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REGULAR ARTICLE

Modelling of the Room-Temperature Ferromagnetism in Hydrogenated Co-Doped ZnO by Rational Function

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Room-temperature ferromagnetism (RTFM) remains challenging to achieve in ZnO-based dilute magnetic semiconductors (DMS) co-doped with transition metals because of complex defect interactions. To explain the non-linear magnetization behavior of hydrogenated $Zn_{0.25}Co_{0.75}O$:H specimen is reported here. The specimen was made by a solid-state process and was hydrogenated at 550 °C for 12 hours. The room temperature magnetic hysteresis was measured with a Vibrating Sample Magnetometer (VSM) and analyzed by non-linear least squares fitting in MATLAB based proposed rational model. The optimized model parameters, i.e., $\beta_{SE} = 0.3782$, $\varphi_I = -0.0222$, and $\delta_d = 2.4433$, indicate increased magnetic saturation, weak inhibitive behavior, and high damping associated with oxygen vacancy-type defects, respectively. The results provide support to the rational model as a powerful approach to describe defect-induced ferromagnetism and provide guidelines to the design and optimization of spintronic materials presenting magnetic ordering at room temperature.

Keywords: Room-temperature ferromagnetism, ZnO, Hydrogenation, Rational function model, Vibrating sample magnetometer.

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1. INTRODUCTION

Spintronics, a frontier in condensed matter physics, controls the intrinsic spin of electrons along with their charge to enrich storage and information processing technologies. In Contrast to conventional electronic devices that are solely contingent on charge transfer mechanisms, spintronic devices rely on spin-polarized current mechanisms that offer steady memory, extremely low power consumption, and enhanced functionalities [1]. The real-world spintronics-based applications require an engineered specimen that can sustain their ferromagnetic ordering at room temperature, such as Dilute Magnetic Semiconductors (DMS), as they integrate magnetic properties with semiconductor resourcefulness [2].

ZnO is an II-VI semiconducting composite material whose ionicity lies at the border line between covalent and ionic semiconducting materials along with wide band gap (~ 3.37 eV), high exciton binding energy (~ 60 meV), transparency, biocompatibility, and non-toxic nature place it as potential material in designing biosensors, bioimaging, and medical diagnostics devices [3].

The functionality of ZnO-based DMS composites relay on the probability of substitution of Zn wurtzite lattice structured sites by doped transition metal ions like Mn, Fe, Co, Ni, or Cu that tends to create localized magnetic moments and can induce ferromagnetic ordering through indirect exchange interactions, such as the RKKY mechanism, mediated by electrons (*n*-type) or holes (*p*-type) in the valence band of ZnO [4]. However, achieving room-temperature ferromagnetism (RTFM) specifically in ZnO-based DMS composite is still a challenging task due to the lack of precise control over the various induced defects like oxygen vacancies [5], zinc interstitials [6], and dopant clustering [7]. These defects can promote or inhibit magnetic interactions, and a balance must be maintained between the two for DMS ZnO-based composites to be successfully applied.

In recent years, hydrogenation has been used as an annealing technique to improve the ferromagnetic TM-doped ZnO-based DMS composites [8-10]. Singhal et al. reported that FM ordering in Co-doped ZnO composites can be switched between "*on*" and "*off*" upon hydrogenation and after that, re-heating the specimen, respectively [11]. Singh et al. [12] reported that the annealing of ZnO films in a hydrogen environment boosts the ferromagnetic properties of ZnO films via forming O-H bonds and shallow donor states along with carrier-mediated exchange interactions among localized magnetic moments.

Our group also studied the effect of hydrogenation on the magnetic properties of Co-doped ZnO DMS composites and reported that hydrogen annealing causes the formation of Co–H–Co complexes along with an increment in oxygen vacancies, both aspects endorse effective magnetic coupling among Co^{2+} ions. Hydrogenation not only modulates the electronic structure but also

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influences the local defects, leading towards a noticeable improvement in saturation magnetization [13-14]. Our findings were attributed to the bound magnetic polaron (BMP) [15] and acceptor impurity band (AIB) [16] models, which attribute the role of hydrogen ions in tailoring the observed enhanced magnetic properties of Co-doped ZnO DMS-like composites [17].

