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SR diffraction studies of the structural inhomogeneities of $CaCu_3Ti_4O_{12}$

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$CaCu_3Ti_4O_{12}$ is a material which shows colossal dielectric constants ~10^4 over a wide range of temperatures and frequencies [1-3]. A dielectric anomaly is observed in $CaCu_3Ti_4O_{12}$: between 100 K and 200 K [1-3] the dielectric constant, ε, jumps up to values about 10^6 between 200K and 600K. At higher temperatures there are pronounced maxima of ε in the 650K – 1050 K region [4,5]. No structural phase transitions were reported from X-ray and neutron diffraction studies of $CaCu_3Ti_4O_{12}$ up to 1270K [3,6].

The crystal structure of $CaCu_3Ti_4O_{12}$ has been studied by using the high resolution synchrotron radiation based X-ray powder diffraction [7]. The observed X-ray diffraction patterns show pronounced Bragg peak asymmetries which should not be present assuming the commonly accepted cubic crystal structure of $CaCu_3Ti_4O_{12}$ described by the space group *Im*-3. Several structural models are discussed. The first model assumes a coexistence of two phases with the cubic symmetry (both space group *Im*-3) and different lattice constants. Next models are based on subgroups of the cubic space group *Im*-3. The best agreement is obtained with the two-phase cubic model [7]. The single cubic phase model gives worse agreement as compared with the two-phase cubic one. None of the models based on the subgroups *C*2*/m, Immm* or *P*2*/c* gives better agreement than the two-phase cubic model.. An inspection of the peak shape shows that for some peaks, see e.g. (4,4,4) in Fig. 1e,f, the two-phase cubic model gives a better agreement.

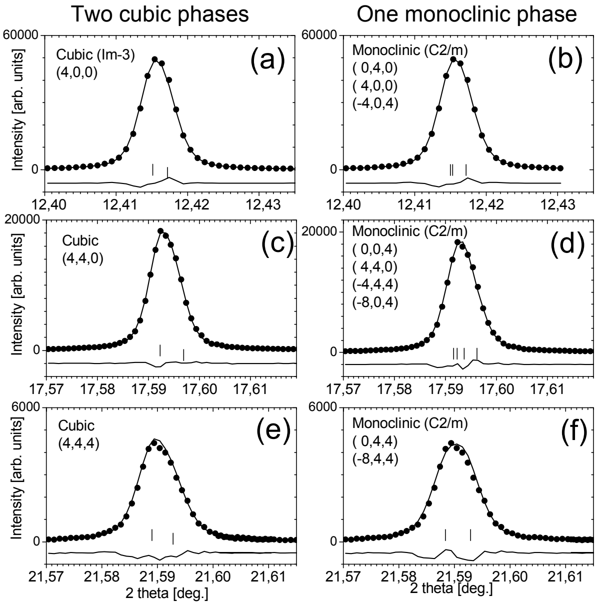

Figure 1. (from [7]) Parts of SR diffraction patterns of $CaCu_3Ti_4O_{12}$ (experimental data = solid symbols). The measurements were performed with λ = 0.39996 Å at RT. Panels a,c,e present the refinement with the two-phase cubic model, space group Im-3 (solid line). Panels b,d,f present the refinement with the monoclinic model, space group *C*2/*m* (solid line). Ticks indicate the positions of the Bragg peaks due to both cubic phases (a,c,e) and the monoclinic phase (b,d,f). The bottom solid lines are difference curves. The corresponding (hkl) are listed.

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