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Atomistic Simulation of Temperature Dependent Magnetic Properties of Hole Doped 2H-VSe_2 Bilayer

Haq Siraj and Jisang Hong*

Department of Physics, Pukyong National University, Busan 48513, Republic of Korea

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Density functional theory calculations provide very accurate physical quantities at zero Kelvin. Nonetheless, it is necessary to understand how the physical quantities are changed at finite temperatures for real device application purposes. Here, we investigate the finite temperature dependent magnetic properties of hole doped 2H-VSe_2 bilayer structure using atomistic simulation. We find that the Curie temperature of 600 K at the hole concentration of 2.27×10^{20} cm^{-3}, and this is enhanced to 620 K at the hole concentration of 3.01×10^{20} cm^{-3}. We fit the temperature dependent magnetization curve (M(T)) using both Curie-Bloch and Kuz'min equations. We also calculate temperature dependent magnetic anisotropy energy. We find that the magnetic anisotropy energy is almost linearly decreased with increasing temperature. Besides, we obtain that the normalized temperature dependent anisotropy constant [K(T)/K(0)] shows the relation to the temperature dependent magnetization curve of $[M(T)/M(0)]^{2.9}$, and this is well converged with the exponent of 2.9 in the Callen-Callen theory.

Keywords : atomistic simulation, temperature dependency, 2D VSe2

1. Introduction

Magnetic materials are used in a wide range of potential applications like spintronics, data storage [1] and also in biomedical engineering [2]. In the study of magnetic materials, the key elements are exchange interaction, magnetization, coercive field, and magnetic anisotropy. Regarding these physical quantities, the density functional calculations provide very accurate values. However, strictly speaking, the first principles calculations are based only at zero Kelvin. But, all the aforementioned technologies are performing at finite temperatures. So, it is necessary to explore the finite temperature properties of all physical quantities. To this end, mostly two approaches are employed; micromagnetic [3-5] and atomistic models [6]. Micromagnetic simulation usually works at large length scale systems so that the periodic boundary conditions can be ignored [3]. The micromagnetic simulation considers small volume elements or cells in terms of a single magnetic moment (macrospin). Thus, the magnetization is assumed to be uniform. Also, the magnetization remains constant at finite temperatures, and this is one of the drawbacks of the micromagnetic model. Consequently, this approach may not explain the temperature dependency of a magnetic material.

As an alternative approach, the atomistic model considers a collection of spins (macrospin) to simulate the temperature dependent magnetic properties. Based on the atomistic model, one can easily calculate the Curie temperature (T_C) from the temperature dependent magnetization curve, and the estimated T_C itself is fairly good enough in many cases. Nonetheless, the temperature dependent magnetization (M(T)) curve deviates from experimental data, particularly at low temperature regions. So, it may require some parameters to fit the experimental data, and two approaches are employed; Curie Bloch equation [7] with a single fitting parameter and Kuz'min [8] equation using two parameters. Note that the Curie Bloch equation is good enough to extract a critical temperature, but it cannot properly reproduce the experimental magnetization curve behavior well. Then, the Kuz'min approach is widely applied if experimental data are available. As mentioned above, the density functional calculations provide the magnetic anisotropy energy of a material only at zero Kevin. To improve this shortcoming, the constraint Monte Carlo (cMC) method is usually applied to calculate the anisotropy energy at finite temperature [9].

*Corresponding author: Tel: +82-51-629-5573
Fax: +82-51-629-5549, e-mail: hongj@pknu.ac.kr

In our previous work [10], we reported the fundamental magnetic properties of the 2H-VSe_2 bilayer system. The pristine 2H-VSe_2 bilayer system had a layer-to-layer antiferromagnetic ground state in the pristine structure. However, we obtained a ferromagnetic ground state by hole carrier doping. Therefore, in this report, we aim to investigate the temperature dependent magnetic properties (temperature dependent magnetization and anisotropy energy) of the hole doped 2H-VSe_2 bilayer system.

