Curie temperatures and critical exponent properties of FePd ferromagnetic materials by data simulations approach

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Abstract. This paper has systematically investigated the Curie temperature of Fe₁₋ₓPdx ferromagnetic materials under the data simulations approach. Using a Monte Carlo model, we calculated the Curie temperatures of Fe₁₋ₓPdx. The Curie temperature of the nanomaterial Fe₁₋ₓPdx was measured on variation of compositions (x) at x = 0.1, 0.3, 0.5, 0.7, and 0.9. The Curie temperature of nanomaterial Fe₁₋ₓPdx was found decreasing when the palladium (Pd) composition was increased. The Curie temperature is the transition temperature of ferromagnetic to a paramagnetic phase which can be analyzed using the calculation of critical exponents. The Curie temperature of data simulations was obtained and compared to the calculation of critical exponents. The results showed no difference of the Curie temperature obtained from both approaches.

1. Introduction
Magnetic materials which bear high perpendicular magnetocrystalline anisotropy (PMA), like FePd, are a competitive candidate for ultrahigh magnetic recording [1]. FePd materials are ferromagnetic materials with high Curie temperature [2]. The raising temperature of a ferromagnetic material will increase movements of atomic thermal thus it will allow the atom magnetic moment to align its direction [3]. This condition occurs when the temperature of ferromagnetic materials is below the Curie temperature. If the ferromagnetic material is heated over the Curie temperature, its spins will randomly orient, leading this material to its paramagnetic phase. Thus, ferromagnetic materials have low even zero saturation magnetization (Ms) if its heat exceeds the Curie temperature. In this case, the Curie temperature as a temperature of transition of a ferromagnetic material becomes a paramagnetic material, a significant parameter since it can help understand better the magnetic materials properties for an ultrahigh recorder media. Therefore, accuracy in Curie temperature calculation is a non-negotiable variable [4]. It, indeed, requires a fundamental study of Curie temperature in FePd materials.

The present study of FePd materials employed the computational theory approach. This approach is intended to observe the properties and characteristics of magnetic materials more appropriately with inexpensive costs, using a micromagnetic simulation. The simulation of this study utilized Vampire software. Furthermore, the method used in the simulation is Monte Carlo method. This method uses a
random number in simulating a physics system which seems impossible to be solved analytically by computing. This method consists of algorithms which are useful for visualizing magnetics of a particular material [5]. Thus, the Monte Carlo method lends itself very naturally to simulating systems in which stochastic processes occur.

2. Simulations
Nanomaterial \(Fe_{1-x}Pd_x\) random alloy model nanocube of FCC structures has been measured with composition variation \(x\) with \(x = 0.1, 0.3, 0.5, 0.7, 0.9\), employing micromagnetic simulations. In this process, the simulation was started by making two script files as inputs, namely one is for the material and the other is for the input. The former comprises information of parameters of FePd materials, such as exchange constant, anisotropy constant, atomic spin moment, uniaxial anisotropy direction, damping factor, and composition of the material. The parameters of FePd materials can be seen in Table 1. On the other hand, the input script file contains information about crystal structure of the material, cell unit (Å), minimum and maximum temperature, and output data, namely magnetization and temperature. The preferable size of the material in the study is 5 nm with uniaxial anisotropy direction by \([0 0 1]\) and damping factor of \(\alpha = 0.01\) at 0 K to 1200 K temperature.

The measurement of Curie temperature was obtained from the graph of magnetization change towards the heat. From the graph, the Curie temperature of FePd materials determined by considering the magnetics point when approximating zero, as illustrated in Figure 1.

| Crystal Structure | Iron (Fe) | Palladium (Pd) | FePd | Unit |
|-------------------|-----------|----------------|------|------|
| Cell Unit         | BCC\(^a\) | FCC\(^c\)      | FCC\(^d\) | -    |
| Exchange \(Jij\) Constant | \(3.028 \times 10^{-21}\) \(^b\) | \(1.289 \times 10^{-21}\) | \(3.277 \times 10^{-21}\) | J/link |
| Atomic Spin Moment | \(2.22\) \(^a\) | \(0.35\) \(^d\) | - | \(\mu B/atom\) |
| Anisotropy Constant \(k\) | - | - | \(2.6487 \times 10^{-23}\) | J/atom |

\(^a\) Evans et al. [6]  
\(^b\) Bazerra-Neto et al. [7]  
\(^c\) Kudasov and Korshunov [8]  
\(^d\) Burzo and Vlaic [9]
\[ M(T) \sim (T_C - T)^\beta \]  

where \( M(T) \) is magnetization saturation, \( T_C \) is Curie temperature, \( T \) is temperature and \( \beta \) is critical exponent. The average of the critical exponent is \( \beta = \frac{1}{2} \).

3. Results and Discussion

The magnetization change curve to temperature for nanomaterial \( \text{Fe}_{1-x}\text{Pd}_x \) random alloy model nanocube of FCC structure with the composition variation of \( x = 0.1, 0.3, 0.5, 0.7, 0.9 \) is shown in Figure 3. It shows that the Curie temperature generated is reliant on the provided composition of the material. The result shown in Table 2 indicates the continuous increase of the Curie temperature of \( \text{Fe}_{1-x}\text{Pd}_x \) along with the increasing composition of Fe. This occurs due to the nature of Fe material as a ferromagnetic material, while that of Pd is paramagnetic material; therefore, the more compositions of Fe, the greater Curie temperature generated. Essentially, only the ferromagnetic materials have Curie temperature.

