STRUCTURAL, MAGNETIC AND HYPERFINE PROPERTIES OF B2–TYPE FeAl DOPED WITH TRANSITION METAL IMPURITIES

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9.7 cm

The structural, electronic and magnetic properties of the transition metal (TM=Ti, V, Cr, Mn, Co, Ni, Cu, Zn) impurities in $Fe_{50}Al_{50}$ matrix with B2-type structure have been investigated applying the the super-cell approach and using the tight-binding linear muffin-tin orbital (TB-LMTO) method of electronic structure calculations. The location of the TM impurity at Fe and Al sites was tested. For each investigated composition $Fe_{44}TM_6Al_{50}$ and $Fe_{50}TM_6Al_{44}$ the volume optimization was performed and the formation energy was estimated. Both magnetically ordered and non magnetic solutions were analysed. Based on the calculated results the following conclusions can be drawn: a) In all investigated cases the magnetic solutions are stable against the non-magnetic one. b) The site preference established shows that the elements of the periodic table on the left of iron (Ti, V, Cr, Mn) prefer to occupy Al sublattice while the heavier atoms (Co, Ni, Cu, Zn) locate at the Fe sites. c) The site preference strictly correlates with the alignment of the impurity local moment. The local moment of the impurities located at the preferred site always show the antiferromagnetic alignment with respect to the bulk magnetization. d) The calculated (optimized) volume and the average ^{57}Fe isomer shift show the similar dependence on the impurity atomic number (Z). The calculated structural and electronic properties follow qualitatively the tendency observed experimentally for the TM impurities in FeAl host and the dilute Fe-TM alloys.

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