2. Numerical Method

For atomistic simulations, VAMPIRE 5.0 simulator is used to determine the temperature dependent magnetization, magnetic susceptibility, and anisotropy for the hole-doped bilayer system. For temperature dependent magnetization curve and magnetic susceptibility calculation, we perform the Monte Carlo simulations with 10,000 equilibration timesteps and 10,000 loop timesteps. To reduce the finite system size effects, we use 30×30 supercells with periodic boundary conditions along x and y. The total Hamiltonian can be written as

$$H = -\sum J_{ij} S_i \cdot S_j - k_u \sum (S_i \cdot e)^2 - \sum \mu_s S_i \cdot H_{app} \quad (1)$$

The first term represents the exchange interaction (J_{ij}) between two spins at atomic sites, and the second term represents the anisotropy energy per atom (k_u). The last term indicates the interaction with an applied magnetic field. All the parameters for the simulations are adopted from our first principles calculations [10]. For determining temperature dependent anisotropy energy, we use the cMC method that operates on two spins and constrains the magnetization along a specific direction to allow the spins to reach thermal equilibrium. Since the system is not in equilibrium, the total internal torque τ acting on the magnetization does not vanish. For a system at a constant temperature, the magnitude of the torque (τ) acting on the system is $\tau = \frac{\partial F}{\partial \theta}$ where 'θ' is the constraining direction, and F is the Helmholtz free energy of the system. We can then compute the magnetic anisotropy energy as the variation of the free energy $\Delta F = -\int d\theta \tau$. The ΔF allows the reconstruction of the anisotropy energy (MAE) at different temperatures. In this way, we can calculate the temperature dependent anisotropy constant from the anisotropy energy.

3. Results and Discussion

We now discuss the temperature dependent magnetic

Table 1. Carrier concentration dependent structural and magnetic information. Here, J_1 and J_2 are the intra-layer and J_2 is the inter-layer exchange interaction.

2H-VSe_2 bilayer	Hole carrier (cm^{-3})	Lattice constant (Å)	J_1 (joule)	J_2 (joule)	μ_s (μ_B)	MAE (meV)
	2.27×10^{20}	a=b= 3.29, c = 13.19	6.95×10^{21}	1.83×10^{22}	0.98	2.01
	3.01×10^{20}	a=b= 3.29, c = 13.19	6.95×10^{21}	2.99×10^{22}	0.97	1.95

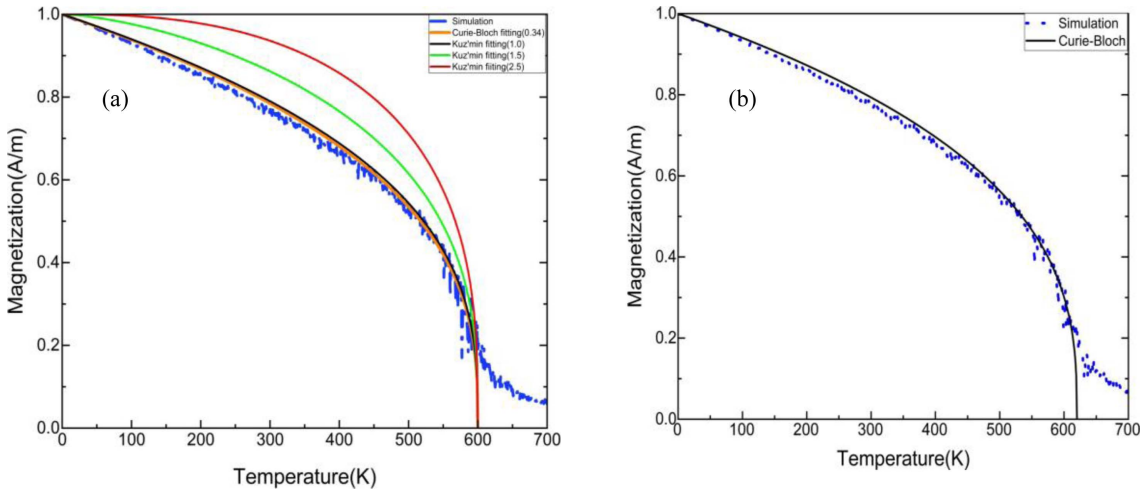

Figure 1. (Color online) Calculated temperature dependent magnetization curve and fitting curves with Curie-Bloch and Kuz'min equation with hole carrier concentrations of (a) 2.27×10^{20} cm^{-3} (b) 3.01×10^{20} cm^{-3}.

properties of the hole-doped 2H-VSe_2 bilayer system. Note that we obtain all parameters from our previous first principles calculations [10], and they are presented in Table 1.

