

Abstract Submitted  
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**Quantitative chemical and structural ordering of Heusler  $\text{Co}_x\text{Mn}_y\text{Ge}_z$  (111) epitaxial films**<sup>1</sup> FRANK TSUI, BRIAN COLLINS, LIANG HE, Physics and Astronomy, University of North Carolina at Chapel Hill, YONG CHU, National Synchrotron Light Source II, Brookhaven National Laboratory — Heusler alloys are attractive spintronic materials, owing to the predicted half-metallicity and their compatibility with epitaxial semiconductor heterostructures. Chemical defects have been suggested as the cause of low spin-polarizations measured in these materials. We report a systematic investigation into the structural and chemical ordering of  $\text{Co}_x\text{Mn}_y\text{Ge}_z$  films grown epitaxially on Ge (111) substrates, as a function of composition near the Heusler  $\text{Co}_2\text{MnGe}$  stoichiometry. X-ray diffraction experiments show that the structural ordering is extremely sensitive to the Co-Mn atomic ratio with the best ordering occurring at compositions rich in Ge, i.e. off the Heusler stoichiometry. A new multi-edge anomalous diffraction technique has been employed to measure the elemental occupancy of the lattice sites. The measurements and analysis reveal that the dominant chemical defect is Mn-Ge site swapping with no detectable Co-Mn swapping, at variance with the predictions based on density functional theory. The observed shift for the most ordered composition from that of the bulk has been attributed to epitaxial constraints. The finding provides impetus for exploring spin polarization at off-stoichiometric compositions.

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