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Anisotropic magnetoelastic coupling and magnetocaloric effect in the Fe_5Si_3-type hexagonal single crystal GUIXIN CAO, Center for Nanophase Materials Sciences, Oak Ridge National Lab, Oak Ridge, TN 37831, SATOSHI OKAMOTO, M.A. MCGUIRE, JUNJIE GUO, Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, LING LI, JIEYU YI, DAVID MANDRUS, Department of Materials Science and Engineering, University of Tennessee, Knoxville, TN 37996, MATTHEW F. CHISHOLM, BRIAN C. SALES, Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, ZHENG GAI, Center for Nanophase Materials Sciences, Oak Ridge National Lab, Oak Ridge, TN 37831 — The structural, magnetic properties, and the magnetocaloric effect (MCE) of Fe_5Si_3 single crystal with trace of Mn and P doping ($Fe_{4.83}Mn_{0.16}Si_{2.91}P_{0.09}$) are investigated. A first-order magnetoelastic transition was found at the magnetic transition temperature T_C, with the magnetic easy axis lying in the ab plane. While the trace of Mn and P doping in the Fe_5Si_3 single crystal was found to increase both the maximum magnetic entropy change and relative cooling power from those in polycrystalline Fe_5Si_3 compound, indicating the intrinsic broaden entropy change in larger temperature span. The anisotropy in the MCE between H//ab and H//c is observed, which originates from the anisotropic spin-lattice coupling between the ab plane and the c axis. The density functional theory calculations were performed to gain microscopic insights into the experimental findings. Our results suggest hexagonal Fe_5Si_3 system may become a new candidate of giant MCE as La-Fe-Si and Fe-Mn-P-Si systems.

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