Influence of the Cu doping on the Electronic Structure and Magnetic Properties of the Mn_2VAl Heusler compound

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Detailed investigations on the electronic and magnetic properties of the Heusler compounds $Mn_{2-x}Cu_xVAl$ (x = 0 to 0.5) with $L2_1$ structure have been performed. The $Mn_{2-x}Cu_xVAl$ ingots were prepared by induction melting under a purified Ar atmosphere. The resulting samples have been studied by X-ray diffraction (XRD) and magnetization measurements. The degrees of the B2 and $L2_1$ atomic ordering were obtained by using the Takamura's extended order model. The Curie temperatures decrease with Cu content, from 771 K (x = 0) to 580 K (x = 0.5). Additionally, electronic band structure calculations using the KKR Greens function method have been performed, taking into account the site occupation obtained by XRD measurements. The substitutional disorder was accounted by the means of the Coherent Potential Approximation (CPA). Our study gives insight on the evolution of the half-metallic fully compensated ferrimagnet (HMF) character with disorder and Cu doping.

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