Theoretical approaches, such as first-principles calculations [18] and empirical models [19], have been used to get valuable insights about complex interactions and underlying mechanisms that are responsible for a deeper comprehension of the material's behavior. Bassi et al. [19] reported that room temperature ferromagnetism of Co and Ni Co: ZnO DMS composites is improved by both Co and Ni dopants using Density Function Theory (DFT). The calculations focused on the strong magnetic interactions between the dopants and oxygen vacancies, providing insight into the electronic structure and magnetic properties of the material.

Accompanying these theoretical approaches, the present study proposed empirical rational function models to correlate experimental magnetization data of hydrogenated $Zn_{0.25}Co_{0.75}O$ specimens obtained using a Vibrating Sample Magnetometer (VSM). The proposed model helps quantify ferromagnetic (FM) coupling, saturation effects, and defect interactions, including their parameters. The present model aims to evolve defect-mediated strategies for next-generation spintronic materials that can be scalable and can sustain as room-temperature magnetic semiconductors.

2. MATERIALS AND METHODS

$Zn_{0.25}Co_{0.75}O$ specimen was prepared by the traditional solid-state reaction route with the powders of very high purity ZnO (99.99 %) and Co_3O_4 (99.999 %). The denser discs were formed by pelletizing, sintering mixtures of powder. Hydrogenation was performed in a quartz tube furnace with 99.999 % ultra-high pure H_2 gas flow at 550 °C for 12 h to achieve defect-induced ferromagnetism. Room-temperature magnetic properties were characterized by a Vibrating Sample Magnetometer (VSM) at an applied field of up to ± 3 Tesla [13]. The measured magnetization data were normalized and fitted by the non-linear least-squares procedures with MATLAB to obtain the model parameters.

3. THE PROPOSED RATIONAL FUNCTION MODEL AND ITS RELATION WITH EXPERIMENTAL DATA

Magnetization (M) as a function of applied magnetic field (H) is modeled using the following rational function:

$$M = \frac{\beta_{SE} H}{1+\varphi_i H+\delta_d H^2} \qquad (3.1)$$

where β_{SE} term quantifies the saturation effect, reflecting how magnetization tends to level off at high magnetic fields, φ_i represents interaction coefficients among magnetic dipoles or clusters within the material, δ_d denotes the impact of defect interactions, especially due to oxygen vacancies or lattice distortions, particularly relevant in hydrogenated samples.

The proposed rational model (Eq. 3.1) is a phenomenological model designed to efficiently capture the nonlinear magnetization behavior of $Zn_{0.25}Co_{0.75}O$:H, predominantly after hydrogenation. In these systems, hydrogen serves as a shallow donor, involving the generation of carriers, while also inducing the formation of oxygen vacancies in the ZnO lattice. Such defects increase the exchange interaction between Co^{2+} at room temperature and establish ferromagnetism. The model is particularly suitable for both intrinsic and extrinsic-doping-related effects (e.g., hydrogenation) on the magnetic response of materials. Unlike more sophisticated physical models, which are, e.g., a bound magnetic polaron (BMP) model using a statistical Langevin description of polaron-induced magnetization, the rational function used here offers a simpler mathematical representation without sacrificing the desirable core mechanisms such as saturation, ion-ion interactions and defect-induced damping.

Table 1 – Parameters of Rational Function Model

No	Parameter	Hydrogenated $Zn_{0.25}Co_{0.75}O$
1	β_{SE}	0.3782
2	φ_i	− 0.0222
3	δ_d	2.4433
4	R^2	0.9960

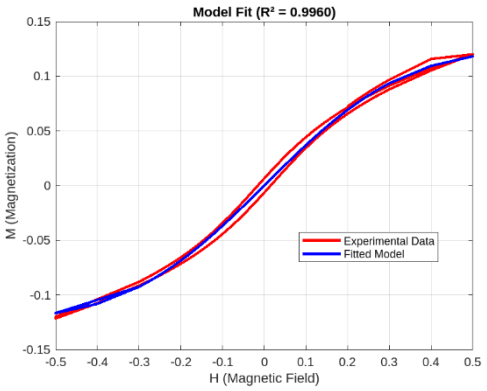

Fig. 1 – Magnetization curve fitted with rational function mod

In the proposed model, each parameter has a clear physical interpretation. Table 1 shows that the non-linear least-squares fitting technique with MATLAB values of, for $Zn_{0.25}Co_{0.75}O$: H case patient material was used for sequence (Fig. 1). The parameter $\beta_{SE} = 0.3782$ represents how well the magnetic moments orient along the direction of the external field in the weak-field limit. A low positive value is evidence of fast initial magnetization newly seen in the sample, indicating the increase of ferromagnetic ordering on hydrogenation [21-24]. The value $\varphi_i = -0.0222$ (which is marginally negative) indicates that there are weak compensatory or inhibitory interactions, which can either come from antiferromagnetic coupling between localized and delocalized magnetic carriers or competitive behaviors between the two contributions.

