

Phy.- Cond. Matter, 1995, 7,3,585.

Keywords: rare earth molybdates, second harmonic generation (SHG), scheelite structure

P08.14.165

Acta Cryst. (2008). A64, C469

Application of statistical methods for the prediction of properties of organic solid forms

Sarah B Carnaby, Michael B Hursthouse, Dave C Woods

University of Southampton, School of Chemistry, Highfield, Southampton, Hampshire, SO17 1BJ, UK, E-mail: sbc103@soton.ac.uk

We are investigating the application of appropriate statistical methods for the prediction of the formation and properties of organic solid forms, taking advantage of the possibility to determine structures and properties of family sets of organic solid forms using High Throughput Chemical Crystallography. Statistical models are being built to relate quantitative descriptors of molecular or crystalline structure to the classification of compounds, and to predict measured properties of the compounds, such as melting point and enthalpy of fusion. In many of these studies, a large number of quantitative variables are available as potential predictors of a response. The sizes of available datasets and feasible experiments (small to medium), often result in there being more potential descriptors than data points. We are therefore exploring the selection of statistically relevant subsets of the possible descriptors. A further complication is the need to consider nonlinearities in the statistical models and interactions between the variables. A variety of data forms are being considered, including binary data for the classification problem, categorical data when considering the occurrence of polymorphs and continuous data for measured properties. Appropriate statistical methods are being developed, where necessary, and applied to each situation, based on methods such as generalised linear and additive models, recursive partitioning and classification trees, and ensemble models. The performance of different methods are being critically assessed and compared. The poster will present results obtained so far.

Keywords: statistical methods, crystal structures, property prediction

P08.14.166

Acta Cryst. (2008). A64, C469

High hardness and incompressibility in transition metal borides

Guenter Krauss, Qinfen Gu, Walter Steurer

Laboratory of Crystallography / ETH Zurich, Department of Materials, Wolfgang-Pauli-Strasse 10, Zurich, Zurich, 8093, Switzerland, E-mail: guenter.krauss@mat.ethz.ch

Transition metal borides have recently gained high interest as potential superhard materials. Despite the high costs for the transition metals, their synthesis is comparably facile and can be done at ambient pressure conditions, what favours them for example against c-BN or advanced nanocomposite materials for a potential use in industrial applications. In a systematic study, we synthesized borides of Ru, W, Re, and Os. The crystal structures of these materials are characterized by a different packing of transition metal and flat and/or puckered boron layers. The mechanical properties were determined by microindentation as well as compressibility measurements using diamond-anvil cells and synchrotron radiation. The observed

properties of the materials can be understood based on their crystal structures and the chemical bonding. The analysis of the chemical bonding of these compounds by means of the electron localization function (ELF) revealed a high degree of covalent boron-boron bonding as a necessity for a high hardness. On the other hand, as it is well known, a high electron concentration yields to an incompressible material. Therefore, OsB was found to be the most incompressible, WB₄ the hardest of the investigated materials. A good compromise between incompressibility and hardness was found for WB₂, (W,Os)B₂ and the isoelectronic ReB₂. We thank the staff of the MS beamline at Swiss Light Source (SLS at PSI, Villigen, Switzerland) for experimental assistance

Keywords: borides, bulk modulus, microhardness

P08.14.167

Acta Cryst. (2008). A64, C469

Structure and magnetic study of solvated and non-solvated spin crossover complex [Fe(SalEen)₂]ClO₄

Chou-Fu Sheu, Szu-Miao Chen, Yuh-Sheng Wen, Gene-Hsiang Lee, Yi-Hung Liu, Yu Wang

National Taiwan University, Chemistry, No. 1, Sec. 4, Roosevelt Road, Taipei, 10617 Taiwan, Taipei, 10617, Taiwan, E-mail: fu@xtal.ch.ntu.edu.tw

