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Identification of singular interfaces with Δg vectors

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Microstructures generated from solid state phase transformations often display a self-resemble morphology characterized with faceted interfaces of unique crystallographic orientations. Being stable in the transformation condition, the reproducible facets are likely singular interfaces, associated with singularity in the interfacial energy. This singularity is believed to be also associated with singularity in the interfacial structures. The structure of a singular interface must consist of certain kind of low energy building blocks in major area, but existence of limited defects is possible. One may identify a singular interface based on elimination of interfacial defects, either ledges or dislocations. Based on elimination of ledges, a typical singular interface is atomic flat, which is usually normal to a low index reciprocal vector, g. Based on elimination of dislocations, an ideal singular interface is free of any dislocations, but these interfaces are rare. A singular interface can be identified according to elimination of at least one type of dislocations which must exist in any vicinal interface. Such a singular interface must be normal to one or more reciprocal vectors,Δg, connected to gα and gβ, of the two phases (Δg = gα - gβ). It is simple to elucidate the puzzling high index orientation of a facet withΔg, since Δg may not be parallel to any low index gα or gβ. The reason behind the Δg approach is mainly based on the O-lattice theory. This will be explained in presentation together with examples from various materials to demonstrate the applications of this approach.

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Crystal growth and efficient second-harmonic generation of quasi one-dimensional centrosymmetric KDP single-crystalline microstructures

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Potassium di-hydrogen phosphate (KH_2PO_4 or KDP) single crystals are important multifunctional crystals, which possess distinct piezoelectric, ferroelectric, electro-optic and second-harmonic generation (SHG) properties. In the past a few decades, studies on KDP crystals mainly focused on the large-size and high optical quality tetragonal phase KDP crystals in order to satisfy the demand for nonlinear and electro-optic applications in laser inertial confinement fusion. However, low-dimensional, self-assembled KDP microstructures and their important nonlinear optical properties have been largely overlooked. In this work, we reported the ambient-condition growth of high optical quality KDP microstructures with large length-to-diameter ratio. The exact X-ray diffraction date indicates that the microstructures possess identical crystal structure with the centrosymmetric high pressure IV phase of KDP, which was never known to crystallize under ambient conditions. However, Laue diffraction also showed the presence of a very small fraction of twin crystal lattice on (hk0) plane of the microstructure. According to the fundamental physics, SHG is strictly forbidden in crystals possessing perfect centrosymmetric properties. However, we observed a highly efficient optical SHG in the centrosymmetric KDP microstructures. The normalized conversion efficiency of 532 nm light is up to 10^{-4} W^{-1} pumped by 1-W CW light at 1064 nm. We explained that the SHG is attributing to the small fraction of twin-crystal-induced symmetry breaking (although possibilities of other weak-symmetry-breaking mechanisms cannot be completely eliminated). Using these microstructures, we also demonstrated the polarization-maintaining features of the KDP microstructures, which can be exploited for advanced optical communication applications.

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