

**P08.14.142***Acta Cryst.* (2008). A64, C462**Jahn-Teller distortions in mixed crystals,  $[\text{Cu}_x\text{Mn}_{1-x}(\text{H}_2\text{O})_4(\text{C}_7\text{H}_4\text{NO}_3\text{S})_2](\text{H}_2\text{O})_2$** Gligor Jovanovski<sup>1,2</sup>, Pance Naumov<sup>1,3</sup>

<sup>1</sup>SS. Cyril and Methodius University, Faculty of Science, Institute of Chemistry, P.O. Box 162, Arhimedova 5, MK-1001, Skopje, Macedonia, <sup>2</sup>Macedonian Academy of Sciences and Arts, P.O. Box 428, MK-1001 Skopje, Macedonia, <sup>3</sup>School of Engineering, Osaka University, 2-1 Yamadaoka, Suita 565-0871, Osaka, Japan, E-mail : gligor@iunona.pmf.ukim.edu.mk

The structure of the isomorphous tetraaquabis(saccharinate)metal(II) dihydrates was employed as structurally flexible coordination framework capable of sustaining large internal distortions to study the competitive inclusion of Jahn-Teller (JT) distorted  $d^9$  ions,  $[\text{Cu}(\text{H}_2\text{O})_4(\text{sac})_2]^{2+}$ , and undistorted  $d^5$  ions,  $[\text{Mn}(\text{H}_2\text{O})_4(\text{sac})_2]^{2+}$ , in a series of mixed crystals of composition  $[\text{Cu}_x\text{Mn}_{1-x}(\text{H}_2\text{O})_4(\text{C}_7\text{H}_4\text{NO}_3\text{S})_2](\text{H}_2\text{O})_2$ , under thermodynamically controlled conditions (sac = saccharinate anion,  $\text{C}_7\text{H}_4\text{NO}_3\text{S}^-$ ). Probing of the metal content of the solid phase showed a two-regime inclusion profile: increasing of the ratio of the distorted cation relative to the undistorted one in the solution phase of up to about 35% results in linear dependence and preferred inclusion of the former with maximum concentration of 100% in the crystal, and complete exclusion of the undistorted ion above that point. A mixed crystal with highest copper ratio of 63% was obtained from solution with 25% copper, which under the  $P2_1/c$  crystal symmetry corresponds to sustainable integrity of the undistorted lattice by substitution of up to 2/3 of its sites. This stability limit shows that four out of six sites around each  $[\text{Mn}(\text{H}_2\text{O})_4(\text{sac})_2]^{2+}$  ion can be substituted by distorted  $[\text{Cu}(\text{H}_2\text{O})_4(\text{sac})_2]^{2+}$  guests under conditions of thermodynamically controlled, statistically averaged exchange. The undistorted ion is tolerant toward inclusion of the strongly distorted guests, whereas the distorted ion is exclusive toward the undistorted ion. Along with the expectation from the JT theory, structural refinement of seven crystals, including a mixed crystal with composition of  $[\text{Cu}_{0.126}\text{Mn}_{0.874}(\text{H}_2\text{O})_4(\text{C}_7\text{H}_4\text{NO}_3\text{S})_2](\text{H}_2\text{O})_2$ , showed that metal-ligand distances are significantly affected by the metal substitution.

Keywords: copper and manganese saccharinates, solid solutions, Jahn-Teller distortions

**P08.14.143***Acta Cryst.* (2008). A64, C462**Evolution of phonon spectra and elastic constants from graphene to graphite**

Karl H Michel, Bart Verberck

University of Antwerp, Department of Physics, Groenenborgerlaan 171, Antwerp, Antwerp, 2020, Belgium, E-mail : karl.michel@ua.ac.be

We present a unified theory of the phonon dispersions and elastic properties of graphene, graphite and graphene multilayer systems. Starting from a fifth-nearest neighbor force constants model derived from full in-plane phonon dispersions of graphite [Mohr et al., Phys. Rev. B 76, 035439 (2007)] we use Born's long wavelength method to calculate the tension and bending coefficients of graphene. Extending the model by interplanar interactions, we study the phonon dispersions and the elastic constants of graphite and the phonon spectra of graphene multilayers. We find that the inner displacement terms due to sublattice shifts between inequivalent C atoms are quantitatively important in determining the elasto-mechanical properties of graphene but not of graphite. We investigate the

evolution from graphene to graphite by studying the increase of the  $wB2g1(N)$  rigid planes optical mode as a function of the number of layers  $N$ . At  $N = 10$  the graphite value  $wB2g1$  127  $\text{cm}^{-1}$  is practically reached near  $N = 15$ .

