

Solar cell production from multicrystalline (mc) silicon presently experiences a yearly growth of about 40%. A lack of cheap scrap silicon from the electronic industry has arisen the last years. Metallurgical silicon is very expensive to purify, and, in order to produce cost effective solar cells, the new trend is to use dirtier source materials in mc ingot production. Higher levels of impurities and structural defects in such materials act as recombination centres and reduce the efficiency of mc silicon solar cells. To come up with good solutions for improving the silicon wafer production, it is important to understand how structural defects are formed and where precipitates of other phases are nucleated and grow during solidification and cooling. In the present work impurity precipitation on extended defects in as-cast mc silicon grown from metallurgical feedstock using a direct route process (i.e. no filtration and one step directional solidification) has been studied using transmission electron microscopy combined with dislocation density measurements and chemical analysis. All observed dislocations and grain boundaries, except for some coherent twins, were contaminated with silicon oxide precipitates. Different types of multi-metal precipitates containing nickel, copper and iron were present randomly distributed in grain boundaries. No measurable gettering of metals by oxides was observed. Slower diffusing elements were not present in the precipitates, in spite of being present at relatively high levels in the bulk. Observations are discussed in terms of the potential for defect engineering to reduce cost by allowing the use of lower purity feedstock.

Keywords: silicon crystal growth and its effect on device pe, transmission electron microscopy, solar cell fabrication

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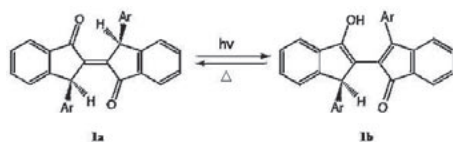
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Crystalline-state photochromic reaction of *trans*-biindenilidenedione derivatives

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It has been found that *trans*-biindenylidenedione (TBID) derivatives show photochromism and the color changes from yellow to red upon irradiation with UV and visible light in the solid state. In our previous study, crystal structure determination of red form was performed in order to reveal the photochromic reaction mechanism. The crystal structure after irradiated with UV light was analyzed to show both the reactant (**1a**) and the photoproduct (**1b**) which were located as a disordered structure, indicating that the photochromism is caused by an intramolecular (Norrish Type II) hydrogen transfer reaction. In this study, several TBID pseudo-polymorphs were prepared and the crystal structures were determined before and after the irradiation in order to make clear the relationship between the structures and photochromic properties. From the comparison of the crystal structures and the life-time of red-colored photoproduct, it is elucidated that the following three factors are important for the photochromism; (1) molecular conformation of the initial crystal, (2) cavity size around the reactive part of the molecule, and (3) cooperative movement of the solvent molecules in the crystal.



Keywords: crystalline-state reaction, photochromism, biindenilidenedione Derivatives

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Structural and physical properties of single crystal $K_xNa_{1-x}NbO_3$ around the $x=0.3$ phase boundary

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Lead zirconium titanate (PZT) is commonly regarded as the leading piezoelectric material for a wide range of applications, and one which all others are assessed against. However, there are growing concerns over the toxicity and environmental issues of lead-based substances [1], which is why attention has turned to other lead-free piezoelectric materials. Sodium potassium niobate (KNN) is of particular interest not only because its piezoelectric properties are comparable to that of PZT [2], but also because the phase diagram contains three morphotropic phase boundaries (MPB), at $x=0.2$, $x=0.3$ and $x=0.5$. MPBs are a very interesting area of study, since dielectric and piezoelectric properties are enhanced in these regions, and the atomic-level structural mechanisms underlying these transitions are poorly understood. Until now, only the MPB at $x=0.5$ in KNN has been studied in any detail, and no information was available on the other two. Several single crystal samples have been grown via the flux method around the $x=0.3$ MPB. X-ray structural analysis has been performed to supplement earlier X-ray and neutron work on powder samples. Birefringence, dielectric, NMR and polarisation measurements have also been taken with a variety of techniques, in order to explain the enhanced physical properties of this potentially interesting material at this previously unstudied MPB.

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Keywords: phase transitions, quantitative X-ray analysis, ferroelectric piezoelectric crystals

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Phase transitions in one-layered Aurivillius phases, $Bi_2W_{1-x}Mo_xO_6$ ($0 < x < 1$)

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One-layered ferroelectric-superionic Aurivillius phases Bi_2WO_6 (BW) and Bi_2MoO_6 (BM) are under investigation more than 50 years but there is no agreement concerning their polymorphism. There are well-established in both compounds two phases: orthorhombic polar phase at room temperature (RT) and monoclinic phase at high temperatures. The data about intermediate phases are extremely inconsistent. In this work the phase transitions peculiarities of BW and BM were investigated by mutual substitution Mo and W cations. Two series of $Bi_2W_{1-x}Mo_xO_6$ ($0 < x < 1$) ceramics have been synthesized at 600–630°C (**I**) and 850°C (**II**). X-ray powder diffraction at RT, differential scanning calorimetry, dielectric permittivity and conductivity measurements were used for phase identification and investigation of polymorphism. The samples of

