Structural Aspects of the Charge Disproportionation Transition in $La_xSr_{1-x}FeO_{3-y}$ (x = 1/10, 1/3, and 1/2)

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The aspects of the charge disproportionation transition for polycrystalline $La_x Sr_{1-x} FeO_{3-y}(x = 1/2, 1/3, \text{ and } 1/10)$ near the transition temperature are investigated using Mössbauerspectroscopy in relevance with their chemical and crystallographic data.

As the lanthanum content x is increased, both the rhombohrdral lattice constant $a_{\rm R}$ and the edge angle $\alpha_{\rm R}$ increase, resulting in a slight increase in the tolerance factor t. For x = 1/3, a first-order-like transition between the low-temperature antiferromagnetic mixed-valence state and the high-temperature paramagnetic average-valence state takes place in the temperature range between 175 K and 200 K. With an increase in x from 1/3 to 1/2, this transition becomes blurred by the weakened p-d hybridization due to the slight decrease in the bond angle (\angle Fe-O-Fe) from 180° with its transition temperature effectively unchanged. For the case of x = 1/10, the electron delocalization takes place at considerably low temperature, and $\text{La}_x \text{Sr}_{1-x} \text{FeO}_{3-y}$ is paramagnetic in the temperature region examined. This comes from a reduction of electron transfer energy due to contractions in the bond lengths.

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