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LETTER

Microscopic strain in synthetic pyrope-grossular solid solutions determined by synchrotron X-ray powder diffraction at 5 K: The relationship to enthalpy of mixing behavior

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ABSTRACT

A series of synthetic pyrope-grossular garnets ($Mg_3Al_2Si_3O_{12}$-$Ca_3Al_2Si_3O_{12}$) were investigated by powder X-ray synchrotron radiation at 5 K to determine their microscopic structural strain, which may be responsible for the observed excess enthalpy of mixing for this binary. This substitutional solid solution provides an excellent system for investigating microscopic-macroscopic relationships and the physical nature behind non-ideal thermodynamic mixing behavior in silicates, because of the measurable nonidealities shown by its enthalpy and volume of mixing. An analysis of the X-ray refection profiles, based on theoretical considerations of X-ray line broadening, permits for the first time a direct experimental determination of crystallite size and the root-mean-square structural strain for a mineral solid solution. The measured microscopic strain shows positive and asymmetric deviations from linearity across the join with the largest excess in pyrope-rich compositions. There is a good correlation between the structural strain and the macroscopic enthalpy of mixing behavior for pyrope-grossular garnets as measured by calorimetry.