The transition temperatures of 2 nm and 2.5 nm Co–Pt NPs are about 530 K and 610 K [20], respectively, but 565 K and 645 K for NWs with similar sizes. These results indicate that the properties of NWs lie in between NPs and bulk materials.

To find the effect of finite size in two dimensions, we also compare the results of NWs with NPs at the same size and shape, namely, disk-like NPs at 3.31 nm, 6.16 nm and 9 nm. In comparison, the transition temperature of NPs is lower than that of NWs in the same size. More specifically, the temperatures are 627 K(3.31 nm), 743 K(6.16 nm) and 756 K (9 nm), which are 99 K, 96 K and 95 K lower than those of NWs with tetragonal cross-section. Although NPs and NWs for simulation contain the same number of atoms, the description for size in NWs is not well suitable for NPs due to the existence of thickness in disk-like NPs. The transition temperature varies with the fluctuation of thickness, and in disk-like NPs with sufficient thickness, the transition temperature will approximate that in NWs. To explain these cases, we have also established a theoretical model expressed as $T_{NW} = \{1 - 0.33[(1/2h) + (1/D)]\} \times T_{Bulk}$, the h of disk-like NPs is 1.48 nm. Thus we plot the transition temperature calculated by this model for comparison. The transition temperature of NWs is

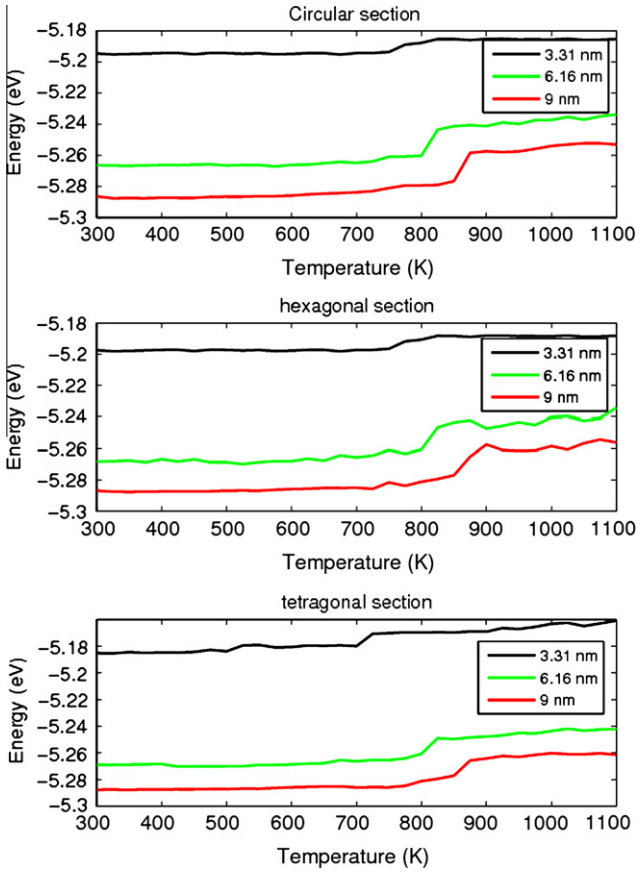

Fig. 2. Energy variation per atom for prism-like and cylindrical nanowires of different sizes.

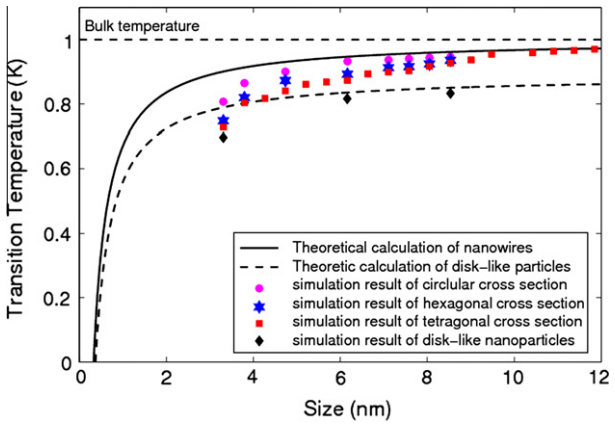

Fig. 3. Size and cross-section dependent order–disorder transition temperature of Co–Pt NWs and its comparison with disk-like nanoparticles.

a bit higher than that of disk-like NPs, which may result from the larger surface area of disk-like NP than that of NW in the same size. The present results indicate that the order–disorder transition of nanosolids is a surface-dominant process.

