Magnetic properties, electronic structure and stability of Heusler alloys $Mn_{2-x}Fe_{1+x}Al$

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Heusler Mn-based alloys are being intensively studied because of complex magnetic properties [1], spintronic applications, electronic structure and band-gap design. We present an investigation of the electronic structure and magnetic properties of the novel composition $Mn_{2-x}Fe_{1+x}Al$. It was found to be stabilized in a cubic β-Mn-type crystal structure with an antiferromagnetic ordering of the Mn and Fe magnetic moments for x = 0.5, similar to the recently reported Mn_2FeAl Heusler alloy [2]. The detailed theoretical study was done to obtain the optimized atomic positions for $Mn_{1.5}Fe_{1.5}Al$ in the β-Mn-type structure for the first time. The calculated total magnetic moment is found to be 1.76 μ_B per formula unit of $Mn_{1.5}Fe_{1.5}Al$. The magnetic ordering in this configuration is composed of the ferro and antiferromagnetically arranged Mn ions, being antiferromagnetically ordered mostly in the 8c-type positions. The average magnetic moment of Mn, Fe and Al are 3.1 (Mn2) and 2.2 (Mn1) μ_B, 0.7 and 0.2 μ_B, correspondingly. These contributions of the Mn ions give the largest contributions to the densities of states and magnetic properties of the $Mn_{1.5}Fe_{1.5}Al$ Heusler alloy. The calculations for the Mn-Al alloys show that with the occupation of the 12d positions with Al results in the decreasing total magnetic moment with the total moment equal to zero in some cases. Our theoretical calculations demonstrate the complex character of the magnetic properties and electronic structure of the Heusler $Mn_{2-x}Fe_{1+x}Al$ alloys.

References:

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