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Brief Reports

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Temperature dependence of hyperfine magnetic fields in Fe-Co alloys

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A Mössbauer spectrometry study of bcc Fe-Co alloys was performed to measure the ^{57}Fe hyperfine-field parameters from 77 to 900 K. The temperature dependence of the ^{57}Fe hyperfine magnetic field in Fe-Co alloys was similar, although not identical, to that of ^{57}Fe in pure Fe. These results are understood if the alignment of magnetic moments at Fe atoms is only slightly more temperature dependent than at Co atoms. This situation for Fe-Co is significantly different from that of Fe-Ni alloys, indicating that the interatomic exchange interactions in Fe-Co alloys are stronger than in Fe-Ni.

It is well known that the Slater-Pauling curve of Fe-Co alloys (saturation magnetization versus Co concentration) displays a sharp maximum. This is accepted as a transition from weak ferromagnetism to strong ferromagnetism as the addition of Co causes the $3d\uparrow$ states to become filled at about 30 at. % Co. We recently performed Mössbauer and electron energy-loss spectrometry studies of Fe-Co alloys and found maxima in the ^{57}Fe hyperfine magnetic field (hmf) and isomer shift near 30 at. % Co.[1] With these data and with magnetization data, we deduced how the occupancies of Fe $3d\uparrow$, $3d\downarrow$, and $4s$ states depend on Co concentration. Making use of these results, we then performed a Mössbauer spectrometry study of the disorder$\rightarrow$$B2$ order transformation in equiatomic FeCo.[2] Brief annealings of the disordered material caused an increase in the variance of the ^{57}Fe hmf spectra distribution in spectra measured at 77 K, but not in spectra measured at room temperature. This suggests that the temperature dependence of the ^{57}Fe hmf depends on the number of Co atoms near the ^{57}Fe atom. In some transition-metal alloys such as Fe-Ni and Fe-Mn, the temperature dependence of the ^{57}Fe hmf is "anomalous" in that it is not proportional to the temperature dependence of the saturation magnetization.[3-5] Here we present the results of a study of the temperature dependence of the ^{57}Fe hmf in Fe-Co alloys across the bcc composition range. Preliminary results were described recently.[6]

Our Mössbauer spectrometer (^{57}Co in Rh source) and our procedures for alloy preparation were described recently.[1] For high-temperature measurements, an evacuated furnace[5] was mounted on the spectrometer, and the cryogenic measurements were performed with the specimen in a He exchange gas at 78 K. The experimental data were analyzed by the method of Le Caër and Dubois[7] to extract hmf distributions and isomer shift data.

We interpreted the ^{57}Fe hmf distribution with the model developed by Stearns for dilute Fe-Co (Ref. 8) and later used by Fultz and Morris for nondilute Fe-Ni (Ref. 5). In this model, the ^{57}Fe hmf is a linear combination of the local core polarization (CP) and the nonlocal conduction-electron polarization (CEP). The CP component is proportional to the local magnetic moment at the ^{57}Fe atom, while the CEP component is proportional to the magnetic moment at the ^{57}Fe atom and the magnetic moments in each surrounding shell of atoms. The magnetic moment of Fe, μ_{Fe}, is calculated by considering its magnetic-moment perturbations due to neighboring Co atoms in the first five nearest-neighbor shells. The magnetic mo-

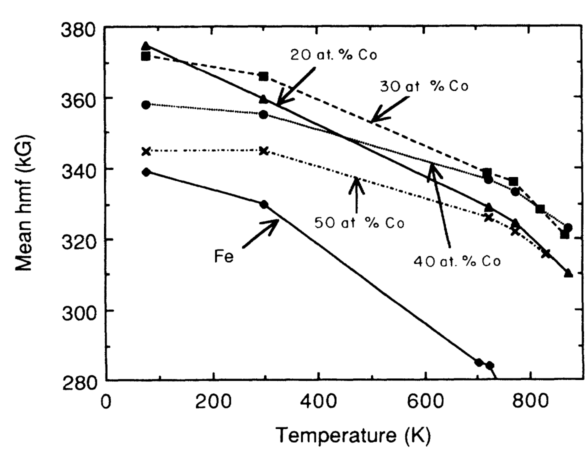

FIG. 1. The mean ^{57}Fe hyperfine magnetic field of disordered Fe-Co alloys vs temperature.

