
This transformation was characterized by the formation of monomeric plenary Lindqvist hybrids (nBu$_4$N)$_2$[MW$_5$O$_{18}$EOR$_3$] (E = Si, Sn). These derivatives were characterized in the solid state by IR and in solution by multinuclear NMR (1H, 13C, 29Si, 119Sn, 183W). The crystallographic study of (nBu$_4$N)$_2$[(TaW$_5$O$_{18}$)O] was characterized by IR spectroscopy and single crystal X-ray diffraction. It crystallizes in the orthorhombic system, space group $Pbnm$ with lattice parameters $a = 15.7981(14)$, $b = 17.939(3)$, $c = 35.216(6)$Å, $V = 9980$ Å$^3$ and $Z = 4$.

The grafting of organic moieties onto the dimeric forms leads to the formation of monomeric plenary Lindqvist hybrids (nBu$_4$N)$_2$[MW$_5$O$_{18}$EOR$_3$] (E = Si, Sn). These derivatives were characterized in the solid state by IR and in solution by multinuclear NMR (1H, 13C, 29Si, 119Sn, 183W). The crystallographic study of (nBu$_4$N)$_2$[(TaW$_5$O$_{18}$)O] shows that the structure of the POM is conserved and (SiPh$_3$)$_2$ is grafted selectively on the surface of the polyanion through the terminal O-Ta oxygen atom.

Keywords: polyoxometalates, crystal structures, NMR spectroscopy

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Domain redistribution in SrTiO$_3$. Holger Gibhard, Jakob Sidorku, Jeaniss Leiss, Claudia Hradia, Martin Meven, Götz Eckold.

At ambient temperatures strontium titanate (SrTiO$_3$) has a cubic perovskite structure. Below 105 K the antiphase rotation of adjacent oxygen octahedra leads to an antiferrodistortive transition into a tetragonal phase [1]. During this transformation three different kinds of domains are formed with their tetragonal axes along each of the cubic principal axes. A ferroelectric phase like in the isotropical barium titanate (BaTiO$_3$) is not observed, even at low temperatures. Long range ferroelectric order is suppressed by quantum fluctuations but can be induced by applying an external electric field [2].

The domain distribution can be changed considerably by applying uniaxial mechanical stress [3]. Since the tetragonal distortion corresponds to a c/a-ratio larger than unity, stress along the [110]-direction results in the preferred formation of domains with a tetragonal axis along [001]. Recently, we reported that even an electric field leads to a redistribution of tetragonal domains [4].

In this contribution we present the results of neutron scattering experiments using the diffractometer HEIDI at the FRM II neutron source in Garching. The intensities of a set of 15 superlattice reflections originating from combinations of different domains were determined and fitted to a structure factor model. This yields a quantitative determination of the domain distribution in SrTiO$_3$ as a function of temperature, uniaxial stress and electric field.

Even untreated samples did not show a uniform domain distribution and consisted to almost 50% of $x$-domains. This may be a result of residual stresses originating in crystal growth or sample preparation. Mechanical stress applied along the [110]-direction caused an increase of $x$-domains and only 15 MPa were sufficient to obtain almost monodomain samples. The changes were temperature independent and irreversible. Even after heating the sample above 120 K the same domain distribution was observed in subsequent measurements. An electric field along [001] showed the opposite effect and favoured the reversible formation of $x$- and $y$-domains. The redistribution was temperature dependent and increased on cooling. A complete suppression of $z$-domains was observed when the field induced ferroelectric phase was entered. The simultaneous application of stress and field showed that it is impossible to obtain monodomain samples. Moreover, the present results show that the polar axis of the field induced ferroelectric phase is always perpendicular to the tetragonal axes, corresponding to orthorhombic symmetry.