

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

### P08.04.26

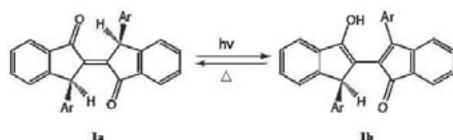
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#### Crystalline-state photochromic reaction of *trans*-biindenilidenedion derivatives

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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, biindenilidenedion 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.

[1] M. Demartin Maeder, D Damjanovic, N. Setter, Journal of Electroceramics 2004, 13, 385 – 392.

[2] Saito et al., Nature 2004, 432, 84

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