Using group-subgroup relations to understand the structural instability in rutile VO_2

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The metal-to-insulator transition in rutile VO_2 occurs along with a structural instability. The nature of the structural instability is not fully understood, let alone whether it is both a necessary and sufficient component of the electronic transition. Moreover, different phases can be formed through the instability depending on small perturbations in chemical conditions or applied pressure.

We will present total x-ray scattering and 3D-ΔPDF data on single crystals with the formula $V_{1-x}Mo_xO_2$, which exhibit disparate types of ordering depending on *x.* We unify the ordering types using isotropic group-subgroup relations, and present a model that maps out all potential distortions within this order parameter. We propose applying this model to most or all families of distorted rutile phases.