

## Poster Sessions

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The two compounds mentioned in the title ( $\text{In}_{1.0}\text{Fe}_{0.1}\text{Te}_{0.9}$ ,  $\text{In}_{1.0}\text{Co}_{0.1}\text{Te}_{0.9}$ ) are semimagnetic semiconducting materials of very useful application. The two compounds were prepared under Vacuum. X-ray diffraction patterns of the two compounds showed the presence of the same two different phases in each sample, one of the phases is InTe and the other is  $\text{In}_4\text{Te}_3$ . No trace of Fe or Co was found in both samples or even as remains in the corresponding diffraction pattern. The quantitative phase analysis showed that InTe phase was a major phase of nearly 80% in both samples. Rietveld analysis were used in order to find the exact location of the Fe and Co atoms in the two phases in both samples, the In and the Te atoms positions were also found. The R factor of the refinement was found to be 0.09. The magnetization curve seems to show a paramagnetic properties for the two samples since the magnetic curves for the two samples pass through the origin. The saturation Flux were found to be 0.04545, 5.117, 2.689 emu/g for the pure InTe sample, the iron and cobalt Sample respectively. The MUD program were used in order to find the Crystallite size and microstrain in both phases for the two samples. The structural, microstructural properties of the two samples were correlated with each other

Keywords: semimagnetic semiconductor, structural analysis, crystallite size, microstrain

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#### Properties and local structure analysis of N or Nb doped $\text{TiO}_2$

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Until now, many kinds of photocatalysts have been developed, and particularly  $\text{TiO}_2$  has been considered most promising for the strong oxidization ability.  $\text{TiO}_2$  is one of most promising photocatalyst because of its optical and electronic properties, stability, low cost and non-toxicity. However, the excitation of pure  $\text{TiO}_2$  by just ultraviolet irradiation has limited realization of effective utilization of solar energy because of 3-4% UV light in solar irradiation. In previous works reported that nitrogen doping could narrow the band gap and hence induce the visible light absorption of  $\text{TiO}_2$ . On the other hand, transparent conducting oxides (TCOs) are key components in many optoelectric devices. Nb doped  $\text{TiO}_2$  is a promising indium-free TCO. The purpose of this study is to examine the correlation between the band gap and the crystal local structure determined by Extended X-ray Absorption Fine Structure (EXAFS) analysis of N or Nb-doped  $\text{TiO}_2$ . Results indicate that nitrogen doping could narrow the band gap and shorten the interatomic distances between Ti and O atoms in  $\text{TiO}_2\text{:N}$ . The reason for this is that in anatase-type structure  $\text{TiO}_2\text{:N}$ , O atoms approaches Ti atoms followed by the repulsive force operates between doped N atoms and O atoms. On the other hand, it was discovered that Ti-O interatomic distances in all samples of  $\text{TiO}_2\text{:Nb}$ , which were synthesized in different temperatures, were shorter than

Ti-O distance in non-doped  $\text{TiO}_2$ . Moreover, it was found that the more the resistivity is low, the more Ti-O distance is long in the samples synthesized in different temperatures. These mean that the doping Nb atoms induces the enlargement of carrier concentration.

Keywords: photocatalysis, EXAFS, crystal structure and properties

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#### Crystal structural determination and SAXS/SANS structural analysis of human thrombomodulin domains

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Thrombomodulin (TM) is a membrane protein distributed in many different tissues with crucial functions in coagulation, fibrinolysis, cell proliferation, adhesion and inflammation. A unique feature of TM is regarding its intronless property. Current comprehension has been proposed to be a restriction in protein expression through regulation of different RNA splicing. Enhancement of blood coagulation function was not supposed to be through blood vessel per se, instead, possibly through pivotal mediations like thrombomodulin. The structures of TM are proposed to be responsible for its functions. The lectin-like domain of TM can be categorized as family containing C-type lectin, which is strongly involved in cell adhesion and inflammations, especially the properties regarding its carbohydrate recognition domain structure. As a consequence, it is absolutely essential to understand the structure of TM, in order to get into more functional details of its regulation in the aforementioned properties. Until present, there have been several NMR structures available for the TM fragments of EGF-4 and EGF-5 domains, Loop conformations as well as EGF-4,5 domain. Through X-ray crystallographic analysis, EGF-4 or EGF-5 fragments and complex structure of EGF-5 and thrombin have been also available. However, these so-far available structures, either through NMR or through X-ray analyses, can not shed light into the decent structural-functional interpretations for TM regulations in its crucial cellular functions. However, we have already got fairly abundant results in the crystallization of extracellular fragments of TM. Hopefully we will get into the structural and functional details of TM's molecular mechanism in the near future.

Keywords: thrombomodulin, X-ray crystallographic analysis, SAXS

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#### Structural and magnetic investigations of nanocrystalline nickel ferrite $\text{NiFe}_2\text{O}_4$

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