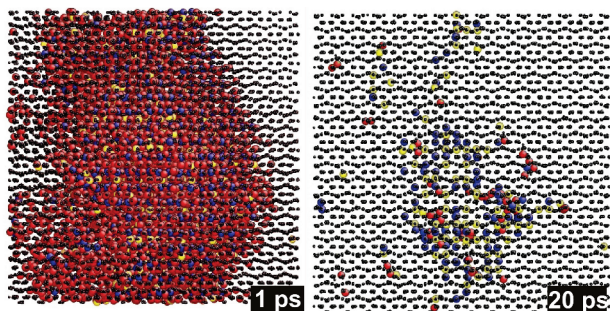


when solving both fundamental and applied problems associated with the isolation and burial of highly active radioactive wastes.

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**Figure 1.** Radiation damage, produced by 20 keV Th recoil in  $\text{Ca}(\text{Zr,Ti,Sn})\text{O}_3$  solid solution at the peak of the damage (left) and after structure relaxation (right).

**Keywords:** radiation resistance of minerals, semiempirical interatomic potentials, molecular dynamics, crystal structure and properties computer simulation, Frenkel defects.

## MS16-P2 Structure relations of the sub-solidus phases in the $\text{CaO-La}_2\text{O}_3\text{-TiO}_2$ system

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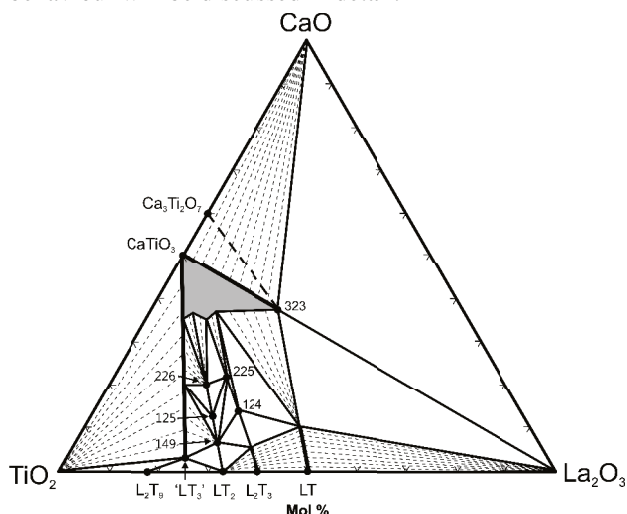
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Sub-solidus phase relations in the ternary  $\text{CaO-La}_2\text{O}_3\text{-TiO}_2$  system at 1400 °C in air were determined. The multi-phase samples were prepared by a solid-state reaction method, whereas the single-phase samples for the structure analysis of selected solid solutions were prepared by a wet-precipitation method in order to provide good homogeneity of the starting mixtures. The phases in the prepared samples were characterized by X-ray powder diffraction (XRD), scanning electron microscopy (SEM) and energy-dispersive spectroscopy (EDS). The oxides form seven ternary compounds in the equilibrium state, many solid solutions (which extend across a broad concentration region), and a large, single-phase area based on the  $\text{CaTiO}_3$  solid solution. The structures of several new phases – solid solutions on the tie lines  $\text{CaTiO}_3\text{-Ca}_3\text{La}_4\text{Ti}_3\text{O}_{15}$  and  $\text{La}_2\text{TiO}_5\text{-Ca}_3\text{La}_4\text{Ti}_3\text{O}_{15}$  – were determined in detail.

The phases studied are denoted with black dots in Fig. 1 and the labels are explained in the figure caption. It was found that the majority of identified ternary phases belong to the perovskite group of structures. The exception is 232, which is isostructural with LT.

The remarkable single-phase region (marked grey in Fig. 1) is due to an extensive solid solubility of lanthanum titanates and the 323 compound in the perovskite  $\text{CaTiO}_3$ . Interesting composition-dependent distortions of the perovskite structure were found. The compositions  $\text{Ca}_{1-x/2}\text{La}_x\text{Ti}_{1-x/2}\text{O}_3$  with  $x > 0.353$  have a monoclinic perovskite structure and those with  $x < 0.353$  an orthorhombic perovskite structure. The origin of such behaviour will be discussed in detail.



**Figure 1.** Sub-solidus phase diagram of the ternary system  $\text{CaO-La}_2\text{O}_3\text{-TiO}_2$  in air, at 1400 °C ( $\text{L}_2\text{T}_9$ :  $\text{La}_4\text{Ti}_9\text{O}_{24}$ ,  $\text{LT}_3^1$ :  $\text{La}_{7/3}\text{TiO}_3$ ,  $\text{LT}_2$ :  $\text{La}_2\text{Ti}_2\text{O}_7$ ,  $\text{L}_3\text{T}_3$ :  $\text{La}_3\text{Ti}_3\text{O}_{12}$ ,  $\text{LT}_4$ :  $\text{La}_4\text{TiO}_5$ , 149:  $\text{CaLa}_8\text{Ti}_6\text{O}_{31}$ , 125:  $\text{CaLa}_4\text{Ti}_5\text{O}_{17}$ , 226:  $\text{Ca}_3\text{La}_4\text{Ti}_6\text{O}_{20}$ , 124:  $\text{CaLa}_4\text{Ti}_4\text{O}_{15}$ , 225:  $\text{Ca}_2\text{La}_4\text{Ti}_5\text{O}_{18}$  and 323:  $\text{Ca}_3\text{La}_4\text{Ti}_3\text{O}_{15}$ ).

**Keywords:** CaO–La<sub>2</sub>O<sub>3</sub>–TiO<sub>2</sub> ternary system, Structure relations, Perovskites, X-Ray powder diffraction, Rietveld refinement

**MS16-P3** Sol–gel synthesis of double perovskite quaternary tellurium-containing metal oxides: Ba<sub>2</sub>NiTeO<sub>6</sub>, Ba<sub>2</sub>CoTeO<sub>6</sub>

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Interest in double perovskite A<sub>2</sub>B'B''O<sub>6</sub> structures comes from the discovery of its colossal magnetoresistance properties exhibited at room temperature by Sr<sub>2</sub>FeMoO<sub>6</sub>.<sup>1</sup> Later it was discovered that perovskites can also act as electrode materials in solid oxide fuel cells (SOFCs),<sup>2,3</sup> and transducers and memories,<sup>4,5</sup> indicating why it is important to invest time to fully understand the nature of their physical and chemical characteristics.

Highly crystalline double perovskite Ba<sub>2</sub>NiTeO<sub>6</sub> and Ba<sub>2</sub>CoTeO<sub>6</sub> have been prepared via novel sol-gel route using citric acid as chelating agent. Both materials have been studied by X-ray diffraction (XRD), scanning electron microscope (SEM), transmission electron microscopy (TEM), and SQUID magnetic measurements. As obtained XRD patterns are carefully analyzed by the Rietveld method using programs X'Pert Highscore Plus and FULLPROF.<sup>6,7</sup>

It was found that at room temperature Ba<sub>2</sub>NiTeO<sub>6</sub> crystallizes in space group *R*-3*m* with *a* = 5.7965(4) Å, *c* = 28.600(3) Å. Ba<sub>2</sub>CoTeO<sub>6</sub> has been refined in the space group *R*-3*m*; *a* = 5.8003(2) Å, *c* = 14.2672(5) are showing trigonal perovskite structure. Average crystallite size is 44 nm for Ba<sub>2</sub>NiTeO<sub>6</sub> and 104 nm for Ba<sub>2</sub>CoTeO<sub>6</sub>, respectively.

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