PHYSICS AND CHEMISTRY OF SOLID STATE
V. 25, No. 3 (2024) pp. 639-649
Section: Physics

DOI: 10.15330/pcss.25.3.639-649

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ФІЗИКА І ХІМІЯ ТВЕРДОГО ТІЛА
Т. 25, № 3 (2024) С. 639-649
Фізико-математичні науки

PACS: 85.75.-d; 75.50.Bb

ISSN 1729-4428 (Print)
ISSN 2309-8589 (Online)

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Ferromagnetic property in transition metal (Mn, Fe, Ni)-doped SnO_2 for spintronic applications: a review of computational and experimental studies

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The development of room temperature ferromagnetic property (RTFM) in TM doped SnO_2 has potential application in the field of spintronic, recently attracted attention. This material exhibits exceptional chemical stability, demonstrates N-type behavior with a high carrier density, and remarkably displays long-range ferromagnetic properties. However, the mechanism behind this ferromagnetic property (FM) is still not fully understood. Numerous surveys of the literature have indicated that factors such as the presence of oxygen vacancies, defects, type and concentration of dopants, temperature, and methods used for sample preparation have a notable impact on the performance of FM. Here we reviewed the FM mechanism which is noticed in Iron, Nickel, Manganese doped Tin dioxide material both experimental and computational method.

Keywords: Spintronic, DMS, RTFM, TM doped, DFT, GGA+U, GGA, PBE, LSDA, LSDA-SIC, SOL-GEL method, XRD.

Received 21 April 2024; Accepted 03 September 2024.

Introduction

The intrinsic spin of the electron and its associated magnetic moment along with the fundamental electronic charge develops the study of spintronics. It deals with fast data processing speed, non-volatile memories with less electrical power consumption. The logic operations, storage and communication of the data can be achieved with the same material technology using diluted magnetic semiconductors (DMS). In recent developments the oxide diluted magnetic semiconductors (ODMS) like HfO_2, TiO_2, ZnO and SnO_2 doped with transition metals are more advantageous than normal DMS materials. The ODMS are wide band gap semiconductors having high n-type carrier concentration, ecologically safe, transparent to light and cheap. The doping of TM results both semiconducting and magnetic property at room temperature. As SnO_2 is a n-type semiconductor with good conductivity, high carrier density and high chemical stability, its TM doped system is a potential candidate for spintronic applications. In this article we reviewed the development of FM by doping transition metals (Ni, Fe, Mn) with SnO_2 both by experimental and theoretical work.

SnO_2 occurs naturally in the form of cassiterite and possesses a rutile tetragonal form, with a 3.6 eV direct band gap [1, 2]. Compared to other oxide diluted magnetic semiconductor (ODMS) materials, SnO_2 boasts a large excitation energy [3] and excellent optical transmittance [4, 5]. As a result, it finds widespread use in a mixture of applications, including photovoltaic devices, solar cells, transparent electrodes, organic LED, gas sensors, touch sensitive screens, and transistors [6-11]. One of the key advantages of SnO_2 is its affordability, combined with its chemical stability in both acidic and basic solutions, thermal stability in high-temperature oxidizing environments and mechanical robustness, all of which make it highly versatile for a broad range of applications.

In recent years, there has been a surge in both experimental and theoretical investigations on SnO_2. When doped with transition metals, SnO_2 exhibits not only useful semiconducting properties but also ferromagnetic behavior. Interestingly, as reported in [12], SnO_2

nanoparticles have already demonstrated magnetic properties without requiring transition metal doping. Additionally, it is crucial to consider the effect of oxygen vacancy, which is familiar to be present in all wide band gap oxide semiconductors [13]. Given that room temperature ferromagnetic property (RTFM) is a necessary characteristic for materials intended for spintronic applications [14-17], further exploration of this property is essential. The d-sp exchange mechanism between the sp free carriers and d-states of the transition metal dopants and the double exchange mechanism between d-states of TM ions, play crucial roles in generating ferromagnetic property in ODMS [18].

We have gone through the Google Search, sciencedirect.com, EBSCO e-resources to review the related published papers basing on development of ferromagnetic property of Mn, Fe and Ni doped SnO_2 both for computational and experimental studies.

We observed for Mn-doped SnO_2 the magnetic moment increased with Oxygen vacancy than the presence of only transition metal. Again, co-doping with W results half metallic behavior and there was increase in magnetic moment. We also observed in some studies reported only para-magnetism, while others suggested the Oxygen vacancy and defect contribute FM with Mn-doping. For Fe-doped SnO_2 it was reported that both O-vacancy and Sn-vacancy increases the magnetic moment. SnO_2 nanoparticles doped with Fe can lead to paramagnetic behavior in the system due to weak antiferromagnetic interaction. But for Ni-doped SnO_2 with increase in doping concentration the magnetic moment was reduced. We also observed, as per one of the paper there was diamagnetism by doping Ni powder in Sn- site of SnO_2.