Fig. 1(a) shows the simulated M(T) curve at a hole carrier concentration of 2.27×10^{20} cm^{-3}. To calculate the Curie temperature, we test two approaches to fit the curve; Curie-Bloch and Kuz'min equations. The Curie-Bloch equation has a form of $M(T) = \left(1 - \frac{T}{T_c}\right)^{\beta}$ whereas the Kuz'min equation has a form of $M(T) = \left[\left(1 - \frac{T}{T_c}\right)^{\alpha}\right]^{\beta}$. Note that the α can only be obtained from the experimental data, and both approaches become equal if α = 1. Since no experimental data for M(T) curve of the hole-doped system are available, we plot the M(T) curve with different α values. The blue dotted line and black line are the M(T) simulation and fitting with the Curie-Bloch method. All other curves are fitting using the Kuz'min equation. As shown, the Kuz'min curve deviates from the Curie-Bloch fitting by increasing the α value. Nonetheless, both approaches indicate the same critical temperature. We also estimate the Curie temperature in the hole concentration of 3.01×10^{20} cm^{-3}, and Fig. 1(b) shows the calculated M(T) curve. Here, we find the T_C of 620 K, and this enhancement is mainly due to the increased inter-layer exchange parameter as displayed in Table 1. To confirm the T_C, we also calculate the temperature dependent magnetic susceptibility function. The magnetic susceptibility of a ferromagnetic material generally decreases with increasing temperature in the Curie-Weiss law $\chi = \frac{c}{T - T_C}$, and also the magnetic susceptibility function shows a sharp peak near the T_C. Fig. 2(a)-(b)

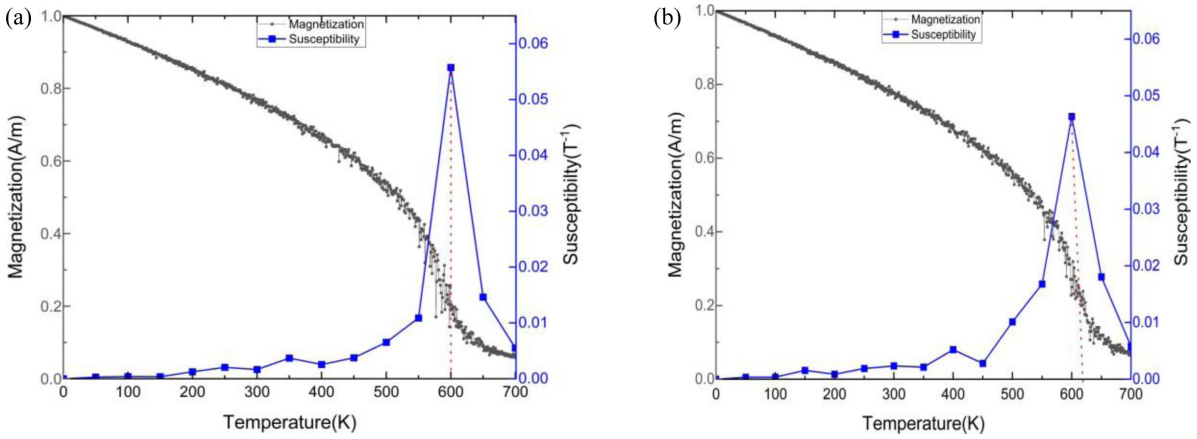

Figure 2. (Color online) Temperature dependent magnetization and magnetic susceptibility function with carrier concentrations (a) 2.27×10^{20} cm^{-3} (b) 3.01×10^{20} cm^{-3}.

