



Mechanism of the morphotropic transformation between the rutile and corundum structural types

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Abstract:

The rutile/corundum structural transformation which is based on crystallographic shear is discussed in terms of a one-dimensional disorder model. The transformation process is described by a simple model based on the structural relationship between the rutile-type and corundum-type phases. The model is able to handle randomly spaced crystallographic shear planes, the so-called Wadsley defects, as well as clustered CS planes. Calculations show that simply modifying the probability parameters of the model can lead to phase segregation. X-ray powder diffraction patterns are calculated for the proposed transformation mechanism as a function of the stoichiometry  $x$  in  $\text{MO}_{2-x}$  in order to show the influence of such defects on the intensities and linewidths of the Bragg reflections.