I. Ferromagnetic property in oxide based DMS

The idea behind the original source of ferromagnetism in ODMS is the most challenging area in solid state physics. The vibrating sample magnetometer (VSM), the superconducting quantum interference device (SQUID), the physical property measurement system (PPMS) and the electron spin resonance (ESR) techniques are used by the experimentalists to explore on this area. Most of the computational researchers are using various computational tools like BIOVIA material studio, Quantum Expresso, Vienna Ab intio Simulation Package (VASP) for these researches. Many literatures [19–25] explains oxygen vacancy, Sample preparation, type of dopant (and its concentration) and co-doping has a role for the magnetic behaviour. As reported in [26] the vacancy-induces ferromagnetism in undoped SnO_2. Similarly, undoped SnO_2 did not shows FM behaviour. But, SnO_2 thin films shows RTFM when doped with Mn, Cr, Fe, Co, or Ni [27–29].

As reported in the literatures [19, 30] the higher doping concentration completely removes the ferromagnetic behaviour of the doped one. Again, the co-doping of Ni-Mn, Fe-Co, Fe-Ni and Fe-Mn enhances the magnetism as reported in the literatures [18, 31]. Besides extensive experimental and theoretical successes, the idea behind RTFM in ODMS is controversial. Here, we present a brief review of the Fe, Ni and Mn doped SnO_2 system both in computational and experimental work.

Ferromagnetic property in Mn-doped SnO_2:

Several computational and experimental studies have shown that Tin dioxide with Manganese doping is a highly promising material for room temperature ferromagnetic property (RTFM). These investigations have been conducted by numerous researchers and have consistently demonstrated the potential of this material as an excellent candidate for RTFM.

Computational

In almost all of the computational literature, the calculation has been conducted the theoretical underpinnings of density functional theory (DFT) [32].The well-known SIESTA code [33-35] has been used in the literature [63] to implement DFT calculations. Specifically, LSDA and Ceperley-Alder functional [37] were used to perform calculations on Tin dioxide with Manganese doping with a doping concentration of 6.25%. The resulting magnetic moment was found to be 3.12 μB. The filled 3d-state of Mn was observed to be greatly hybridized with the 2p states of oxygen, leading to a large similar to the breadth of the oxygen 2p states. The outcome of these calculations indicates that Tin dioxide with Manganese doping was a semiconductor (as shown in Figure 1).

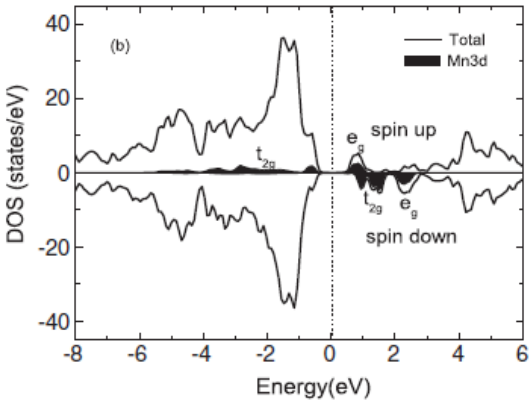


Fig. 1. In the case of 6.25% doping, the shaded 3d states of the TM ion (Mn) and the solid total states are shown for SnO_2 doped with the TM ion [36].

It is also reported that by changing the doping concentration up to 12.5%, the magnetic moment is observed as 3.12 μB for separated configuration and 3.13μB for closed configuration. Weak p-d coupling, hopping and super exchange in doped Tin Oxide results paramagnetism in ground state with O- vacancy. As a result, both the magnetic moments of the super cells and the transition metal ions grow. The magnetic moments of the 1st, 2nd TM as well as the overall magnetic moments of the super cells are included in Table 1 as information on the magnetic characteristics of the Oxygen vacancy containing systems. It is interesting to notice that when transition metal ions and Oxygen vacancy were in the same octahedron, with a distance of 2.06 Å between them, the magnetic moments of the TM ions sharply increase.

Table 1.
Referring to [36], the magnetic moments (in μB) of the 1st, 2nd TM (Mn) and the super cell in the presence of three types of vacancies (one, two, three oxygen vacancy) were given.

System	μTM-1 in μB	μTM-2 in μB	μSC in μB
$(O)_1$ Vacancy	3.25	3.27	6.15
$(O)_2$ Vacancy	3.29	3.82	7.11
$(O)_3$ Vacancy	3.84	3.85	7.93

Table 2.
In the same study mentioned earlier [36], the distances (in Å) between oxygen-vacancy and 1st TM, 2nd TM have also been reported.

