UNUSUAL COMPRESSIBILITY IN THE NEGATIVE-THERMAL-EXPANSION MATERIAL ZRW_2O_8

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The negative thermal expansion (NTE) compound ZrW_2O_8 has been well-studied because it remains cubic with a nearly constant, isotropic NTE coefficient over a broad temperature range [1]. However, its elastic moduli seem just as strange as its volume because NTE makes temperature act as positive pressure, decreasing volume on warming and, unlike most materials, the thermally-compressed solid softens [2]. Does ZrW_2O_8 also soften when pressure alone is applied? Using pulse-echo ultrasound in a hydrostatic SiC anvil cell, we determine the elastic tensor of monocrystalline ZrW_2O_8 near 300 K as a function of pressure. We indeed find an unusual decrease in bulk modulus with pressure [3]. Our results are inconsistent with conventional lattice dynamics, but we show that a framework-solid-based [4] non-linear model with many degrees of freedom predicts elastic softening as increases in either temperature or pressure reduce volume. ReO_3, a similar framework solid, but lacking the necessary degrees of freedom fails to display softening.

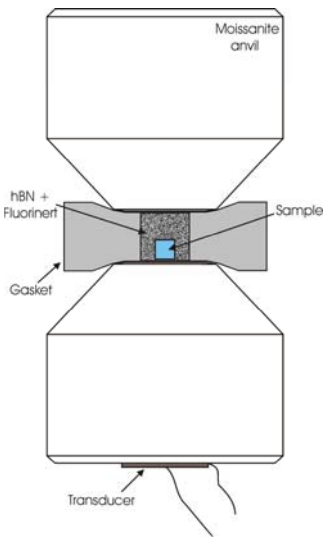

Fig. 1. Schematic of the high-pressure SiC-anvil cell used for determination of elastic moduli at high pressure.

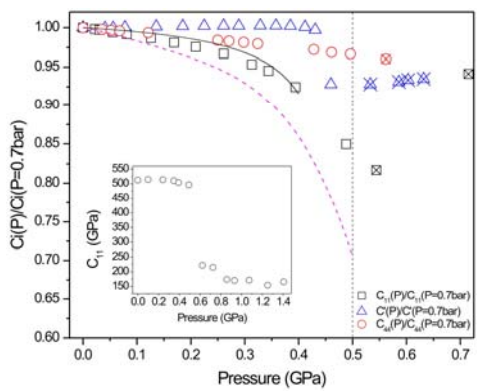

Fig. 2. Relative changes in elastic moduli of ZrW_2O_8 relative to atmospheric pressure at 295K. The bulk modulus B (magenta dashed curve) is computed from a smooth fit to the measured elastic moduli (symbols). The black line represents the fit of C_{11} to Eq.(2). Crosses indicate measurements in the γ-phase of ZrW_2O_8. The vertical dotted line is our fit to the phase-transition pressure. Inset, C_{11} for ReO_3 versus pressure at 295K. The sample was a monocrystal 0.6 mm thick. Measurements were performed in the same system as for ZrW_2O_8.

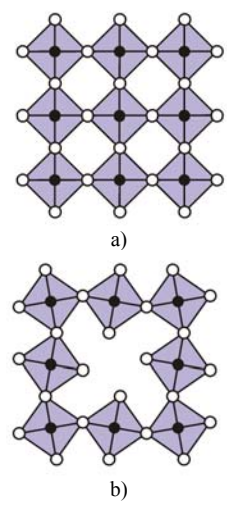

Fig. 3. a) a rigid solid like ReO_3, that does not display NTE. b) a simple picture of a framework solid showing how approximately rigid structures that twist can reduce volume because the open space is reduced when twisting occurs. The twisting can be either thermal-motion induced or pressure induced.

Acknowledgements

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