The water solvated [Fe^{III}(SalEen)₂]ClO₄·0.5H₂O (**1**) and non-solvated [Fe^{III}(SalEen)₂]ClO₄ (**2**) complexes were synthesized and structure characterized (SalEen = N-(2-ethylamino)ethyl-salicylaldehyde). Complex **1** crystallizes in the polar orthorhombic space group *Fdd2* with cell parameters $a = 18.4301(7)$, $b = 55.7300(20)$, $c = 9.9021(3)$ Å, $V = 10171.1(6)$ Å³, $Z = 16$, while complex **2** crystallizes in the monoclinic space group *P2₁/c* with $a = 9.9440(2)$, $b = 21.1875(5)$, $c = 12.3637(3)$ Å, $\beta = 104.311(1)^\circ$, $V = 2524.1(1)$ Å³, and $Z = 4$. The water molecule induces a very different molecular packing situation which causes distinct magnetic property between the solvated and non-solvated complexes. The thermal dependent magnetic measurement shows gradual spin transition property for both complexes, both are in the high spin (HS) state $S = 5/2$ at 350 K and convert to the full low spin (LS) state $S = 1/2$ below 30 K for **1** ($T_{1/2} = 155$ K) and 120 K for **2** ($T_{1/2} = 230$ K). A two-step spin transition is interested found in complex **1**, which represents the first Fe(III) system with such behavior. Crystal structures of the LS state at 25 K for **1** and at 100 K for **2** are collected for comparison to the HS state structures at 300 K. The bond lengths associated with the FeN₄O₂ octahedron in the HS and LS states are consisted with the magnetic result. The Fe-N_{avg} and Fe-O_{avg} differences are 0.148 and 0.034 Å shorter for **1** and 0.132 and 0.027 Å shorter for **2** in the LS state, respectively. Also the octahedral distortion parameters Σ and Θ , defined as the sum of the absolute values of the deviation from 90° of the 12 cis angles and deviations from 60° of the 24 possible angles in the coordination sphere, show the more closely to normal octahedral environment in the LS state as expected.

Keywords: structural and magnetic phase transitions, magnetic behaviour, single-crystal characterization

P08.14.168

Acta Cryst. (2008). A64, C469-470

Structural-microstructural & magnetic properties relationships of In_{1.0}Fe_{0.1}Te_{0.9}, In_{1.0}Co_{0.1}Te_{0.9}

Karimat M EL-Sayed¹, Zein Heiba², Kamelia Saddek³,

Poster Sessions

Hanan Hantour⁴

¹Ain-Shams University, Faculty of Science, Physics Department, P.O.Box 8014 Masaken Nassr City, Cairo 11371, Egypt, Cairo, Egypt, 11371, Egypt, ²Professor At Ain-Shams University, Faculty of Science, Physics Department, Cairo 1655, Egypt, ³Professor at Al-Azhar University (Girl Section) Faculty of Science, Physics Department, Nassr City Cairo 11371, Egypt, ⁴Post Graduate student at Al-Azhar University (Girl Section) Faculty of Science, Physics Department, Nassr City, Cairo 11371. Egypt, E-mail: elkarimat@yahoo.com

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 In_4Te_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

P08.14.169

Acta Cryst. (2008). A64, C470

Properties and local structure analysis of N or Nb doped TiO_2

Kei-ichiro Murai, Doji Suzuki, Dan Kirishima, Toshihiro Moriga
the University of Tokushima, Institute of Technology and Science,
Minami-josanjima 2-1, Tokushima, Tokushima, 770-8506, Japan, E-mail :
murai@chem.tokushima-u.ac.jp

Until now, many kinds of photocatalysts have been developed, and particularly TiO_2 has been considered most promising for the strong oxidization ability. 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 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 TiO_2 . On the other hand, transparent conducting oxides (TCOs) are key components in many optoelectric devices. Nb doped 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 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 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

P08.14.170

Acta Cryst. (2008). A64, C470

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

Po-Tsang Huang^{1,2}, Kuo-Long Lou^{1,2}, Guey-Yueh Shi^{3,4,5}, Hua-Lin Hu^{3,4,5}

¹National Taiwan University Medical College, Institute of Biochemistry and Molecular Biology, 9F, No.1, Sec. 1, Jen-Ai Rd., Taipei, Taiwan, 100, Taiwan, ²Graduate Institute of Oral Biology, Medical College, National Taiwan University, Taipei, Taiwan., ³Department of Biochemistry and Molecular Biology, College of Medicine, National Cheng Kung University, Tainan, Taiwan, ⁴Institute of Basic Medical Sciences, College of Medicine, National Cheng Kung, ⁵Cardiovascular Research Center, College of Medicine, National Cheng Kung, E-mail: d91442010@ntu.edu.tw

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

P08.14.171

Acta Cryst. (2008). A64, C470-471

Structural and magnetic investigations of nanocrystalline nickel ferrite NiFe_2O_4

Yehia M. Abbas¹, Alia A Adam², Zienab A Ali², Islam Abdeltawab²

¹Suez Canal University, Physics Department, Faculty of Science,