![Figure 3. Curie Temperature of \( \text{Fe}_{1-x}\text{Pd}_x \) random alloy model nanocube of FCC structure](image)

| Composition | \( \text{Fe}_{0.1}\text{Pd}_{0.9} \) | \( \text{Fe}_{0.3}\text{Pd}_{0.7} \) | \( \text{Fe}_{0.5}\text{Pd}_{0.5} \) | \( \text{Fe}_{0.7}\text{Pd}_{0.3} \) | \( \text{Fe}_{0.9}\text{Pd}_{0.1} \) |
|-------------|-------------------------------|-------------------------------|-------------------------------|-------------------------------|-------------------------------|
| Curie T (K) | 380                           | 520                           | 620                           | 660                           | 680                           |

![Table 2. Measurement of Curie temperature of \( \text{Fe}_{1-x}\text{Pd}_x \) materials with FCC structure](image)

![Figure 4. Curie temperature models of alloy \( \text{Fe}_{1-x}\text{Pd}_x \) nanocube by polynomials fitting](image)
As seen in Figure 4, curie temperature of alloy Fe$_{1-x}$Pd$_x$ nanocube can be modeled by polynomials fitting and the model is, \( y \) (K) is curie temperature of alloy Fe$_{1-x}$Pd$_x$, and \( x \) is compositions of Pd)

\[
y = -535x^2 + 165.71x + 665.93
\]  

(2)

As seen in Figure 3, it was known that the magnetization declines along with the raise of temperature. This could happen when the temperature rises, the atomic spin which initially winds in the same direction gradually turns to random. The random spin orientation causes the ferromagnetic materials to have smaller to zero magnetization value. The magnetization will rise to maximum if the temperature is 0 K and will reach zero if the the material temperature is equal to the Curie temperature. For example, Figure 5 depicts the change of spin orientation of Fe$_{0.9}$Pd$_{0.1}$ material, from the same direction to random.

![Figure 5](image)

**Figure 5.** Analysis of spin orientation of Fe$_{0.9}$Pd$_{0.1}$ material at the change of magnetisation value

The simulation results were further analyzed using the critical exponent equation. Figure 6 describes the curve combination of Curie temperature from the simulation data and exact measurement, from equation (1), which is intended to strengthen the validity of the obtained result. As seen in Figure 6, it is known that the obtained result from the simulation and exact measurement of the critical exponent are equal. This exponent is essential to the sense that it offers a universal characteristic for differing data collected. The combination of the magnetization curve shows a striking result because this illustrates a more apparent continuous phase transition.
Figure 6. Analysis of Curie temperature of Fe$_{1-x}$Pd$_x$ material with composition variation ($x$)

4. Conclusion
The measurement of Curie temperature of Fe$_{1-x}$Pd$_x$ random alloy model nanocube with FCC structure material was done at composition variation ($x$) with $x = 0.1, 0.3, 0.5, 0.7, 0.9$. The result indicates that material composition significantly affects the generated Curie temperature. The result is further analyzed and evaluated using the critical exponent equation. The simulation results match well with the calculation of critical exponents.

References
[1] Wang L, Fan Z, Roy A G and Laughlin D E 2004 J. Appl. Phys. 95 (11) 7483
[2] Goo N H 2007 Formation of Hard Magnetic L10-FePt/FePd Monolayers from Elemental Multilayers Thesis Seoul: Max-Planck-Institut fur Metallforschung
[3] Askeland D R, Fulay P P and Wright W J 2011 *The Science and Engineering of Materials 6th ed.* (USA: Cengage Learning)

[4] Sudjatmoko 2007 Kajian Transisi Fase Lapisan Tipis Feromagnetik melalui Pengamatan Nilai Resistivitas Listrik Sebagai Fungsi Suhu. Yogyakarta: Pusat Teknologi Akcelerator dan Proses Bahan–BATAN Prosiding PPIPDIPTN ISSN: 0216 - 3128

[5] Newman M E J and Barkema G T 1999 *Montecarlo Methoden In Statistical Physics* (New York: Oxford University Press)

[6] Evans R F L, Fan W J, Chureemart P, Ostler T A, Ellis M O A and Chantrell R W 2013 *Atomistic spin model simulations of magnetic nanomaterials* (York: University of York)

[7] Bazerra-Neto M M, Ribeiro M S, Sanyal B, Bregman A, Muniz R B, Eriksson O and Klatau A B 2013 *Complex Magnetic Structure of Clusters and Chains of Ni and Fe on Pt (111)* Scientific Reports (Brazil: Universidade Federal do Para)

[8] Kudasov Y B and Korshunov A S 2006 *Phys. Lett. A* 364 348

[9] Burzo E and Vlaic P 2010 *J. Optoelectron. Adv. Mater.* 12 186.