Magnetoelectricity of Lu$_2$Fe$_{16.5}$Ru$_{0.5}$

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$_\text{R}_2$Fe$_17$ (R is a rare earth) are compounds with very strong magnetoelectric coupling and often exhibit Invar-like properties such as anomalous and anisotropic spontaneous magnetostriction and negative thermal expansion in a wide temperature range [1]. For Lu$_2$Fe$_{17}$, with the smallest non-magnetic R, the competition of positive and negative exchange interactions between the Fe atoms at various crystallographic positions [2] of the hexagonal (Th$_2$Ni$_{17}$ type) crystal structure results in the transformation of the low-temperature ferromagnetic (F) phase to the antiferromagnetic phase at the Curie temperature $T_C = 274$ K. The application of external pressure and hydrogenation act in the opposite way. While pressure suppresses ferromagnetism in Lu$_2$Fe$_{17}$, hydrogenation (can be considered as a positive pressure) completely removes the AF phase, and the compound Lu$_2$Fe$_{17}$H becomes ferromagnetic [3]. Small substitution of Ru for Fe in Lu$_2$Fe$_{17}$ leads to stabilization of the AF state down to the lowest temperatures. The Néel temperature of Lu$_2$Fe$_{16.5}$Ru$_{0.5}$ is 208 K (Fig. 1) [4].

Neutron diffraction data were collected on the diffractometer D1B ($\lambda = 2.529$ Å). The data analysis done using the FULLPROF program showed that Lu$_2$Fe$_{16.5}$Ru$_{0.5}$ has a helimagnetic antiferromagnetic structure. The propagation vector of the helix varies from 0.236* directly below $T_N$ down to 0.219* at 2 K [4]. External pressure pushes the Néel transition towards the lower temperature. The $T_N$ is $\approx 190$ K under the pressure of 0.5 GPa (Fig 1).

Magnetostriiction of Lu$_2$Fe$_{16.5}$Ru$_{0.5}$ was measured by two independent methods. As the highly sensitive and accurate method, the capacitor dilatometer was employed for the measurement of the single-crystalline sample. The X-ray dilatometry, on the other hand has a much lower sensitivity and accuracy but is a direct method of determination of the interatomic distances changes. Furthermore, possible field-induced structure changes can be observed by means of X-ray diffraction. The atomic coordinates deduced from the powder neutron diffraction experiment were used for the refinement of the obtained X-ray diffraction patterns.

The magnetostrictive strains along the a- and c-axis and the volume effect at 5 T in Lu$_2$Fe$_{16.5}$Ru$_{0.5}$ are $\lambda_a = 0.5*10^{-3}$, $\lambda_c = 1.0*10^{-3}$, $\omega = 2.1*10^{-3}$, respectively. The lattice a parameter remains nearly unchanged as the temperature decreases while the c parameter increases noticeably. The spontaneous volume magnetostriiction reaches the value of $\alpha_v = 6*10^{-5}$. The applied pressure compensates for the unit cell expansion at low temperatures and the AF interactions remain strong in Lu$_2$Fe$_{16.5}$Ru$_{0.5}$.

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