I series existed at RT in polar orthorhombic phase are isostructural to BW at $0 < x < 0.6$ and BM at $0.7 < x < 1$. Part of solid solutions at $0 < x < 0.3$ and $0.8 < x < 1$ transforms into monoclinic phase through intermediate unpolar orthorhombic phase. The transition temperatures depended considerably on doping level and heating rate. The only reconstructive transition into monoclinic phase without intermediate phase was observed at $0.4 < x < 0.7$. The restricted solid solutions in series II with the polar BW structure ($0 < x < 0.3$) have also exhibited two transitions. The monoclinic phase based on BM exists in series II at $x > 0.3$. Obtained results have shown that the BW and BM compounds, which existed in polar phase at RT, at heating are similar in respect of numbers and sequences of their transition phases.

Keywords: phase transitions, Aurivillius phases, solid solutions

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Structural investigations of crystallization processes in amorphous rare earth borates

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Calcite, vaterite and aragonite phases are well known for rare earth borate system. As a rule, different phases in thermodynamic equilibrium states are observed for different rare earth elements. For example, YBO_3 , YbBO_3 and GdBO_3 are crystallized in vaterite phase while ScBO_3 is crystallized in calcite phase only. At the same time LuBO_3 could be crystallized in the both calcite and vaterite phases. Our studies showed that the structures, which do not exist in equilibrium phase diagram, can be obtained during the crystallization of amorphous borates in non-equilibrium conditions. By non-equilibrium conditions a quick heating up to high temperature and subsequent quench is implied. Moreover by means of this method we have produced the x-phase for ScBO_3 with so far unknown structural type. Two methods have been used for amorphous borate synthesis. These are thermolysis of the solution-melt and precipitation from the solution. We found that the synthesis method influences considerably on the phase states of the material upon further treatment. Considering this feature we have undertaken the studies of the borate phase crystallization from different starting material under different crystallization conditions such as starting temperature, heat rate, annealing time at final temperature. By this report crystal structure data of the obtained phases and possible routes of the x-phase-vaterite-calcite transformations will be presented.

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Keywords: complex oxides, nanomaterials, phase transitions

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Structures and transitions in praseodymium at high pressure

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The trivalent lanthanide elements exhibit a range of different close-packed structures as a function of increasing 4f occupancy (hcp \rightarrow Sm-type \rightarrow dhcp \rightarrow fcc) [1]. The same series of structures is also accessible in individual lanthanides by the application of pressure. Two further phases can also be accessed on compression. The first, the distorted fcc phase (d-fcc), has a structure that is closely related to the fcc structure, while the second phase, with the alpha-Uranium structure, arises from the delocalisation of the 4f electrons and marks the end of the sequence of close-packed structures. Despite numerous X-ray diffraction studies dating back 30 years, the structure of the d-fcc phase remains ambiguous. Here we present details of our own structural studies of d-fcc Pr made using powder diffraction methods. In Pr, the d-fcc phase, previously reported to be stable between 9 and ~ 20 GPa, is found to comprise two different structures. Between 9 and 14 GPa, we find the structure to be rhombohedral [2], and can rule out previous reports of a C-centred monoclinic structure. At 14 GPa, we find a structural transition to a second phase, the structure of which does not agree with that reported recently [3]. Further studies reveal that this second phase also exists in Nd, suggesting that there may be a new high-pressure phase in the general lanthanide phase-transition sequence.

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Keywords: lanthanide, distorted FCC, high pressure

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Phase transformations induced by point defects studied by group-subgroup relationships

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Symmetry determination for new compounds, structural relations between crystal structures, phase transition paths and new phases generated by point defects, are some of the structural aspects that can be performed by mean of group-subgroup relationships. This work is focused in the analysis of phase transformations induced by point defects *v.gr.* vacancies, interstitial or substitutional impurities. For instance, in monoclinic hydroxylapatite ($P112_1/b$, No.14) defects are created in the Wyckoff position $6h$ for phosphorus substituting the PO_4^{3-} by CO_3^{2-} ; and the symmetry changes to give the hexagonal hydroxylapatite ($P6_3/m$, No.176). Since direct structural relations cannot be established in going from $P112_1/b$ to $P6_3/m$, a common subgroup between these two space groups was considered, *i.e.* the non-centrosymmetric space group $P2_1$ (No.4) reported for monoclinic chlorapatite under the action of a weak electric field [1]. In the phase transformation from YPO_4 ($P4_1/amd$, No.141) to YPO_4 ($Fddd$, No.70), the orthorhombic phase is induced by Li_2CO_3 during the reaction process, its transformation can be described by a translationengleiche subgroup of index 2. The last case considered, was the α -quartz type germanium oxide ($P3_21$, No.154), which phase transformation to GeO_2 stishovite type ($P4_2/mnm$, No.136) was promoted, doping the phase with vanadium. In this phase