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Epitaxial and stoichiometric effects on structural and chemical ordering in Heusler alloys BRIAN A. COLLINS, LIANG HE, FRANK TSUI, University of North Carolina at Chapel Hill, YUNCHENG ZHONG, YONG S. CHU, Argonne National Laboratory — The Heusler alloys of Co_2MnGe and Co_2MnSi have been predicted to be half-metallic, where the minority spin density of states shows a gap at the Fermi Level. However, half-metallicity has not yet been realized owing to its expected sensitivity to atomic disorders associated with off-stoichiometry and epitaxial constraints. Combinatorial epitaxial films of $Co_xMn_yGe_z$ and $Co_xMn_ySi_z$ have been grown on Ge (111) substrates in and around the Heusler stoichiometry using molecular beam epitaxy. The structural and chemical ordering of the films has been examined using synchrotron x-ray microbeam techniques, including x-ray diffraction and energy dependent anomalous diffraction. A comprehensive model has been developed for anomalous diffraction, allowing for detection and quantification of various disorders even at small amounts, including site-dependent vacancies and elemental site swapping. The x-ray experiments reveal that the ordering is very sensitive to the Co:Mn atomic ratio and that epitaxial strain can cause a shift in the composition of highest structural ordering away from the Heusler stoichiometry, accompanied by increased chemical disorders. These findings have made it possible to explore spin dependent states as a function of structural and chemical ordering.

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