Keywords: graphene, graphite, phonons, elastic constants

**P08.14.144***Acta Cryst.* (2008). A64, C462**Lattice strain tuning in  $\text{SrTiO}_3/\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$  films by inverse piezoelectric effect of PMN-PT wafer**Alexandr A. Levin<sup>1</sup>, Hartmut Stoecker<sup>1</sup>, Stephan Ritter<sup>1</sup>, Torsten Weissbach<sup>1</sup>, Orkidia Bilani-Zeneli<sup>2</sup>, Dirk C. Meyer<sup>1</sup>

<sup>1</sup>Dresden University of Technology, Institute of Structural Physics, Zellescher Weg. 16, Dresden, Sachsen, 01069, Germany, <sup>2</sup>IFW Dresden, Institute for Metallic Materials, P. O. Box 270116, 01171 Dresden, Sachsen, Germany, E-mail : levin@physik.phy.tu-dresden.de

Due to properties favorable for technical applications, ferroic nanometer film composites with perovskite-related structures have received great attention. In this report, the results of an *in-situ* X-Ray Diffraction (XRD) investigation under the influence of a static electric field are presented for 30 nm...100 nm  $\text{SrTiO}_3$  (STO; cubic perovskite; paraelectric)/30 nm  $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$  (LSMO; trigonal perovskite-related lattice; ferromagnetic) film composites grown on a (001)  $\text{Pb}(\text{Mg}_{0.33}\text{Nb}_{0.67})\text{O}_3$ -28%  $\text{PbTiO}_3$  (PMN - PT; pseudo-cubic rhombohedral perovskite; relaxor ferroelectric (RFE) with high piezoelectric properties) wafer. XRD reflection profiles ( $\text{Cu-K}\alpha$ ) of the 001, 002 and 013 PMN-PT (corresponding to attenuation depths of 500 nm, 1000 nm and 1300 nm, resp.) as well as 002 LSMO (pseudo-cubic indexing) and 002 and 013 STO were recorded for every stage of electric field strength  $E$ . The lattice strain  $s(E)$  dependence obtained for the bulk of the PMN-PT substrate exhibited a butterfly-like low-hysteresis shape, which is typical for a RFE. The piezoelectric lattice strain of the substrate induced strain in the films. Initially, for the sample with 30 nm STO film, the near-surface PMN-PT region and films showed a wide smoothed asymmetrical  $s(E)$ . After extended electric field processing, the sample exhibited a low  $s(E)$  hysteresis similar to bulk PMN-PT. In contrast, the sample with 100 nm STO film exhibited a  $s(E)$  response closer to the bulk material at all stages. The differences in the  $s(E)$  behavior of the STO/LSMO film composite structure with different thickness of the top STO film are discussed. A conclusion is drawn that the strained state of the 30 nm...100 nm STO/30 nm LSMO films can be effectively controlled by the inverse piezoelectric effect of the PMN-PT substrate.

Keywords: X-ray diffraction, ferroics, strain

**P08.14.145***Acta Cryst.* (2008). A64, C462-463**Coupling between magnetic and dielectric properties in a triangular lattice antiferromagnet  $\text{CuCrO}_2$** Kenta Kimura<sup>1</sup>, Hiroyuki Nakamura<sup>1</sup>, Kenya Ohgushi<sup>2</sup>, Tsuyoshi Kimura<sup>1</sup>

<sup>1</sup>Osaka University, Graduate School of Engineering Science, 1-3 Machikaneyama-cho, Toyonaka, Osaka, 560-8531, Japan, <sup>2</sup>Institute for Solid State Physics, University of Tokyo, Kashiwa 277-8581, Japan, E-mail : kenta@crystal.mp.es.osaka-u.ac.jp

Coupling between magnetic and dielectric properties has been attracting much attention in the past few years. Recent experimental