ATOM-PAIR CORRELATIONS IN Fe-13.5% V

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J. W. Cable, H. R. Child, and Y. Nakai*

Oak Ridge National Laboratory

P.O. Box 2008

Oak Ridge, Tennessee 37831-6031

U.S.A.

*Faculty of Science

Osaka University

Toyonaka, Osaka 560

Japan

Diffuse neutron scattering data were used to determine the atom-pair correlations for Fe-13.5% V in terms of both the Warren-Cowley ASRO parameters and the Krivoglaз-Clapp-Moss pair-potentials. These agree reasonably well with those calculated by Hennion from alloy band structure parameters.

Keywords: Atom-pair Correlations, Fe-V Alloy

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The pair potentials in ferromagnetic Fe-based alloys were recently treated by Hennion[1] using band structure parameters obtained by the CPA method generalized to the ferromagnetic state. The calculated potentials are strongly dependent on both the atomic separation and the concentration, and in the Fe-Cr case, the first neighbor potential even changes sign with increasing Cr content. This sign inversion has since been verified by a neutron diffuse scattering study of the atomic short range order (ASRO) for Fe-Cr.[2] This agreement provides some confidence that the effective pair potentials extracted from diffuse scattering measurements can be related to those calculated from the band structure of disordered alloys. In this paper, we report a neutron study of the ASRO in an Fe-rich, Fe-V alloy. The Fe-V alloy system is particularly well suited for neutron diffuse scattering studies because the atoms are similar in size but quite different in scattering amplitude. The diffuse scattering should therefore be relatively

intense with little distortion due to static lattice displacement effects.

The neutron measurements were made at the High Flux Isotope Reactor (HFIR) in Oak Ridge using unpolarized neutrons and a triple-axis spectrometer set for elastic scattering with 35 meV incident neutrons ($\lambda = 1.529 \text{ \AA}$). The nuclear and magnetic diffuse scattering intensities for this alloy are comparable and must be separated for the measurement of either. In the present experiment, this is readily accomplished by the application of a saturating magnetic field parallel to the scattering vector. With the magnetic scattering thereby extinguished, the remaining diffuse intensity was measured at room temperature along the [100], [110], and [111] directions. The data, corrected for background and placed on an absolute cross section basis by a vanadium calibration, are shown in Fig. 1. These cross sections are almost entirely nuclear in origin and contain contributions from the nuclear disorder scattering, the spin

incoherent scattering, and the multiple scattering. The observed cross sections exhibit considerable structure which we attribute to the nuclear disorder scattering. The most intense diffuse peaks occur at (100) and (111) which indicates an anti-correlation for first neighbor atom pairs and a tendency toward the β -CuZn type of ordering.

The cross section can be written as

$$\frac{d\sigma}{d\Omega}(\vec{K}) = \frac{d\sigma}{d\Omega}(\text{inc.}) + \frac{d\sigma}{d\Omega}(\text{mult.}) + c(1-c) \Delta b^2 S(\vec{K}) \quad (1)$$

where $S(\vec{K})$ can be expressed either in terms of the Warren-Cowley ASRO parameters or in terms of the Krivoglaz-Clapp-Moss (KCM) pair potentials.[3-5] For the former, the scattering law becomes

$$S(h_1, h_2, h_3) = \sum_{lmn} \alpha_{lmn} \cos \pi l h_1 \cos \pi m h_2 \cos \pi n h_3, \quad (2)$$

where the scattering vector is

$$\vec{K} = 2\pi(h_1 \vec{b}_1 + h_2 \vec{b}_2 + h_3 \vec{b}_3) \quad (3)$$

and the atomic position vectors are defined by

$$\vec{R} = 1/2 (\ell \vec{a}_1 + m \vec{a}_2 + n \vec{a}_3), \quad (4)$$

where l , m , and n are integers that are either all odd or all even for this bcc lattice. All α 's in the same neighbor shell have also been assumed equal.

The data were fitted to Eqs. 1 and 2 with the result shown in Fig. 1 by the dashed curves which correspond to a 10 parameter fit. The α_l variation with the number of parameters included in the fit is shown in Fig. 2. Here, only 6 parameters are shown for clarity of presentation; however, 8 parameters are required to reproduce the double peak near $(1/2, 1/2, 1/2)$ and the sharpness of the diffuse peak at (111) .

