

MODULATED STRUCTURE AND SUPERCONDUCTING MICROMECHANISM IN YBCO COMPOUNDS

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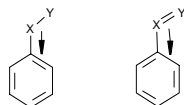
From the experimental results with ESR in combination with other methods, a Modulated Crystal Structure with the twined Y-unit-cells in $\text{YBa}_2\text{Cu}_3\text{O}_x$ (YBCO) ceramics have been revealed, in which appear two different types of the Electron Spin Superexchange Coupled Pairs [Cu-Y-Cu]: A Singlet Pair on the long diagonal of the twined Y-unit-cell by the modulated angle of 72° corresponds to the superconducting phase and a Triplet Pair on the short diagonal of the twined Y-unit-cell by the modulated angle of 78° corresponds to the semiconducting phase. The persistence of the Spin Coupled Pairs as well as the Superconducting Mechanism in YBCO are in close connection with this Modulated Structure. On the basis of the behaviour of the quasi-free electrons in the Y-unit-cell as a Nano Resonant Cavity of the Short-Range Order Structure it can be explained and derived some fundamental problems of the superconductivity in YBCO such as the existence of the spin gap $E_{gs}(T)$, the role playing of the Singlet [Cu-Y-Cu] Electron Coupled Pair as a new type of the Cooper Pair, an equation determining the superconducting transition temperature T_c , and an equation determining the temperature T_x for the conductivity maximum point in the semiconducting phase. The calculated results are in a very good correspondence to the respective measured data.

Keywords: MODULATED STRUCTURE AND SUPERCONDUCTIVITY

ANGULAR GROUP INDUCED BOND ALTERNATION (AGIBA) OBSERVED IN AROMATIC AZINE DERIVATIVES

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Angular groups $-X-Y$ and $-X=Y$ attached to the η -electron ring(s) with a delocalised system of electrons influence the structure in two opposite ways as shown in the scheme below:^[1-4]



This effect has also been observed experimentally for $-X-Y$ substituents in other ring systems with equalised bond lengths like boraxine⁵ and borazine⁶ which are not considered as aromatic.^[7-10]

We report here the low temperature (100K) x-ray diffraction study of 2, 3, 6, 7-tetrahydro-1h, 5h-pyrido [3, 2, 1-ij] quinoline-9-carbaldehyde(E, E)-azine provided the molecular geometry allowing to study a competition between the AGIBA and through resonance effects. The study of four of its analogues where the molecular geometry was retrieved from CSD and of a simplified derivative for which geometry was obtained by optimization at B3LYP/6-311G** level of theory, supported the results for the title compound and the conclusion that the AGIBA effect and the through resonance may exist simultaneously in systems with appropriate substituents. The implications of the findings will be discussed.

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Keywords: SUBSTITUENT EFFECTS, AZINE DERIVATIVES, AB-INITIO

INVESTIGATION ON THE STRUCTURAL DIFFERENCES AMONG LANGASITES BY SINGLE-CRYSTAL X-RAY STRUCTURE ANALYSIS

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Recently, langasite-type single crystals have attracted an attention as new piezoelectric materials for surface acoustic wave (SAW) device because of the large electromechanical coupling factor and the high thermal stability of frequency. The crystal data of langasite ($\text{La}_3\text{Ga}_5\text{SiO}_{14}$, LGS) is as follows; trigonal, space group $P321$ (No. 150), $Z=1$, $a=8.1674$, $c=5.0964$ Å. They have four different cation sites; A decahedron, B octahedron, C and D tetrahedron. The structural formulae are shown as $[\text{La}_3]\text{A}[\text{Ga}]\text{B}[\text{Ga}_3]\text{C}[\text{GaSi}]\text{DO}_{14}$ for LGS and $[\text{Ca}_3]\text{A}[\text{Ta}]\text{B}[\text{Ga}_3]\text{C}[\text{Si}_2]\text{DO}_{14}$ for CTGS. In this work, we refined the crystal structures of three-element compounds; LGS, $\text{Pr}_3\text{Ga}_5\text{SiO}_{14}$ (PGS) and $\text{Nd}_3\text{Ga}_5\text{SiO}_{14}$ (NGS), and four-element compounds; $\text{Ca}_3\text{TaGa}_3\text{Si}_2\text{O}_{14}$ (CTGS), $\text{Ca}_3\text{NbGa}_3\text{Si}_2\text{O}_{14}$ (CNGS), $\text{Sr}_3\text{TaGa}_3\text{Si}_2\text{O}_{14}$ (STGS) and $\text{Sr}_3\text{NbGa}_3\text{Si}_2\text{O}_{14}$ (SNGS) by single-crystal X-ray diffraction analysis. Diffraction intensity data were collected with a Rigaku AFC-7R four-circle diffractometer using graphite monochromized Mo $K\alpha$ radiation. The refinement of the crystal structure was performed by the full-matrix least-square program RADY (S. Sasaki, 1982). A site of three-element compounds with different rare earth atoms, La, Pr and Nd, in decahedron expands in [100] direction, but shrink in [120] direction when the bigger cation occupies A site. This tendency was also shown in CTGS, CNGS, SNGS, and STGS. Furthermore, in these four-element langasite-type of crystals, B site occupied by Nb or Ta expands in a whole, not only [100] direction when Ta ion occupies B site. Corporation because piezoelectric properties are affected by these crystal structure deformations, we have also clarified the relationship between the crystal structure and piezoelectric properties.

Keywords: LANGASITE PIEZOELECTRIC PROPERTY SAW FILTER

STRUCTURE EVOLUTION OF Al-10.4 AT.% LI ALLOY DEFORMED AT ROOM AND LOW TEMPERATURES

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The high strength and plasticity of light Al-Li alloys reaches for account of controlled phase transformations, which in its turn depend on deformation. The effect of deformation on the phase state of quenched and aged alloy Al-10.4 at.% Li was studied in the work by X-ray diffraction powder-pattern method. The powders were prepared by crushing the polycrystalline samples, initially quenched, aged at 473 K and deformed by tension at two temperatures: 295 or 4,2 K. On the diffraction patterns of as-quenched alloy except the solid solution the additional peaks are observed, which corresponds to equilibrium AlLi - phase and metastable ordered Al_3Li -phase. After aging the intensity of all additional diffraction peaks increases. Oppositely, after a plastic deformation of the aged alloy the intensity of additional peaks is decreased noticeably. It is shown, that observed decrease of reflections corresponding to ordered Al_3Li - phase, depends on the deformation temperature: after deformation at 295 K the peaks intensity are found essentially less, than after deformation at 4,2 K. The change of diffraction peaks intensity due to plastic deformation is conditioned by changing of the amount of ordered Al_3Li -phase. The cutting of Al_3Li -particles by mobile dislocations make decrease their effective radius. The particles with effective radius less than some critical value, dissolve in the matrix as faster, as higher the deformation temperature.

Keywords: TEMPERATURE, DEFORMATION, X-RAY