Abstract: Fe hyperfine fields in Fe$_{3-x}$V$_x$Si alloys

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Transition metal elements substituted into Fe$_3$Si were found to preferentially select one of the two inequivalent Fe sites in the Fe$_3$Si structure, according to their location in the periodic table. The atoms of elements to the left of Fe in the table choose the Fe site which has 8 Fe 1st nearest neighbors, inn, while those under Fe or to the right of Fe go into the Fe site with 4 Fe + 4 Si inn. A similar pattern of site occupation is observed in the Heusler alloys. This conclusion was initially based on a variety of hyperfine field studies and has been confirmed by neutron diffraction results. This selectivity allows some careful studies of spin polarization produced by a limited number of specific near neighbor environments. A model including only those spin changes produced by inn explains the internal fields at the transition metal nuclei in Fe$_{3-x}$Mn$_x$Si and Fe$_{3-x}$V$_x$Si alloys. Examination of the electronegativity of the transition metal impurities shows that the Fe site with 8 Fe inn is preferred by the less electronegative substitutions.

REFERENCES
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