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Temperature-driven Phase Transformation in Y_3Co: Neutron Scattering and DFT Studies[1] A. PODLESNYAK, G. EHLERS, H. CAO, M. MATSUDA, Neutron Sciences Directorate, ORNL, Oak Ridge, TN 37831, USA, M. FRONTZEK, O. ZAHARKO, Laboratory for Neutron Scattering, Paul Scherrer Institut, CH-5232, Switzerland, V.A. KAZANTSEV, A.F. GUBKIN, N.V. BARANOV, Institute for Metal Physics RAS, 620041 Ekaterinburg, Russia — The effects of a crystal structure deformation due to subtle atomic displacements have attracted much attention because they can result in colossal changes of the electronic and magnetic properties of solids. The R_3Co binary intermetallic systems exhibit a number of complicated phenomena, including field-induced magnetic phase transitions (R=Er, Ho, Tb), giant magnetoresistance (R=Dy), a substantial magnetocaloric effect (R=Gd) and superconductivity (R=La). Contrary to previous studies that defined the ground state crystal structure of the entire R_3Co series as orthorhombic Pnma, we find that Y_3Co undergoes a structural phase transition upon cooling around Tc 160K. Density functional theory calculations reveal a dynamical instability of the Pnma structure of Y_3Co. Employing inelastic neutron scattering measurements we find a strong damping of the (00ξ) acoustic phonon mode below the critical temperature Tc. We suggest that some other members of the R_3Co series (or even all of them) have ground state crystal symmetry lower than reported Pnma. This raises a question about the true magnetic structures and hence the influence of magnetic properties of the entire R_3Co series.

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