Nevertheless, the prevailing behavior is still ferromagnetic, indicated by a dominant tendency towards saturation. The factor $\delta_d = 2.4433$ accounts for the nonlinearity of the magnetization curve at higher fields, which is caused by structural imperfection. Its relatively large value from the result may be attributed to consid-

erable damping of hydrogenated oxygen vacancies, which locally suppress the alignment of spins and lead to the superparamagnetic saturation [25-27].

These parameters allow the model to closely track experimental data with a very high coefficient of determination, $R^2 = 0.9960$. This high-quality match verifies that the rational function not only makes mathematical sense, but also reflects the physics of the real magnetization behavior of the material. It very well captures the increase in the magnetization with applied field at lower fields, followed by saturation, as is expected for hydrogenated Co: ZnO. Thereby, the model is a reliable and practical model for the analysis of magnetic properties in DMS, and gives an accurate account of the competition between defect chemistry, carrier concentration and magnetic order [28-30].

4. CONCLUSION

The work proposed a rational function model to describe the scroll-like and symmetric non-linear *M-H* loops of hydrogenated Co-doped ZnO. It was successfully used to describe hydrogenation-induced defects on RTFM, with good agreement on R^2 for the experimental data (0.996). Important parameters – $\beta_{SE} = 0.3782$, $\varphi i = -0.0222$ and $\delta_d = 2.4433$ – account for the enhanced magnetic saturation, minor suppression interactions and significant defect-induced damping contributed by oxygen vacancies. These results reveal the effectiveness of hydrogenation in tuning magnetic properties in dilute magnetic semiconductors and a promising route for controlling spintronics materials. The model is a robust and straightforward representative to explain complicated magnetic phenomena. But the investigation has limitations, because only one composition and fixed hydrogenation conditions have been used, for which a generalization could be no more obvious. Further studies need to be extended to more dopants and temperatures and to deal with the condition parameters. The results in this work are meaningful in promoting the development of defect-engineered ferromagnetic materials towards applications in future devices.

