Abstract: Fe hyperfine fields in $Fe_{3-x}V_xSi$ alloys

T. J. Burch and C. A. Weiler

Marquette University, Milwaukee, Wisconsin 53233

K. Raj[b] and J. I. Budnick

University of Connecticut,[a] Storrs, Connecticut 06084

V. Niculescu

Virginia Commonwealth University, Richmond, Virginia 23284

G. C. Papefthymiou and R. B. Frankel

Francis Bitter National Magnetic Laboratory,[c] Massachusetts Institute of Technology, Cambridge, Massachusetts 02139

PACS numbers: 75.50.Bb, 75.30.Hx, 76.60.Lz, 61.16.Hn

Transition metal elements substituted into Fe_3Si were found to preferentially select one of the two inequivalent Fe sites in the Fe_3Si structure, according to their location in the periodic table.[1] The atoms of elements to the left of Fe in the table choose the Fe site which has 8 Fe 1st nearest neighbors, 1nn, while those under Fe or to the right of Fe go into the Fe site with 4 Fe + 4 Si 1nn. 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.[2] 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 1nn explains the internal fields at the transition metal nuclei in $Fe_{3-x}Mn_xSi$ and $Fe_{3-x}VxSi$ alloys.[3] Examination of the electronegativity of the transition metal impurities shows that the Fe site with 8 Fe 1nn is preferred by the less electronegative substitutions. This phenomenological conclusion is reinforced by a band structure calculation of Switendick.

REFERENCES

* Supported by the University of Connecticut Research Foundation.

1. T.J. Burch, T. Litrenta, and J.I. Budnick, Phys. Rev. Lett. 33, 421 (1974).
2. S. Pickart, T. Litrenta, T.J. Burch, and J.I. Budnick, Phys. Lett. A 53, 321 (1975).
3. V. Niculescu, K. Raj, J.I. Budnick, T.J. Burch, W.A. Hines, and A.H. Menotti, Phys. Rev. B 14, 4160 (1976).
4. A.C. Switendick, Solid State Commun. 19, 511 (1976).

 0021-8979/79/032079-01$01.10