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Chemical-disorder effects in half-metallic Heusler alloys RALPH SKOMSKI, YUNLONG JIN, University of Nebraska, Lincoln, JACE WAYBRIGHT, PARASHU KHAREL, South Dakota State University, ROHIT PATHAK, RENU CHOUDHARY, ARTI KASHYAP, Indian Institute of Technology, Mandi, HP, India, D. J. SELLMYER, University of Nebraska, Lincoln — The electronic structure, magnetism, and conductivity of disordered Heusler alloys are investigated theoretically and experimentally. Emphasis is on Heuslers that are predicted to be half-metallic or spin-gapless semiconducting in their fully ordered states, such as CoFeCrAl. Experimental alloys often exhibit resistivities of the order of 200 $\mu\Omega$cm, which is consistent with both dirty-metal and spin-gapless semiconducting behaviors, but a distinction can be made by comparing the residual resistivities of samples having different degrees of order. The corresponding analysis shows that careful processing is necessary to keep the alloys in the spin-gapless semiconducting regime. Several types of disorder occur in Y-type Heusler alloys, with different negative effects on half-metallicity and spin-gapless semiconductivity. A2 (or bcc) disorder is most harmful but can be limited experimentally in CoFeCrAl thin films. B2 (or CsCl) disorder is less harmful, whereas $L2_1$ (normal Heusler) disorder, corresponding to Fe-Co solid solubility is least harmful. The residual resistivity of the partially diorderd alluys is discussed as a carrier-localization effect. — This work is supported by DOE BES (DE-FG02-04ER46152, R.S.) and NSF DMREF (SusChEM 1436385, D.J.S.)

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