Fig. 3 shows that the theoretical results agree with the simulated ones at larger particle size, but disagree in smaller size. It was reported that the transitions of some nanophases do not well coincide with the predictions because the transition temperature range of small particles is much smoother than that of larger ones [7,24–26]. From Fig. 4, it can be found that the transition curve of smaller NWs becomes much smoother, and the transition region expands to ~150 K, which is different from larger NWs. Some bimetallic clusters have continuous transition as a second-order type [20,26], confirming the fact that the structure transformation of small size is very special. The order and disorder phases may coexist or the segregation of disordered phase has also been found [6,25,27].

In order to obtain details in the order–disorder transition, two more parameters are introduced to analyze the simulating results. One parameter is the mixing index μ, proposed by Calvo and Mottet by considering the connectivity between first neighbors [20], and the numbers of Co–Co pairs n_{CoCo}, Pt–Pt pairs n_{PtPt} and Co–Pt pairs n_{CoPt},

$$\mu(R) = \frac{n_{CoCo} + n_{PtPt} - n_{CoPt}}{n_{CoCo} + n_{PtPt} + n_{CoPt}} \tag{7}$$

This parameter would be practical, regarding the mixing and separation behaviors in a certain system. For a fully mixed rock salt structure, $\mu = -1$, but for a fully separated system, $\mu = 1$. The other parameter is the dimensionless asphericity χ, which describes the change of tetragonalization ratio during the order–disorder transition in the FCC structure. In the bulk system, the χ equals 1 – c/a, but this geometric quantity cannot be applied directly to a finite-size system. For NPs, Calvo and Mottet defined it as [20]

$$\chi(R) = 3\frac{A - (B + C)/2}{A + B + C} \tag{8}$$

where A, B and C ($A \geqslant B \geqslant C$) are the three principal momenta of inertia of the NPs. If the truncated octahedron is deformed into an oblate ellipsoid, χ is strictly positive. For NWs, Z-direction is periodical while the sizes at the other two directions are in nanometer. Namely, the shape of the cross-section would change during tetragonalization. For instance, the circular section would deform into an elipse while the square section would deform into a rectangle. In order to deal with these situations, we modify the parameter χ for NWs as:

$$\chi(R) = 2\frac{A - B}{A + B} \tag{9}$$

where A and B ($A \geqslant B$) are the principal momenta of inertia of the cross-section in NWs. Similar to the NPs and bulk size, the ordered NWs will have a larger value than that of the disordered ones. This parameter can be used not only to describe the formation in NWs during order–disorder transition, but to compare the structural transformations between bulk size and nanoscale.

The two quantities μ and χ show a similar behavior (Fig. 5), such as smooth variation within 300–1100 K but a great slope near the transition region. The behavior of mixing parameter for NWs is quite similar for NPs, but the initial mixing parameter for NWs is smaller [20], indicating larger mixing degree for NWs. However,

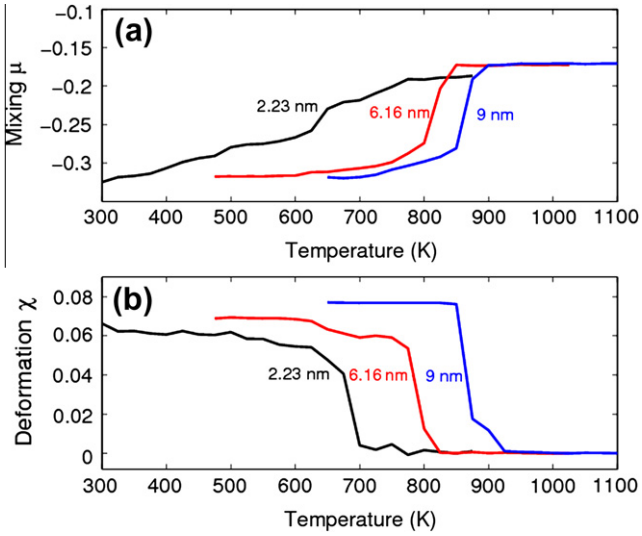

Fig. 5. Thermal averages of the two order parameters obtained from Monte Carlo simulation for Co–Pt NWs of sizes 2.23 nm, 6.16 nm and 9 nm. (a) Mixing order parameter. (b) Shape deformation χ.