Composition	**One oxygen Vacancy**	**Two oxygen Vacancies**	**Three oxygen Vacancies**
1st TM - (O) Vacancy	3.60	4.65	2.06
2nd TM - (O) Vacancy	4.24	2.06	2.06

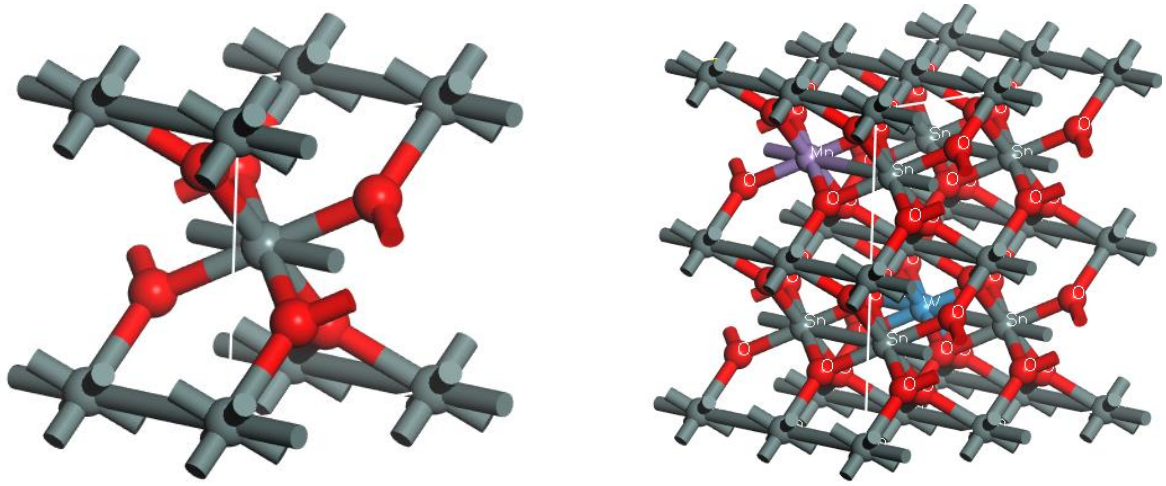
It's important to remember that the magnetic properties of Tin Dioxide with TM doping can vary significantly depending on different conditions. Generally, paramagnetism has been found to be more stable than ferromagnetic property in Transition Metal doped SnO_2. The presence of an oxygen vacancy has an impact on the magnetic characteristics of the doped system.

In a study conducted by A. Fakhim Lamrani *et al.* [38], the calculations are done by GGA-ZY formalism [39] and the local density formalism the parameters are considered according to VBH [40]. Also, it is used to calculate the magnetic properties of $Sn_{1-x}Mn_xO_2$ with x=0.0625. The rutile SnO_2's magnetic characteristics with Mn-doping was studied after employing the spherical augmented wave method. The results indicated that the total magnetic moment in $Sn_{15}MnO_{32}$ is 3μB, which is consistent with the magnetic moment of 3.12 μB obtained by the SIESTA code. Furthermore, the study found that co-doping with W in $Sn_{1-2x}Mn_xW_xO_2$ resulted in half metallic behavior with a semiconducting nature and a high magnetic moment of 5μB, making it suitable for spintronic systems.

The electronic structure of SnO_2 was calculated [41] using LSDA and SIC-LSDA formalism [42,43]. This results a non-metallic character with a direct (at Γ point) band gap. In SIC-LSDA formalism energy band gap found as 3.3 eV, which matches well to the reported experimental data of 3.6 electron volts. A better half metallic behavior was observed for Tin dioxide doped with Manganese, with 5 % doping leading to a ferromagnetic system on LDA formalism and checked accuracy with Monte Carlo simulation with a transition temperature (Tc) of 500 K.

In their work, Sujata Roy *et al.* [44] utilized the MedeA-VASP [45-48] simulation package and the DFT framework with GGA and PBE exchange and correlation methods [49] to calculate the magnetic and electronic properties of Tin dioxide with manganese doping. Cut off energy was 400 eV with 10^{-5} eV tolerance, a 4x4x4 grid of K- points sampled [50]. The total DOS plot showed an asymmetric distribution of down-spin and up-spin electrons which results in a net magnetic moment value of 5.95 μB in $Sn_{22}X_2O_{48}$. The dopant is primarily responsible for magnetic density while the oxygen atoms nearby had a minor contribution. Furthermore, the system was found to be highly P-type which is crucial for the development of transparent electronic devices. Intrinsic oxygen vacancies in SnO_2 lead to N-type electronic conduction. The generation of P-type conducting materials based on SnO_2 was previously demonstrated both theoretically and experimentally. [51]

As reported by Long Lin *et.al.*52, as the distance between two Tin dioxide doped with Manganese increases, then the ferromagnetic property changes to paramagnetism. Where, all the computations were performed using CASTEP package [53]. This result is nearly matched with results obtained by Zhang *et.al.* [54] using the WIEN2K code. According to a study by J. Wang *et al.*, the introduction of Ga into the system results in



a *b*

Fig. 2. (a) The primitive rutile unit cell of Tin Dioxide can be visualized with gray colored balls representing tin atoms and Oxygen atoms are represented by red balls. (b) The $Sn_{14}MnWO_{48}$ unit cell was generated by substituting Manganese and Tungsten atoms for Sn atoms in a 2×2×2 super cell of SnO_2.

