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Interactive comment on "Is there a layer deep in the Earth that uncouples heat from mechanical work?" *by* S. J. Burns and S. P. Burns

Anonymous Referee #1

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This paper points out that if the volume thermal expansion coefficient of the major mineral phases comprising the Earth's mantle were to fall to zero at the P and T conditions of the mantle, then solid state convection would be suppressed. That conclusion would have profound geodynamic consequences. However, as I discuss below, there is no significant evidence for zero or negative thermal expansion in the major lower mantle minerals (silicate perovskite and (Mg,Fe)O), while the thermodynamic argument presented by the authors has previously shown to be flawed.

Negative thermal expansion is known, as the authors point out, in a number of materials at ambient pressures. The negative thermal expansion of Type IV elements that they mention in the Introduction is exclusively a low-T effect. The negative thermal expansion claimed for diamond (Xie et al., 1999) does occur at high pressures but is also

restricted exclusively to low temperatures (< 500K). These examples are therefore not relevant to the structure of the minerals, nor to the P and T, of the Earth's lower mantle.

There are indeed, as the authors note, a significant number of minerals that exhibit negative volume thermal expansion over significant temperature ranges at low pressures. The negative thermal expansion is well-understood and arises from large anharmonic correlated motions of strongly-bonded cation-anion polyhedra joined at the corners (e.g Dove et al, 2000). Such anharmonic motion can occur in perovskites , especially in the neighbourhood of structural phase transitions, where the anharmonic motion can be very significant. Such large-magnitude anharmonic motions require open space within the structure, and are thus expected to normally be suppressed at high pressures. Both the most recent DFT simulations (Zhang et al, 2013) and extensive experimental measurements confirm this view. They show that actually structures of perovskites with compositions relevant to the Earth's lower mantle (i.e. (Mg,Fe)SiO3) become more distorted with increasing pressure. Therefore a phase-transition related mechanism for negative thermal expansion in (Mg,Fe)SiO3 perovskite is unlikely because the increased tilting takes the structure further away from a transition to higher symmetry; no lower-symmetry perovskite structures exist than the Pbnm structure of (Mg,Fe)SiO3. That is why it transforms to the 'post-perovskite' phase. That transition is not a structural phase transition but is completely reconstructive, and no anomalous behaviour can be expected in the vicinity of the transition. DFT simulations of perovskites at mantle conditions confirm this picture; no structural phase transitions, and the thermal expansion coefficient always remains in excess of 10-5 K-1 (e.g. Table 1 in Zhang et al., 2013).

The authors claim that the measurements of Meng et al (1994) on magnesium silicate spinel show evidence for zero thermal expansion at high pressures. Examination of Figure 1 of that paper shows that the current authors' conclusions are based on an estimated extrapolation of the reported data. Leaving aside the difficulty of these experiments in terms of pressure calibration at high temperatures, and the lack of precision of the measurements, and non-hydrostatic stresses imposed by both grain-grain contacts in the sample and by the pressure medium, such an extrapolation is not supported by the original analysis of the paper.

Therefore, allowing for the uncertainties in experimental measurements at the extreme pressures and temperatures of the Earth's mantle, I am not aware of any experimental evidence for negative volume thermal expansion in major mantle minerals at the appropriate conditions. This conclusion is supported by recent DFT simulations, of which I have only cited one of many.

The authors other line of argument is based on EoS theory. They show that, if one makes certain assumptions about linearity of parameters, one can show that extrapolation of such an EoS can lead at extreme conditions to the prediction of negative thermal expansion. This was previously demonstrated by Hellfrich and Connolly (2009) among others, and arises from non-physical assumptions in the EoS formulation that may appear to be valid over narrow ranges in P and T (perhaps in an experimental range) but are not valid for larger ranges or extrapolations.

I therefore conclude that the authors offer no concrete evidence in this manuscript for negative volume thermal expansion in major mantle minerals at the conditions relevant for the Earth's mantle.

References additional to those in the manuscript:

Hellfrich, G., and Connolly, J.A.D. (2009) Physical contradictions and remedies using simple polythermal equations of state. American Mineralogist, 94, 1616-1619.

Zhang, Z., Stixrude, L., and Brodholt, J. (2013) Elastic properties of MgSiO3 perovskite under lower-mantle conditions and the composition of the deep Earth. Earth and Planetary Science Letters, 379, 1-12.

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