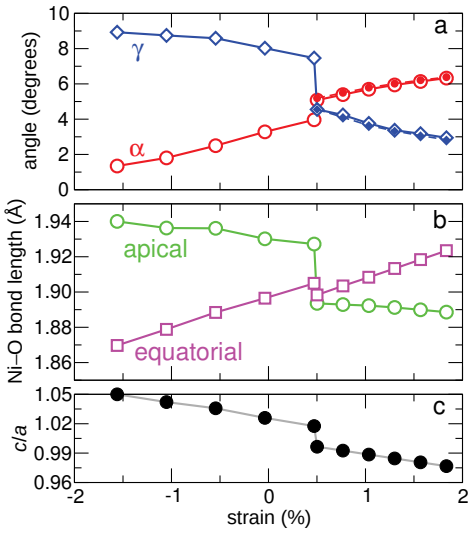

Figure 4: The DFT calculated rotation angles α and γ (**a**), Ni–O bond lengths (**b**) and the c/a axial ratio (**c**) for the monoclinic nickelate structure as a function of strain (open symbols). A sharp first-order transition induced by heteroepitaxy occurs at approximately $c/a = 1$. The solid symbols (broken lines) in (**a**) indicate the bond angles associated with a lower symmetry structure described in the text.

tiling of corner-connected octahedra that is incompatible with size of the unit cell. Recently a strain-induced isosymmetric phase transition, with the axial ratio being the order parameter has also been reported in insulating thin films of the rhombohedral antiferromagnetic and ferroelectric $BiFeO_3$ [6]. Since LNO and $BiFeO_3$ have distinctly different physical properties (LNO is metallic and non-polar), we suggest this intriguing strain-induced isosymmetric phase transition may be a universal feature of epitaxially strained rhombohedral oxide films with the $a^-a^-c^-$ rotation pattern. In principle such strain-induced changes to the rotation patterns can be used to tailor the bandwidth anisotropy, and thus macroscopic properties such as conductivity and magnetism in the thin film. In the case of the large bandwidth compound LNO, however, our DFT calculations (Supplementary Fig. S6) and experiments indicate that the strain induced by the STO and LAO substrates is insufficient to produce dramatic changes in the electronic structure.

In summary, we have demonstrated a general strategy for quantifying oxygen octahedral rotations in strained complex oxide films. We have determined the atomic structure of strained $LaNiO_3$, in which the NiO_6 octahedra are distorted and rotated to accommodate strain. It is anticipated that the future application of this method will enhance fundamental