stable ferromagnetic property, and the calculated density of states and spatial distribution of spin density indicate that the ferromagnetic coupling between the magnetic moments induced by doping is due to the p-d interaction between the 2p orbitals of the Oxygen and 3d orbitals of the Manganese. Furthermore, the study found that oxygen vacancies do not support the stabilization of ferromagnetic property. In a reported study, the experimental band gap of 3.6 eV for bulk SnO_2 was successfully replicated using the (GGA+HUBBARD U) approach, while the Mn-doped system exhibited semiconducting magnetic behavior in both (GGA+HUBBARD U) and GGA methods, with a

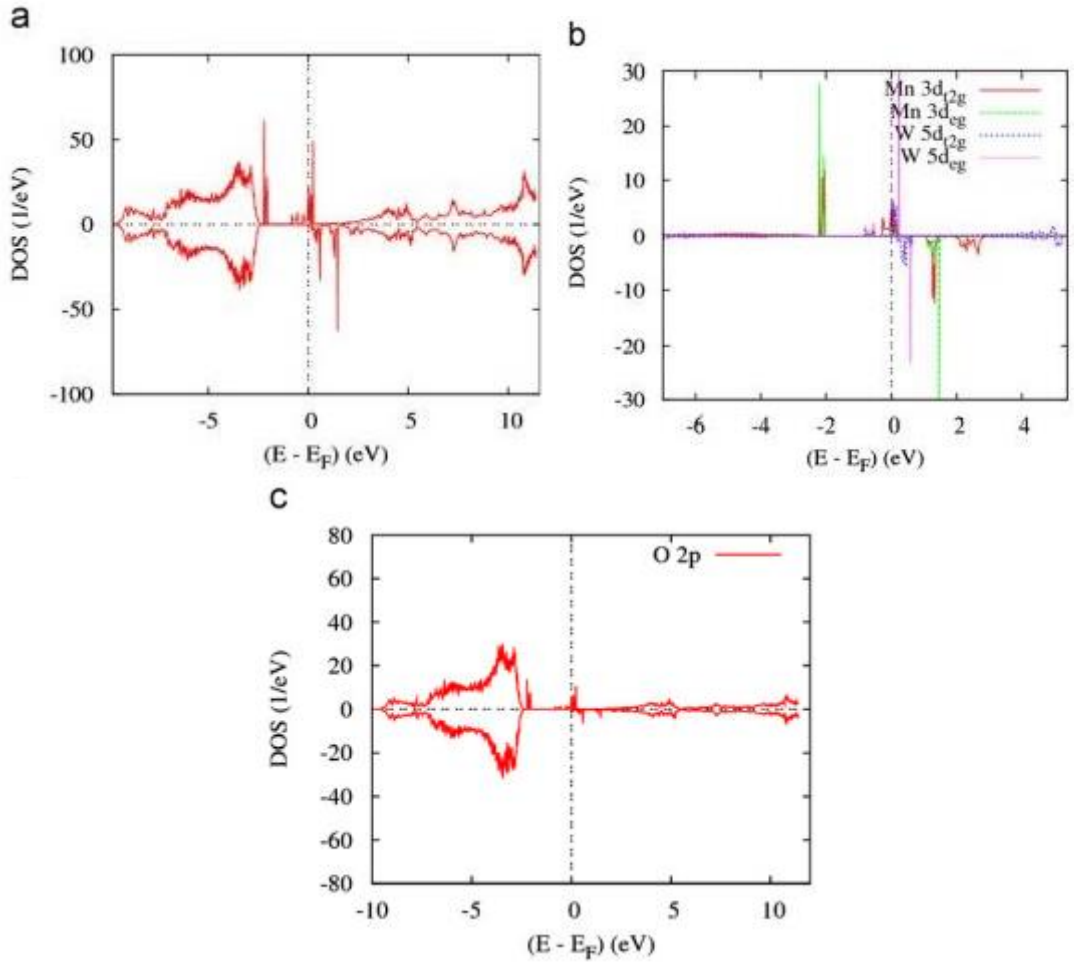


Fig. 3. The spin-polarized DOS of $Sn_{14}MnWO_{48}$, including the TDOS, 3d state PDOS of Mn and 5d state of W, neighboring O-2p states for a 3.7 Å Mn-W distance, were calculated [38].

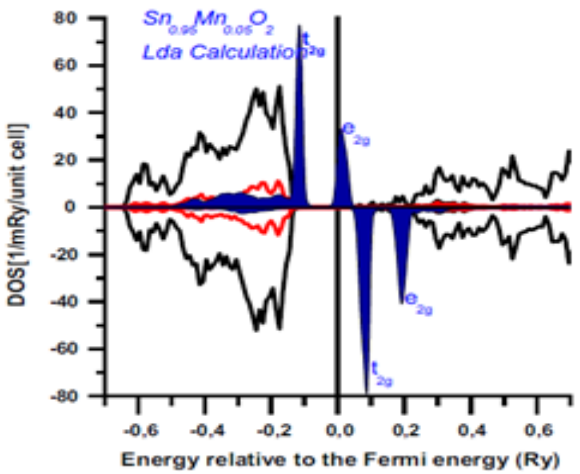


Fig. 4 The TDOS and the 3d state of TM (Mn) projected DOS of SnO_2 calculations carried out using SIC-LSDA formalism, where the TDOS is represented by a solid black line and the blue zone represents the 3d-state of Transition Metal (Mn) [41].