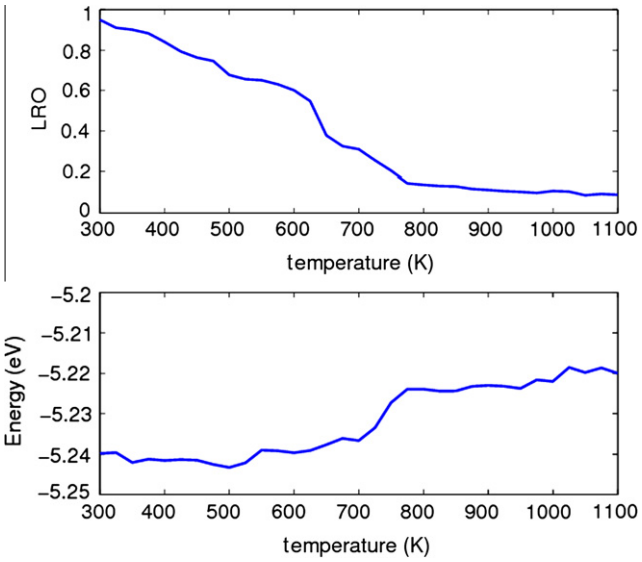

Fig. 4. Variation of energy per atom and order parameter of 2.23 nm Co–Pt NWs as the function of temperature.

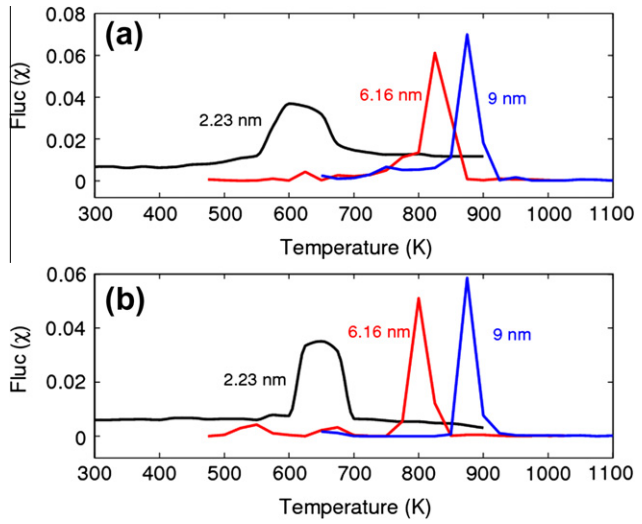

Fig. 6. Statistic fluctuations corresponding to the transition of cylindrical and prism-like Co–Pt NWs. (a) Fluctuations of the mixing order parameter. (b) Fluctuations of shape deformation χ.

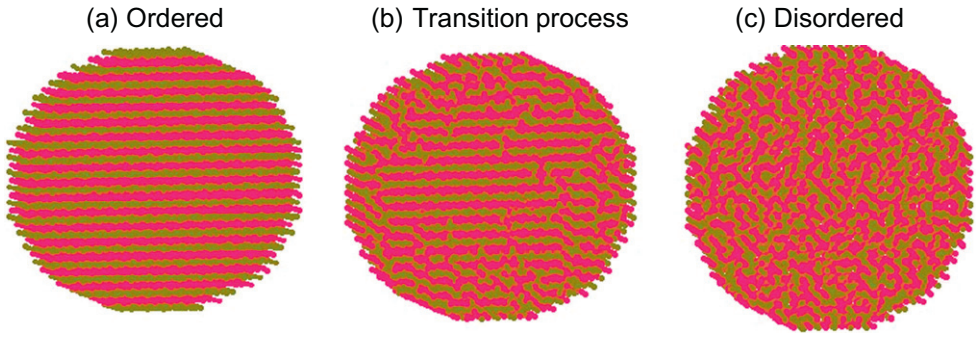

Fig. 7. Snapshots of the cross-section of cylindrical and prism-like NWs from order to disorder. (a) Order. (b) Surface disorder. (c) Full disorder.

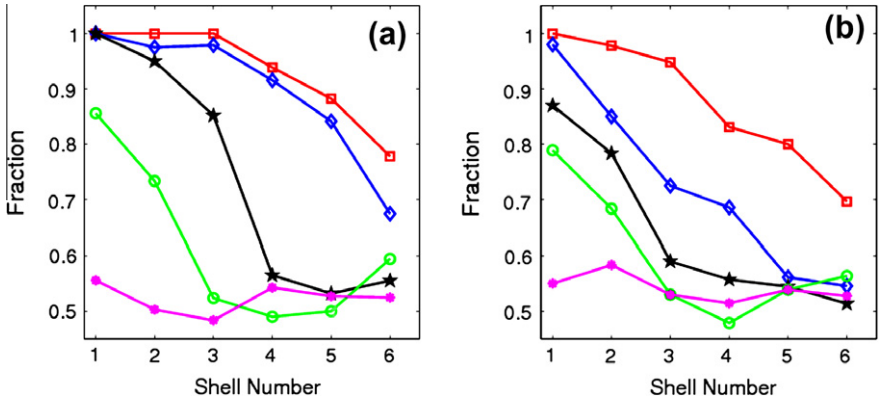

Fig. 8. Fraction of atoms in ordered sub-lattices in two sizes 2.23 nm (a) and 3.72 nm (b). The symbols correspond to different temperature: $T = 0.38T_0$ (red squares), $T = 0.55T_0$ (blue diamonds), $T = 0.69T_0$ (black stars), $T = 0.87T_0$ (green circles), and $T = T_0$ (purple points). Shell 6 is surface shell, and shell 1 refers to the core shell. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