REFERENCES

1. P.J. Rajput, S.U. Bhandari, G. Wadhwa, *Silicon* **14** No 15, 9195 (2022) https://doi.org/10.1007/s12633-021-01643-x.
2. P.H. Dederichs, K. Sato, H. Katayama-Yoshida, *Phase Transit.* **78** No 9-11, 851 (2005).
3. P. Kumari, et al., *Mater. Today Proc.* **43**, 3297 (2021) https://doi.org/10.1016/j.matpr.2021.02.299.
4. Aravind, M.K. Jayaraj, *Nanostruct. Metal Oxides Devices*, 233 (2020) https://doi.org/10.1007/978-981-15-3314-3_8.
5. H. Liu, et al., *J. Mater. Sci. Mater. Electron.* **26**, 2466 (2015) https://doi.org/10.1007/s10854-015-2707-y.
6. T. Shi, et al., *Appl. Phys. Lett.* **96** No 21 (2010) https://doi.org/10.1063/1.3432447.
7. J.C.A. Huang, et al., *Appl. Phys. Lett.* **85** No 17, 3815 (2004) https://doi.org/10.1063/1.1812844.
8. A. Singhal, *J. Alloys Compd.* **507** No 1, 312 (2010) https://doi.org/10.1016/j.jallcom.2010.07.189.
9. M.N. Mehathaj, N. Padmanathan, E. Sivasenthil, *J. Mater. Sci. Mater. Electron.* **33** No 14, 11523 (2022) https://doi.org/10.1007/s10854-022-08126-8.
10. M.P.F. De Godoy, et al., *J. Alloy. Compd.* **555**, 315 (2013) https://doi.org/10.1016/j.jallcom.2012.11.105.
11. R.K. Singhal, et al., *J. Alloy. Compd.* **496** No 1-2, 324 (2010) https://doi.org/10.1016/j.jallcom.2010.02.005.
12. P. Singh, et al., *J. Alloy. Compd.* **889**, 161663 (2021) https://doi.org/10.1016/j.jallcom.2021.161663.
13. R. Mukherji, et al., *Adv. Compos. Hybrid Mater.* **1**, 809 (2018) https://doi.org/10.1007/s42114-018-0052-3.
14. R. Mukherji, V. Mathur, *J. Nano- Electron. Phys.* **11** No 4, 03039-1 (2019) https://doi.org/10.21272/jnep.11(3).03039.
15. P. Kaur, et al., *Appl. Surf. Sci. Adv.* **5**, 100100 (2021) https://doi.org/10.1016/j.apsadv.2021.100100.
16. A. Di Trolio, A.M. Testa, A.A.°Bonapasta, *Nanomaterials* **12** No 9, 1525 (2022) https://doi.org/10.3390/nano12091525.
17. R. Mukherji, et al., *Philos. Mag.* **11** (2019) https://doi.org/10.1080/14786435.2019.1624851.
18. M.S. Khan, L. Shi, B. Zou, *J. Appl. Phys.* **127** No 6 (2020) https://doi.org/10.1063/1.5143487.
19. K.P. Misra, et al., *Semiconductors* **54**, 311 (2020) https://doi.org/10.1134/S1063782620030136.
20. M. Bassi, et al., *Appl. Phys. A* **130** No 11, 850 (2024) https://doi.org/10.1007/s00339-024-08018-0.
21. R. Mukherji, et al., *Mater. Focus* **7** No 6, 842 (2018).
22. R. Mukherji, et al., *Journal Nano- Electron. Phys.* **10** No 5, 05008 (2018) https://doi.org/10.21272/jnep.10(5).05008.
23. A.A. Dakhel, *Appl. Phys. A* **123**, 1 (2017) https://doi.org/10.1007/s00339-017-0867-8.
24. H.M. Lu, W.T. Zheng, Q. Jiang, *J. Phys. D: Appl. Phys.* **40** No 2, 320 (2007) https://doi.org/10.1088/0022-3727/40/2/006.
25. C.Y. Yang, et al., *J. Phys. D: Appl. Phys.* **47** No 34, 345003 (2014) https://doi.org/10.1088/0022-3727/47/34/345003.
26. S.H. Liu, H.S. Hsu, C.R. Lin, C.S. Lue, J.C.A. Huang, *Appl. Phys. Lett.* **90** No 22 (2007) https://doi.org/10.1063/1.2745642.
27. Z. Ke, Y. Li, C. Hou, Y. Liu, *Phys. Sci. Rev.* **3** No 10, 20170038 (2018) https://doi.org/10.1515/psr-2017-0038.
28. S. Dhieb, A. Krichene, N.C. Boudjada, W. Boujelben, *J. Phys. Chem. C* **124** No 32, 17762 (2020) https://doi.org/10.1021/acs.jpcc.0c04910.
29. H. Kumari, et al., *J. Photochem. Photobiol. A: Chem.* **453**, 115673 (2024) https://doi.org/10.1016/j.jphotochem.2024.115673.
30. P. Gao, et al., *Chem. Eng. J.* **359**, 828 (2019) https://doi.org/10.1016/j.cej.2018.11.184.

Моделювання феромагнетизму кімнатної температури в гідрованому колегованому ZnO за раціональною функцією

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Феромагнетизм за кімнатної температури (RTFM) залишається складним завданням для досягнення в розбавлених магнітних напівпровідниках (DMS) на основі ZnO, спільно легованих перехідними металами, через складні взаємодії дефектів. У цій роботі описано нелінійну поведінку намагнічування гідрогенізованого зразка $Zn_{0.25}Co_{0.75}O$:H. Зразок був виготовлений твердотільним методом і гідрогенізований при 550 °C протягом 12 годин. Магнітний гістерезис за кімнатної температури був виміряний за допомогою вібраційного магнітометра зразка (VSM) і проаналізований за допомогою нелінійного методу найменших квадратів у запропонованій раціональній моделі на основі MATLAB. Оптимізовані параметри моделі, тобто $\beta_{SE} = 0.3782$, $\varphi_I = -0.0222$ та $\delta_I = 2.4433$, вказують на підвищене магнітне насичення, слабку гальмівну поведінку та високе затухання, пов'язане з дефектами типу вакансій кисню, відповідно. Результати підтверджують раціональну модель як потужний підхід до опису феромагнетизму, індукованого дефектами, та надають рекомендації щодо проектування та оптимізації спінтронних матеріалів, що демонструють магнітне впорядкування за кімнатної температури.

Ключові слова: Феромагнетизм за кімнатної температури, ZnO, Гідрування, Модель раціональних функцій, Магнітометр з вібраційним зразком.