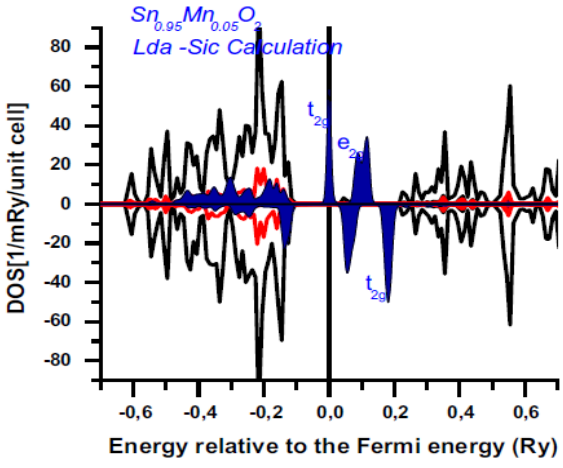


Fig. 5 The LSDA-based TDOS and d (TM)-DOS projected of SnO_2 are shown, with the TDOS represented by black solid line and the 3d-DOS of TM (Manganese) indicated by the blue region.[41].

calculated magnetic moment of 3.0 μB using U=4.0 eV where the WIEN2K code and the Full potential-LAPW method were carried out. [55, 56]

Experimental:

The ferromagnetic (FM) behavior in Tin dioxide with Manganese doping is dependent on multiple factors, with some studies reporting only paramagnetic behavior [57] while others suggest that oxygen vacancies and defects contribute to FM with Mn doping playing a role [58], and still others reporting that oxygen vacancies are the cause of FM in Mn-SnO_2 powder and Mn doping is significant for room-temperature FM, and high levels of Manganese dopant can even degrade the Ferromagnetic behavior [59, 60].

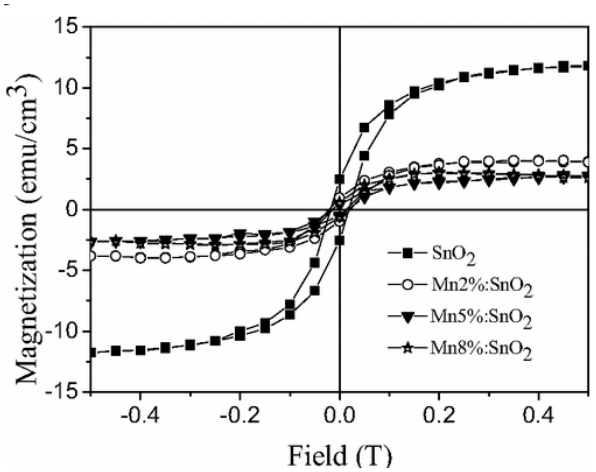


Fig.6. RTFM for undoped and Mn-doped tin oxide thin films [58].

The magnetic property in Mn: SnO_2 nanoparticles was influenced by both the sintering temperature and the concentration of doping [61]. According to previous reports, the Sol-Gel synthesis of Mn: SnO_2 thin films has demonstrated that both dopants and interactions between electronic clouds have a notable impact on the FM properties [62]. The exact reason for the FM observed in the Mn: SnO_2 system is still uncertain, and it remains a topic of controversy.

Ferromagnetic property in Fe: SnO_2 :

Various computational and experimental researchers reported SnO_2 doped with Fe exhibits ferromagnetic behavior in its ground state and the Curie temperature are of high value [63, 65] where, Oxygen vacancy attracts Fe ions.

Computational:

The software is based on DFT for most of the computational research. In the work done by X L Wang *et.al*.[36], an electronic metallic structure generated in Tin dioxide with Iron doping and AFM is more unstable than FM. Curie temperature is reported to be 610K using pulsed- laser deposition [64]. Others [65] Fe-doped synthesized powder samples of SnO_2, which display a Curie temp of 850K.It is reported that with O-vacancy magnetic moment of TM ions as well as the super cells increases and maximum has been achieved when the distance between the Vac(O) and TM ion is $2.06A^0$ (Table-2, [36])

Table 3.
Magnetic moments of the 1ST TM ($\mu^{1ST\ TM}$), 2ND TM ($\mu^{2ND\ TM}$) (Fe) and the super cell total moments in the presence of one, two and three oxygen vacancies [36].

