

MS24 P01

Ionic path in oxygen-ionic conductor
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Oxygen-ionic conductors are very important materials for various kinds of applications such as fuel cells and oxygen-gas sensors. In 1995, Nakayama found new type of oxygen-ionic conductor; Ln-Si-O apatites (Ln = Lanthanoids). [1,2] These compounds show better oxygen ionic conductivity in middle range of temperature compared with other famous oxygen-ionic conductors (ZrO₂ and/or CeO₂-based materials). Recently, Yoshioka reported that Mg-doped apatites show the best ionic conduction. [3] However, in all of the apatite system, details of mechanism of ionic conduction are still unknown.

Therefore, we carried out high-temperature diffraction study using synchrotron radiation to suppose mechanism from a change of electronic density. In this study, we selected 20 % Mg-doped compound, which showed the highest conductivity. Intensity data was measured by powder method at BL-19XU beam line, SPring-8, Japan, and the temperature range was from room temperature to 1283 K. The crystal structures were refined by Rietveld method using RIETAN-FP [4], the electron distributions were investigated by whole-pattern fitting approach based on the maximum-entropy method (MEM) using PRIMA [5], and the structure and electron distributions were drawn by VESTA [6,7].

In whole temperature range, this compound belongs to P6₃/m. The Rietveld refinement suggested an interstitial oxygen site O5 located at (-0.01,-0.003,-0.002). Electron density map derived from the MEM analyses revealed that oxide ions O4 located at 2a site were diffused along the *c*-axis. In addition, a short-range curved diffusion path through the interstitial site was clearly visualized between two oxygen atoms O3 within the SiO₄ tetrahedra.

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MS24 P02

Experimental charge density study of (*E*)-4-(2,4-diisopropylphenyl)-4-oxo-2-butenoic acid

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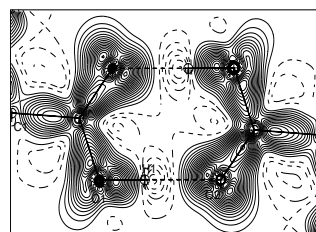
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4-Aryl-4-oxo-2-butenoic acids (AAA) exert antibacterial and antineoplastic activity [1]. The (*E*)-4-(2,4-diisopropylphenyl)-4-oxo-2-butenoic acid was a precursor of one of most active CSAB derivative [2] that selectively suppress proliferation of neoplastic HeLa cells in submicromolar concentration. The activity of AAA are ascribed to high affinity of their ketovinyl moieties (-C(O)-CH=CH-) toward octagonal thiol groups of biomolecules. Introduction of branched alkyl chains on phenyl ring significantly increases activities within the congeneric group of compounds. Here, we present the results of the experimental charge density study of the (*E*)-4-(2,4-diisopropylphenyl)-4-oxo-2-butenoic acid. The Hansen-Copens multipole model was used to describe the electron density distribution within this compound. Subsequently, the topological analysis was performed to characterize the properties of the covalent bonds and interactions. The values of ρ in the sixteen C-C bonds are ranging from 1.64-2.46 e.Å⁻³. The highest value is found for the formally double bond of the ketovinyl moiety. The strongest interaction in the structure is the cyclic O-H...O hydrogen bond formed between the carboxyl moieties (Scheme). In the aim to understand the further reactivity of this molecule the molecular electrostatic potential was also determined.

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**MS24 P03**

Crystal geometry and scale levels of plastic flow localization in metals and alloys Lev B. Zuev, Svetlana A. Barannikova Institute of Strength Physics and Materials Science, SB RAS, Tomsk, Russia.

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Keywords: single-crystal orientation, crystal geometry, wavelength

Using a holographic technique, plastic flow investigations were carried on for FCC, BCC and HCP monocrystals tested in tension. The experimental evidence obtained points to the existence of hitherto unknown wave processes involved in deformation localization. Waves of this kind are generated in the deforming crystals as an ensemble of localized plastic deformation nuclei moving in a concerted manner and evolving with time. Wave