In the KCM formalism, the scattering law is given by

$$S(h_1, h_2, h_3) = \quad (5)$$

$$A [1 + 2c (1-c) \beta V(h_1, h_2, h_3)]^{-1},$$

where A is a normalization constant and $\beta = (k_B T)^{-1}$. The Fourier transform of the interatomic pair potential is

$$V(h_1, h_2, h_3) = \quad (6)$$

$$\sum_{lmn} V_{lmn} \cos \pi l h_1 \cos \pi m h_2 \cos \pi n h_3,$$

with the same l, m, n restrictions and neighboring-shell assumptions as for the α_{lmn} . The data were fitted to Eqs. 1 and 5 in the $A = 1$, or high temperature limit, and the 10 parameter fit is shown by the solid curves in Fig. 1. The dependence of the βV_l parameters on the number of parameters is shown in Fig. 2. Here again, only a limited number of parameters are represented for purposes of clarity, but at least 8 parameters are required to reproduce the features of the $[h h h]$ cross section.

The atom-pair correlations obtained from these fitting procedures are summarized in Table I. These α_{lmn} are qualitatively consistent with those previously obtained[6] for polycrystalline samples. In that paper, an average α for first and second neighbors was defined as $\alpha_{12} = (8\alpha_1 + 6\alpha_2)/14$ and $\alpha_{12} = -0.084$ was obtained for an Fe -14.7% V alloy. This is in reasonable agreement with the average of $\alpha_{12} = -0.071$ for the present Fe-13.5% V alloy. The third and fourth neighbor parameters obtained in reference 6

are larger than the present results but have the same signs. First and second neighbor ASRO parameters were also obtained from NMR data using a model which attributes spectral lines in the hyperfine field distribution of ^{51}V nuclei to specific configurations of V atoms in the first and second neighbor shells of a central V atom.[6] If these NMR lines are properly assigned, then the present ASRO results indicate that a second neighbor V atom produces a larger NMR frequency shift than does a first neighbor.

In accordance with the theoretical calculations,[1] the fitted pair potentials decrease rapidly with increasing interatomic separation. However, the calculated V_2/V_1 ratio is only about 0.22, and this is much too small to account for the observed intensity at $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ which is strongly dependent on this ratio. We note that the observed V_2/V_1 ratio of 0.63 lies properly below the $V_2/V_1 = \frac{2}{3}$ value that defines the stability limit for the β - CuZn type of ordering.[7] To place these fitted pair potential parameters on an energy scale, an

effective temperature must be assigned to the quenched-in, high-temperature state of the alloy. For this sample, which was quenched from about 1270 K, we estimate an effective temperature of about 900 K or $k_B T \sim 80$ meV. The first three observed pair potentials therefore have energies corresponding to 34, 22, and -4 meV compared to the calculated[1] values of 46, 10 and 2 meV. We consider this good agreement, especially in view of the fact that the experimental results correspond to the high temperature limit while the calculations are carried out in the $T = 0$ limit. The double peak near $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ and the sharpness of the diffuse peak at (111) indicate atom-pair correlations extending to the 8th neighbor shell. It will be quite interesting to see if first-principles calculations[8] can reproduce this unexpected long-range feature of the atom-pair correlations in Fe-V alloys.

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* Faculty of Science, Osaka University, Toyonaka, Osaka 560, Japan.

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TABLE

Neighbor Shell	lmn	α_{lmn}	βV_{lmn}
1	111	-0.092	0.43
2	200	-0.044	0.27
3	220	0.033	-0.05
4	311	-0.003	0.00
5	222	0.008	0.00
6	400	0.000	0.01
7	331	-0.008	-0.01
8	420	0.011	-0.03
9	422	0.003	0.00

Table I. Atom-Pair Correlations for
Fe-13.5% V

FIGURE CAPTIONS

Fig. 1. Cross sections along high symmetry directions in Fe-13.5% V. The solid and dashed curves are fitted to the data with pair-potential and ASRO parameters, respectively.

Fig. 2. Dependence of the fitting parameters on the number of parameters included in the fit. The effective temperature of the quenched-in alloy state is defined by $\beta = (k_B T)^{-1}$.

Fe-13.5% V

Fig. 2