System	μTM 1 in μB	μTM 2 in μB	μSC in μB
$(O)_1$ Vacancy	3.88	3.87	9.02
$(O)_2$ Vacancy	3.89	4.05	9.41
$(O)_3$ Vacancy	4.05	4.07	9.93

Ab initio study [66] of magnetic properties of Iron doped rutile SnO_2, for different concentration and distribution of Fe atoms and O-vacancy reports, O-vacancies are fundamental for the magnetic response of Fe-doped SnO_2. In this computation, it is observed that two Fe ions participate in sharing an oxygen vacancy and exhibit ferromagnetic coupling, resulting in the formation of a bound-magnetic polaron (BMP). Additionally, it is noted that two adjacent BMPs are aligned in an anti-parallel configuration. The overall magnetic properties involve the interplay between Oxygen vacancy and doping atoms. A quantum chemical study [67] of O-vacancy with Fe and Ni co-doping in SnO_2 crystal has been performed using DFT +U method using GGA formalism. It is reported that magnetic moment increased by the significant hybridization between the 3-d state of Iron and 2p state of Oxygen. (Fig-07). It is also reported that the Oxygen vacancy is essential to magnify magnetism in SnO_2, but it not only induces a magnetic moment but also backed by some experimental [68] and theoretical [69] confirmation of local magnetic moment with only Sn-vacancy.

Some reported [70] ferromagnetic stability in Tin dioxide with Moments of iron doping thin films range from 1.06 to 4.76 μB. With LSDA- SIC and LSDA formalism a good half metallic behavior was predicted for Iron-doped SnO_2 [41]. It is also reported that, the more precise Monte Carlo Method was used to determine the Curie temperature within the surrounding conditions. In the case of (Sn, TM) O_2 with 5% doping, the system is ferromagnetic, LSDA spin glass phase and SIC-LSDA formalism is more unstable than the ferromagnetic phase.

Fu *et al.* [71] used RF magnetron sputtering to create a Sn_{1-x} Fe_xO_2 film.No clusters and secondary phases were discovered. According to reports, the saturated ferromagnetic strength increases with increased iron doping concentration while the carrier concentration drops, suggesting that the ferromagnetic feature may be generated by Vo. Some reported [72] the order of magnetic moments as $Sn_{14}FeO_{32} > Sn_{15}FeO_{31} > Sn_{15}FeO_{32} > SnO_2$ Where, $Sn_{14}FeO_{32}$ and $Sn_{15}FeO_{31}$ are in the most reliable ground condition. Additionally, it has been noted that systems with Tc above room temperature have variable magnetic moments when iron is doped with one O-vacancy or one Sn-vacancy at various concentrations. Iron-doped SnO_2 with Sn-vacancy demonstrates half-metallic property that is incredibly helpful as a source for hole injection for DMS. The most stable form of iron-doped SnO_2 contains O-vacancy, and the strongest magnetic moment is found in Sn-vacancy. Some others [44] also reports, Iron doped SnO_2 doped at Sn-site give a ferromagnetic (Parallel spin ordering) ground state with

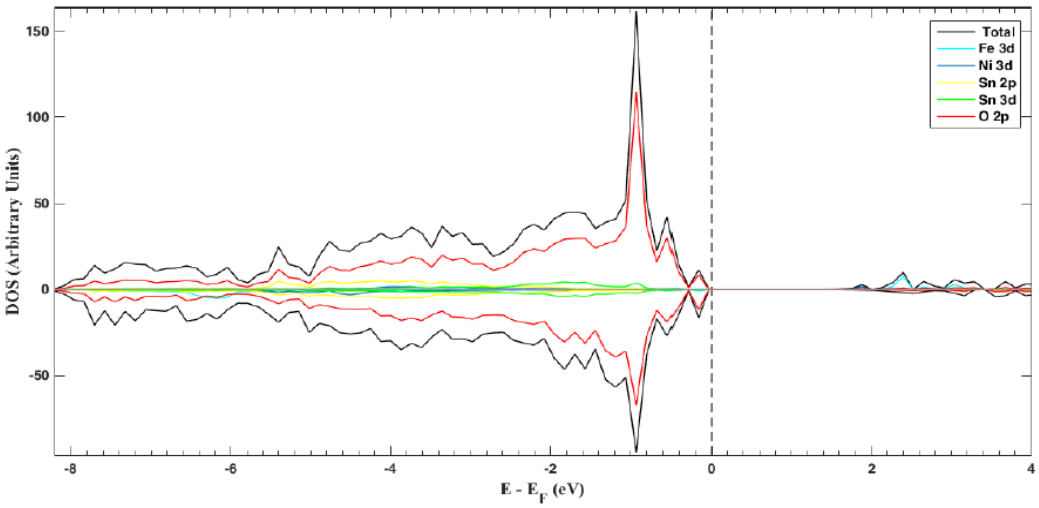


Fig. 7. The most stable DOS pattern co doping configuration. The Fermi Level is indicated by the vertical dotted line [67].

magnetic moment around 4.5 μB. Work done by Milman *et.al.*[73] reports 5% of Iron doped SnO_2 film grown with PLD shows RTFM with magnetic moment of 1.8 μB per Iron. It is also reported that the electronic configuration of the dopant plays major role in the magnetic behavior of the doped system. Others report [74], Comparing the Fe^{2+} doped case with the Fe^{3+} doped case, the Fe^{3+} doped SnO_2 is more likely to achieve high Curie temperature and magnetic moment at the same doping concentration and position. SnO_2 with Fe^{3+} doping demonstrates complete polarizability of the conduction holes. This is incredibly helpful as a source for hole injection and may eventually be utilized as a DMS.