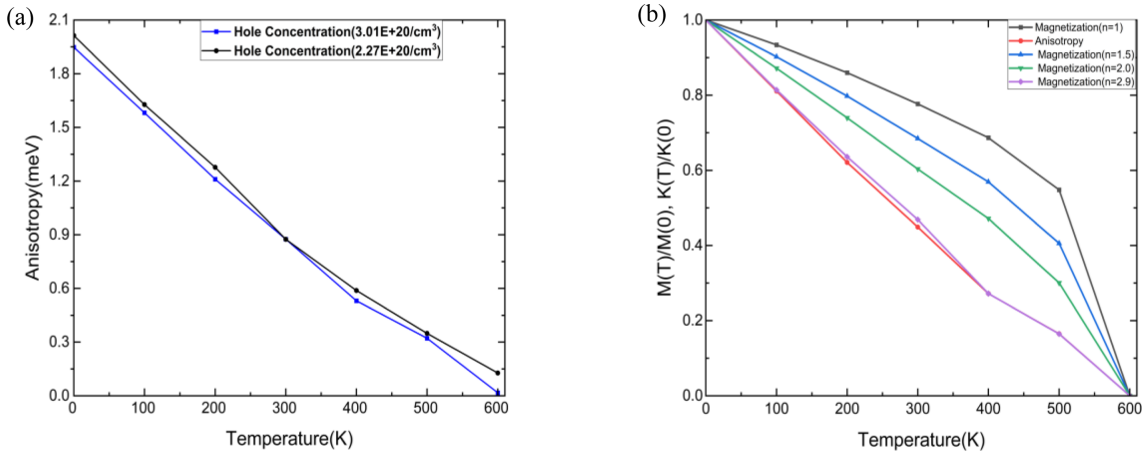

Figure 3. (Color online) (a) Temperature dependent anisotropy energy (b) correlation of the normalized magnetization and anisotropy constant using Callen-Callen power law.

shows the M(T) curves and magnetic susceptibility functions at the hole concentrations of 2.27×10^{20} cm^{-3} and 3.01×10^{20} cm^{-3}. As shown, the magnetic susceptibility function confirms the reliability of our estimated Tc.

We now present the temperature and carrier concentration dependent magnetic anisotropy energy using the cMC method. Fig. 3(a) shows the temperature and hole carrier concentration dependent magnetic anisotropy energy. The black and blue colors are for the hole carrier concentrations of 2.27×10^{20} and 3.01×10^{20} cm^{-3}. Due to the thermal effect, the anisotropy energy gradually decreases with increasing temperature. For instance, the anisotropy energy of the hole carrier 2.27×10^{20} and 3.01×10^{20} cm^{-3} are 2.01 meV and 1.95 meV at zero Kelvin, and it becomes 0.74 meV and 0.70 meV at room temperature. Note that the anisotropy constant (K) can be easily extracted by dividing the temperature dependent anisotropy energy over the volume. Regarding the relation of anisotropy constant and magnetization, Callen-Callen proposed the power law of $K(T) \propto M^n$ where $n = l(l+1)/2$ [11]. Although this law is originally proposed for a ferromagnetic insulator, we display the correlation between K(T) and M(T) i.e. $K(T)/K(0) = [M(T)/M(0)]^n$. In Fig. 3(b), we show the relation between normalized magnetization and normalized magnetic anisotropy constant at the hole concentration of 2.27×10^{20} cm^{-3}. The red color shows the normalized anisotropy constant; K(T)/K(0) while all other lines are the magnetization fitting curves with different exponent n. We find that the temperature dependent magnetic anisotropy constant and magnetization have a correlation of an exponent of 2.9 in the hole doped 2H-VSe_2 bilayer system. Note that we find the same exponent of 2.9 at the hole concentration of 3.01×10^{20} cm^3.

4. Conclusion

In summary, we perform the atomistic simulation to investigate the temperature dependent magnetic properties of the hole-doped 2H VSe_2 bilayer system. From the simulated M(T) curve, we fit using two different approaches; Curie-Bloch equation and Kuz'min fitting approach. We find that both approaches predict the same critical temperature although the temperature dependent magnetization curve itself may depend on the fitting parameters. We also calculate the temperature dependent magnetic susceptibility function to confirm the Curie temperature, and the estimated Curie temperature agrees with each other. Besides, we calculate the temperature dependent magnetic anisotropy energy, and the anisotropy energy is linearly decreased with increasing temperature. Moreover, we find that the normalized anisotropy constant K(T)/K(0) can be correlated to the magnetization with the exponent of 2.9 i.e. $K(T)/K(0) = [M(T)/M(0)]^{2.9}$.

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