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Tunable cobalt vacancies and related properties in LaCoxAs2 GANG WANG, SHIJIE SHEN, SHIFENG JIN, Institute of Physics, Chinese Academy of Sciences, QINGZHEN HUANG, NIST Center for Neutron Research, NIST, TIANPING YING, DANDAN LI, XIAOLONG CHEN, Institute of Physics, Chinese Academy of Sciences, QINGZHEN HUANG COLLABORATION — The ThCr2Si2-type structure, composed of covalently bonded transition metal-metalloid layers and the intermediate metals, is a common structure to around 1000 compounds. However the origin of transition metal vacancies and their effects on the properties of corresponding compounds have been poorly understood. Here we will report the investigation of structure, physical properties, and electronic structure for a series of nominal LaCoxAs2 (1.6 ? x ? 2.1). It is revealed that the Co occupancy can be tuned between 1.98(1) and 1.61(1). The structural analyses show that the existence of Co vacancies results from charge balance due to the formation of bond between As-As. These Co vacancies adjust the Curie temperature from 205 K to 47 K and increase the resistivity by more than 100%. First-principles calculations indicate that the Co vacancies weaken the spin polarization and reduce the density of states at the Fermi level, resulting in decreased Curie temperature and increased resistivity, respectively. The results address the importance of transition metal vacancies in ThCr2Si2-type structure and offer a reliable route to tune the magnetism of ThCr2Si2-type structure.

Gang Wang
Institute of Physics, Chinese Academy of Sciences

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