Others reports [55] Iron-doped system illustrates magnetic semiconducting states within both Generalized Gradient Approximation and (GGA+HUBBARD U) scheme with total internal magnetic moment of 2.0 μB both in GGA and (GGA+HUBBARD U) Iron-doped SnO_2 system.

Experimental:

The X-ray diffraction technique was employed to determine the crystallographic structures of Iron-doped SnO_2, and magnetic measurements were carried out using a SQUID magnetometer. There are reports in the literature suggesting that defects in un-doped Tin dioxide may contribute to the observed ferromagnetic property [75, 76]. It has been observed that both un-doped Tin dioxide and with Iron doping thin films exhibit the FM property, which is attributed to O-vacancy, and a component of magnetism is observed in Tin dioxide as well, as illustrated in figure [77].Some studies have reported a decrease in the magnetic moment with an increase in the concentration of transition metals (TM) in Iron-doped SnO_2 [78]. Co-doping of Iron- SnO_2 induces lattice distortion, which enhances ferromagnetic saturation magnetization compared to non-co-doped samples, according to other reports [79]. The ferromagnetic behaviour of iron doped tin dioxide is significantly influenced by oxygen vacancies, according to some studies [80]. The iron-doped tin dioxide's ferromagnetic properties thin films are believed to result from the ferric ion coupling through an electron confined to an oxygen vacancy, as reported by another group [81]. Iron doping in SnO_2 nanoparticles can lead to a paramagnetic behaviour in the system due to weak anti-ferromagnetic interaction, as reported by one study [82]. However, the decline in anti-ferromagnetic interaction was found to decrease with an increase in Fe concentration, according to another study [83]. Increasing the Fe concentration in Tin dioxide nano powders was reported by some to reduce oxygen-related vacancies and change the magnetic properties to paramagnetic. It has been observed that the magnetic characteristics of a system can be influenced by doping Tin dioxide and SnO with Iron during the sample preparation process [84]. Additionally, a study has reported that magnetic transition (MT), which occurs when behaviour changes from paramagnetic to ferromagnetic at low and ambient temperature can be influenced by changes in temperature.

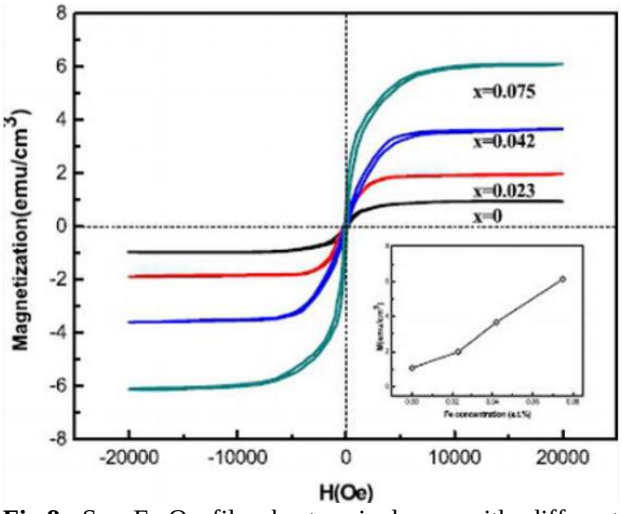


Fig.8. $Sn_{1-x}Fe_xO_2$ film hysteresis loops with different concentration at 300K.The insert is the difference in the concentration of Fe doping in saturation magnetization [80].

Ferromagnetic property in Ni doped SnO_2:

RTFM is reported in Tin dioxide with Nickel doping in different computational and experimental researches.

Computational:

Most of the computational work is done by VASP computer code [87] which is based in DFT [86,87] within GGA method. As reported in the literature [44] Tin dioxide with Nickel doping is not able to initiate magnetic moment ($Sn_{22}X_2O_{48}$) system. Dopant like Ni Initiate P-type system analogous to the pristine one. In literature [55] it is reported that Tin dioxide with Nickel doping holds magnetic/non-magnetic character of semiconductors for GGA +HUBBARD U or GGA functional. Insulating non-magnetic states (Both GGA and GGA+HUBBARD U) were reported in rutile tin dioxide with nickel doping, with U=3.8 electron volts on Nickel 3-d states at 6.25 percentage of occurrence [88]. Nickel -doped SnO_2 displays a degenerate semiconducting Total DOS including a 0.91eV band gap [figure 4(g); L-55] by GGA spin- polarized method. With (GGA+HUBBARD U) method (U=3.5 eV) Nickel-doped structure shown a non-degenerate semiconducting Total DOS with 0.37 eV band gap, which leads in magnetic property as shown in figure 5(g) of literature – [55]. Hence, we conclude that the system found to be a magnetic semiconductor. Total integral magnetic moment of 0μB/4 μB are calculated in GGA/(GGA+HUBBARD U) methods. As previously reported that Tin dioxide with Nickel doping can-not produce magnetic property without vacancy of oxygen even in (GGA+HUBBARD U) method[88], which contradicts the result of integral magnetic moment of 4μB with (GGA+HUBBARD U) method as reported in literature [55].

