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Structural, electronic, magnetic and transport properties of $Co_2Fe_{1-x}Cr_xSi$ Heusler alloys

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The effect of Cr substitution in place of Fe on the structural, electronic, magnetic and transport properties of the Co_2FeSi alloy is studied. A comprehensive structural analysis is done using X-ray diffraction (XRD) and extended X-ray absorption fine structure (EXAFS) spectroscopy. Quaternary Heusler compounds $Co_2Fe_{1-x}Cr_xSi$ with Cr content (x = 0.1, 0.3, 0.5) were found to crystallize in cubic structure. The synchrotron-based EXAFS studies reveal that the anti-site disorder increases with the increase in Cr concentration. The saturation magnetization values in all the alloys are found to be less than those expected from the Slater-Pauling rule, which may be due to some inherent disorder. A detailed resistivity analysis in the temperature range of 5-300 K is done, taking into account different scattering mechanisms. The residual resistivity ratio is found to decrease with increasing Cr concentration. A disorder induced resistivity minimum due to weak localization effect is seen for x=0.5. The resistivity measurements also indicate that the half-metallic character survives up to 100 K for x=0.1, whereas the alloys with x=0.3 and 0.5 show signature of half-metallic nature even at higher temperatures. First-principles calculation done with a more robust exchange-correlation functional (namely HSE-06) confirms the half-metallicity in the entire concentration range. Theoretically simulated band gap and magnetic moments compliment the experimental findings. All these properties make $Co_2Fe_{1-x}Cr_xSi$ a promising material for spintronics.

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