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Fe-excess ions as the electronic charge suppliers in Fe1+xTe1-ySey for development of a ferromagnetic component in the superconducting state and a zero thermal expansion in the normal state

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Superconductivity in α-FeSe has received special attention due to its simple crystalline structure. It is known that the wavy layered α-FeSe structure can accommodate a significant amount of extra Fe ions. These non-stoichiometric Fe ions occupy the interstitial sites that are slightly below the center positions of the Se square sublattice. The general picture established so far for the links between superconductivity and magnetic ordering in iron chalcogenide Fe1+y(Te1-xSex) is that the substitution of Se for Te directly drives the system from the antiferromagnetic end into the superconducting regime. Here, we report on the observation of a ferromagnetic component that developed together with the superconducting transition and a zero thermal expansion of the crystalline lattice in the normal state in Fe-excess crystals, using neutron and X-ray diffractions, resistivity, magnetic susceptibility and magnetization measurements. The superconducting transition is accompanied by a negative thermal expansion of the crystalline unit cell and an electronic charge redistribution, where a small portion of the electronic charge flows from around the Fe sites toward the Te/Se sites. Two magnetic phases are identified. The low-temperature magnetic phase, which coexists with superconductivity, involves the ordering of the lattice Fe and interstitial Fe ions. An extremely large thermal expansion of the lattice is observed in the superconducting state. Thermal expansion coefficients of the lattice are quenched upon loss of superconductivity. Zero thermal expansion is retained over a very broad temperature range from 20 to 200 K. These behaviors are understood as being due to the electronic charge redistribution, in which the excess Fe ions on the interstitial sites act as electronic charge suppliers that strengthen the electronic connections between the Te/Se and Fe ions on the lattice sites once the temperature is raised.

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