Single crystal elastic constants (SCEC) for new materials not available as single crystals can not be measured using conventional techniques. In principle, neutron diffraction patterns from a polycrystalline solid under known uni-axial stress contain sufficient information. The direction dependent strains and known applied stress yield the diffraction elastic constants (DEC) which may be used to estimate the SCEC via a tensor transformation and appropriate averaging. However, the external stress is not experienced identically by each crystal orientation and a micromechanical model is needed.

It is a long standing problem that, for a given set of DEC, to determine the micro-mechanical state has required known SCEC and *vice versa*. We report a novel method to solve this problem by adopting a parameter similar to the 'volume fraction' in the non-dilute Eshelby model [1] for overlapping strain fields in a polycrystalline solid. In detail, this parameter indicates how the elastic anisotropy of the crystallite affects its averaged internal stress when it is treated as an inclusion embedded in a matrix material – in this case the averaged effect of all the other crystals. Moreover the strain gradient solution for Eshelby's ellipsoidal inclusion [2] has been applied in this method to verify how the grain size and shape affect the micro-mechanical state and hence the experimental SCEC. In addition, the influence of crystallographic texture on both the micro-mechanical state and the experimental SCEC has been integrated into the new method. Taken together, the method demonstrates how the micro-mechanical state of a polycrystalline material is dependent not only on the macroscopic elastic properties, but also on the grain size and orientation of the crystallites. For given Young's modulus, Poisson's ratio, grain size, texture and a set of carefully determined diffraction elastic compliances, the proposed method is capable of simultaneously optimizing the micro-mechanical model AND the single-crystal elastic constants. This is achieved by an iterative routine that minimises the usual least squares residual constrained to be self consistent through balancing the microscopic and macroscopic strain energies and constrained to give the correct computed Young's modulus and Poisson's ratio compared with those measured independently.

Two MAX phase polycrystalline materials (Ti_3SiC_2, Ti_3AlC_2) and a ceramic (ZrO_2) have been analysed using DEC from *in situ* neutron diffraction patterns, neutron diffraction texture measurements, the crystallite size, macroscopic Young's modulus and Poisson's ratio. According to these inputs, the optimized micro-mechanical state was then estimated as well as the SCEC for those materials. The SCEC of Ti_3SiC_2 were determined to be s_{11}=5.094, s_{12}=-1.859, s_{13}=-1.199, s_{14}=4.823 and s_{44}=2.243 and this outcome matches fairly well with our recently published results from an independent method [3].

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Keywords: single-crystal elastic constants, micro-mechanical state, ellipsoidal inclusion

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Morphotropic phase transition in a lead-free system (1-x)$NaNbO_3$-x$CaTiO_3$

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The phase diagram of solid solutions of $PbTiO_3$ with several ABO_3 type perovskites contains a morphotropic phase boundary (MPB) separating tetragonal and pseudo-rhombohedral (monoclinic) phase fields. The MPB composition has been found to be of special technological significance for numerous sensor and actuator devices, as the dielectric permittivity, electromechanical coupling coefficients and piezoelectric strain coefficients are maximized around this composition. In the well known commercial MPB systems, like $Pb(Zr_xTi_{(1-x)})O_3$(PZT), (1-x)[$Pb(Mg_{(1/3)}Nb_{(2/3)})O_3$]-x$PbTiO_3$(PMN-xPT) and (1-x) [$Pb(Zn_{(1/3)}Nb_{(2/3)}O_3$]-x$PbTiO_3$(PZN-xPT), this peak in the composition dependence of dielectric and piezoelectric properties around the MPB has been linked with a change of crystal structure from tetragonal to rhombohedral through a narrow range of stability of monoclinic phases. The toxicity of lead oxide and its high vapour pressure during processing of these MPB ceramics have led to the search for alternative environmentally friendly materials free from lead. We present here the results of powder x-ray diffraction, powder neutron diffraction and electron diffraction studies in conjunction with dielectric measurements on a new lead free system, (1-x)$NaNbO_3$-x$CaTiO_3$ (NN-xCT), which reveal morphotropic phase transition. This morphotropic phase transition is unique as none of the end members are non-centrosymmetric ($NaNbO_3$ and $CaTiO_3$ are well known antiferroelectric and paraelectric materials, respectively under ambient conditions). The composition dependence of the room temperature dielectric permittivity of this mixed system exhibits a sharp rise in the composition range $0.12<x<0.20$ with a peak at $x\approx0.16$. This anomalous rise in the dielectric permittivity is linked with a change of crystal structure from an orthorhombic structure in the Pbma space group for $x\leq0.10$ to another orthorhombic structure but in the Pbnm space group for $x\geq0.20$. This behavior is reminiscent of a similar rise in the dielectric permittivity near the MPB composition of the technologically important PZT and PMN-xPT ceramics due to a change of crystal structure from tetragonal to rhombohedral/monoclinic. We have also shown that the huge dielectric response in the morphotropic phase transition region $0.12<x<0.20$ is due to the presence of an incommensurately modulated structure in the morphotropic phase boundary region as confirmed by transmission electron microscopic studies. The peak in the room temperature value of dielectric permittivity of NN-xCT at $x=0.16$ is linked with a relaxor ferroelectric instability below the room temperature. The low temperature electron diffraction and powder x-ray diffraction studies suggest the possibility of a lock-in phase transition associated with the relaxor ferroelectric behaviour.

Keywords: morphotropic phase transition, incommensurate modulation, relaxor ferroelectric transition

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Structural characterization of Tm:Lu_2O_3 nanocrystals for laser ceramics

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Highly transparent cubic ceramic materials have received great attention due to the improvement reached in nanocrystalline technology [1] to obtain optimum isotropic precursor. Cubic materials, such as