

**MS34-05** Model of short range order in 5,6-dichlorochinolino-5,8-dion organic compound. Maciej Zubko,<sup>a</sup> Joachim Kusz,<sup>b</sup> Maria Jastrzębska,<sup>b</sup> Stanisław Boryczka,<sup>c</sup> Monika Kadela,<sup>c</sup> <sup>a</sup>Institute of Materials Science, University of Silesia, Katowice, Poland, <sup>b</sup>Institute of Physics, University of Silesia, Katowice, Poland, <sup>c</sup>Department of Organic Chemistry, Silesian Medical University, Sosnowiec, Poland  
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5,6-dichlorochinolino-5,8-dion is an interesting organic compound with potential application in pharmaceutical industry. It has promising anti-inflammatory properties and is a starting agent for synthesis a variety of 6,7-substituted 5,8-quinolinequinolines with biological activity as anti-cancer, anti-inflammatory or tuberculostatic agents [1].

Observation of diffuse scattering in X-ray diffraction patterns is unambiguous sign of breaking of long range order in crystal structure. Such phenomenon gives information about real crystal structure and short range interaction of molecules building studied crystals. Thanks to improvements in experimental techniques and increasing computation power nowadays not only qualitatively but also quantitative analysis of diffuse scattering is possible. Analysis of short range order is performed mainly by means of computer simulations, which are powerful tools to study local crystal structure. During single crystal diffraction measurements of 5,6-dichlorochinolino-5,8-dion strong diffuse scattering is observed in forms of stripes on *hk* planes at RT as well as at 100 K. Stripes are located on *hk* planes with *l* odd and are parallel to [-110] direction. The diffuse scattering is temperature independent and has the same form at RT and at 100 K. Based on Bragg peaks average unit cell was determined in tetragonal system with lattice parameters  $a=b=9.2271(15)$  Å,  $c=10.143(3)$  Å. Although diffraction pattern tends to possess tetragonal symmetry any attempts to determine space group in tetragonal system failed. Due to that issue average structure has been determined in *P1* space group by means of charge flipping method with SuperFlip program [2]. Average structure is formed with molecules arranged in (1-10) layers. Average structure contains overlaid molecules with head to tail patterns and refined occupancy parameter for both molecules is approximately 0.5. Based on observed diffuse scattering model of real crystal structure was proposed. Computer simulations of real crystal structure based on proposed model were performed using DISCUS program package [3,4]. The refinements of the model parameters were done through the differential evolutionary algorithm implemented in the DISCUS software package.

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**MS35-01** Structural Origin of the Ferroelectric Fatigue in Lead Zirconate Titanate (PZT). J. Rouquette,<sup>a</sup> M. Hinterstein,<sup>b</sup> J. Haines,<sup>a</sup> Ph. Papet,<sup>a</sup> M. Knap,<sup>c</sup> J. Glaum,<sup>d</sup> H. Fuess,<sup>e</sup> <sup>a</sup>Institut Charles Gerhardt UMR CNRS 5253 Equipe C2M, Montpellier cedex 5, France., <sup>b</sup>Institut für Werkstoffwissenschaften, Technische Universität Dresden, Germany, <sup>c</sup>CELLS-ALBA, Barcelona, Spain, <sup>d</sup>School of Materials Science and Engineering, Australian, <sup>e</sup>Institute for Materials Science, Technische Universität Darmstadt, Germany.  
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Ferroelectric materials exhibit great potential for microelectronic applications. In ferroelectric random access memories, information is stored and read by switching the polarization orientation in the ferroelectric material. However the decrease of switchable polarization (polarization fatigue) is one of the limiting factors hindering the commercialization of ferroelectric memories, i.e. the amount of switched charge decreases with use. The mechanisms of the ferroelectric fatigue are not well understood in spite of intensive study; ferroelectric fatigue is either proposed to be caused by the formation of interfacial layers between the metal electrode and the ferroelectric material, 90-degree domains and resultant strains, electromigration of oxygen vacancies to form extended defects capable of pinning domains, interface nucleation inhibition mechanisms induced by charge injection, macro- and/or micro-cracking, and so on, but to the best of our knowledge a structural origin for fatigue has never been proposed.

In this study, the ferroelectric fatigue of commercial PZT ceramics was investigated by in situ x-ray synchrotron diffraction experiments as a function of the applied electric field. Using the procedure recently reported[1], we unambiguously characterized the structural origin of the fatigue based on a reduced degree of tetragonal-to-monoclinic transformation, which accounts for the reduction of the piezoelectric efficiency. Loss of the switchable remanent polarization could also be evidenced by a significantly less intense and more diffuse anomaly of Biso (Pb) for fatigued sample, which accounts for polarisation flipping. We were also able to characterize structurally the field induced response on a millisecond time scale, which comforts without any doubt the structural origin of the ferroelectric fatigue on a shorter timescale. These results will be useful to design and optimize high performance fatigue free materials.

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