Experimental

XRD and VSM measurements accustomed to determine the crystallographic Magnetic and structural characteristics of $SnNiO_2$ thin films and powders. Studies have shown that oxygen vacancies and defects contributes to ferromagnetic property in Tin dioxide with Nickel doping [89]. However, in some cases, nano structured crystalline Tin dioxide with Nickel doping exhibits ferromagnetism as the Ni content increases up to ~ 3 mol%, but further increasing the Ni content, the ferromagnetism rapidly falls and paramagnetism was noted, which may be due to the accumulation of Ni ions on the particle surface and changes the magnetic behavior by reducing the available oxygen vacancies and/or the free electrons[90]. It has been reported that an increase in concentration of Nickel doping reduces in the magnetic moment [90]. Tin dioxide with Nickel doping powder in the Sn-site leads to a diamagnetic state [91]. The introduction of room-temperature ferromagnetic property in SnO_2 nano-particles via Ni-ion doping involves the creation of multiple defects or vacancies of Oxygen [92]. It has also been reported that the observed ferromagnetic property in Ni: SnO_2 thin films could be described in the BMP mode [93].

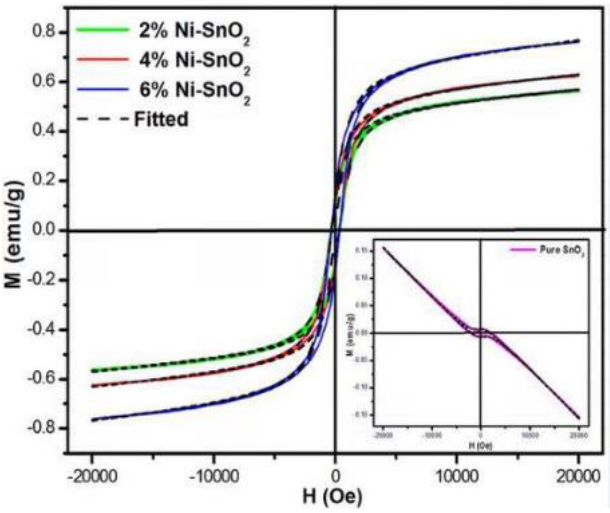


Fig. 9. Room temperature magnetization for pure and Ni doped SnO_2 [90].

Conclusion

As reviewed, the cause of RTFM in SnO_2 doped with Manganese, Nickel and Iron is intrinsic to the material itself. It can be influenced by factors such as O-vacancy, Sn- vacancy, doping concentration and defects in the crystal structure resulting from sample preparation. In some cases, the magnetic moment increases or decreases and even the developed magnetism may be ferromagnetism/ para-magnetism /diamagnetism. However, the reported types of FM property are not consistent and indicates the need for further research in this area. One can extend the research by doping all the TM ions(Sc,Ti,V,Cr,Mn,Fe,Co,Ni,Cu,Zn) considering both O-vacancy and Sn-vacancy and also keeping the TM ions in a suitable separation. One can increase the % of doping. Additionally, co-doping with different transition metals has been suggested as a potential way to enhance the RTFM. One may observe p-type conductivity along with magnetic property which are basic requirements for various spintronic applications.

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Феромагнітні властивості SnO_2, легованого перехідними металами (Mn, Fe, Ni) для спінтроніки: огляд обчислювальних та експериментальних досліджень

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Дослідження феромагнітних властивостей при кімнатній температурі (ФВКТ) у легованому перехідними металами (ПМ) SnO_2, має потенційне застосування в галузі спінтроніки. Цей матеріал демонструє виняткову хімічну стабільність, поведінку N-типу провідності із високою густиною носіїв, а також чудово проявляє феромагнітні властивості на великій відстані. Однак, механізм цих феромагнітних властивостей (ФМ) досі не повністю зрозумілий. Детальний аналіз літератури показав, що такі фактори, як наявність кисневих вакансій, дефекти, тип і концентрація легуючих домішок, температура та методи, які використовуються для підготовки зразків, мають значний вплив на продуктивність ФМ. У статті розглянуто механізм ФМ, який помічено в матеріалі діоксиду олова, легованого залізом, нікелем, марганцем, як експериментальним, так і обчислювальним методами.

Ключові слова: спінтроніка, DMS, RTFM, TM легування, DFT, GGA+U, GGA, PBE, LSDA, LSDA-SIC, золь-гель метод, XRD.