the phase separation is not likely to occur because the parameter in the disordered state is far smaller than one (full separation). The shape deformation χ, from the form 1 – c/a in the bulk size, perfectly reflects the real tetragonalization ratio in the disordered phase of NWs. The NWs with the size larger than 9 nm have similar qualities in bulk size and the simulated tetragonalization ratio is 0.07 near room temperature, close to the experimental value 0.05. The results of tetragonalization ratio are mainly from expansion during Monte Carlo simulation, while the common expansion method produces the tetragonalization ratio of 0.1 in bulk system. From this view, our method proves to be more practical in the simulation of transitions in NW system [14].

As in Fig. 5, the temperature difference ΔT in transition region decreases with the increase of cluster size. Moreover, the mixing parameter indicates the existence of short range ordering in a Co–Pt system. The transition temperature T^* clearly increases and the features are in agreement with the behavior for a first-order phase transition [28,29]. In order to prove the reliability of our simulating results, we take a simple test for the possible memory effects during Monte Carlo simulation. The transition of cylindrical nanowire with diameter of 6.16 nm was chosen as example. The same initial cells were developed to be simulated at different temperatures until they reach the steady state. Two kinds of order parameters were calculated during different temperature. Compared with the results from heating protocol, the relative error is less than 1.3%, which indicates that the hysteretic behavior could be neglected in our discussion. Therefore, we can calculate the fluctuations of the quantities, as illustrated in Fig. 6. Similar to the thermal averages of the order parameters, the fluctuations are mostly smooth except near the transition region. This character is demonstrated by the decrease of peak width and the increase of height. The maximum peaks are almost the same as the transition temperatures showed in Figs. 1 and 4. We pointed out in our previous model [13] that the transition of Co–Pt NWs is also surface dominant. In the present simulation, we obtained supplementary information to support our ideas. The inner structure of NWs could be divided by shells according to the distance from the center of cross-section. To explore the transition of inner structure of NWs, we track the snapshots of cross-sections during the order–disorder transition.

In Fig. 7, three snapshots of cross-section are presented from the ordered state to a disordered one, while the shape deformation accounting for tetragonalization is clearly presented. Moreover, the inner part of the nanowires remains orderly, while the surface is disordered. To obtain more details about the transition shell-by-shell, we divide the NWs into six shells according to their distances from the center. The thickness of the shell is defined as $R/6$ where R represents the radius of the cross-section. Like the definition of long-range order parameter, the fraction of two kinds of atoms in the ordered sub-lattices is calculated to represent the degree of order of the shells. In a fully ordered state, the fraction of two atoms is approximate to one, while in a fully disordered state, the fraction will fluctuate around 0.5 because either Co or Pt will randomly occupy all the sub-lattices. The two sizes are discussed and the results are demonstrated in Fig. 8.

Fig. 8 shows a numerical description of the surface-dominant phenomenon. The fraction of atoms drops from 1 to around 0.5, which clearly shows that inner atoms would not begin to transform until the outer atoms become disordered. The shell-by-shell transition is less obvious in smaller size because almost no atoms

have all their first and second neighbors occupied, which indicates that almost all the atoms are unstable surface ones. There may be an overlap of transformation because all the atoms could be considered as in the surface shell, and the interaction of different shells would also lead to a smoother transition curve. The surface atoms are supposedly in higher energy state, which will be more unstable than the inner atoms, and thus the extremely small nanosolids would be special systems.

4. Conclusions

The transition temperature of Co–Pt NWs increases with the rise of wire size, and approaches the bulk value. The transition temperature also depends on the shape of cross-section, while the shape effect is smaller than the size effect. These predictions are consistent with available data in literature. Furthermore, the present work confirms the efficiency of Bond-Energy model in predicting the order–disorder transition of bimetallic NWs. Further discussions on the mixing conditions of order–disorder transition show a lower tendency of phase separation in NWs than in NPs. Also, a smaller tetragonalization ratio was found in NWs, which is quite similar to the case in NPs. The order–disorder transition of NWs was proved to be surface dominant by comparing order conditions in different shells, while the atoms in the surface would become disordered firstly due to the effect of dangling bonds. The present study could deepen one's understanding on the mechanism of order–disorder transition at nanoscale.

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