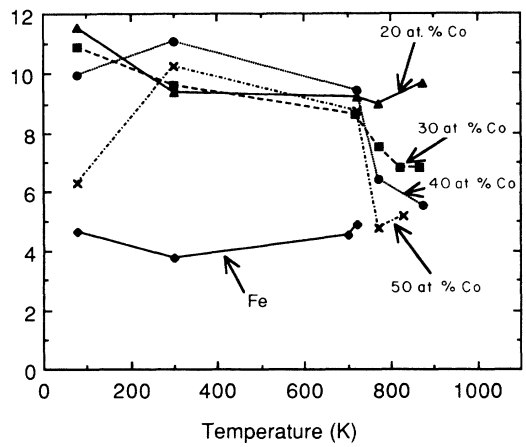

FIG. 2. The square root of the variance of the ^{57}Fe hyperfine magnetic field of disordered Fe-Co alloys vs temperature.

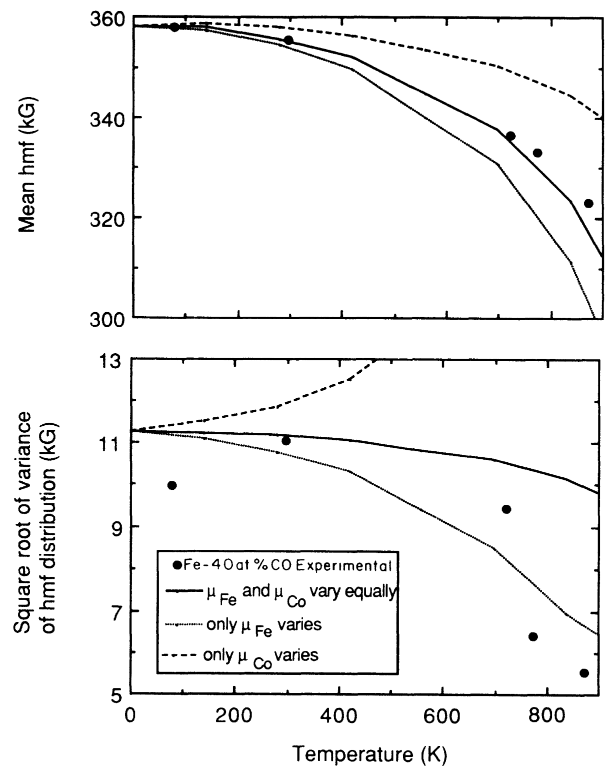

FIG. 3. Calculations of the mean and square root of the ^{57}Fe hmf distribution vs temperature for Fe–40 at. % Co, assuming the extreme cases: (i) only μ_{Co} depends on temperature, (ii) only μ_{Fe} depends on temperature, and (iii) μ_{Co} and μ_{Fe} depend equally on temperature.

ment of Co is unperturbed by variations in its local chemical environment.[9] Details of these calculations are given elsewhere.[1,5]

The mean ^{57}Fe hmf in Fe-Co alloys from 77 to 900 K is presented in Fig. 1. No strongly anomalous behavior was observed; the measured ^{57}Fe hmf was similar, although not identical, to the saturation magnetization measured by Eguchi *et al.*[10] The temperature dependence of the variance of the ^{57}Fe hmf is presented in Fig. 2. These data are less reliable than those of Fig. 1 because they are harder to extract from experimental spectra. (Additionally, a small part of the reduction in variance at high temperatures could arise from a decreased thickness distortion and from a reduced distribution of domain demagnetizing fields of the sample.)

The ^{57}Fe hmf could depend on temperature through a temperature dependence of the CP and CEP constants, or through the temperature dependence of $\mu_{Fe}(T)$ or $\mu_{Co}(T)$. The CP constant is not expected to be temperature dependent because it involves strongly localized electrons at the ^{57}Fe atom. Our evidence that the CEP constants are largely independent of temperature is as follows. We obtained the Mössbauer spectra from chemically disordered alloys of Fe–48 at. % Co–4Mo at temperatures up to 623 K (in times less than required for significant short-range ordering in the material[11]). The Mo atom has no magnetic moment and causes a strong perturbation of the ^{57}Fe hmf through CEP; this is seen as a satellite peak on the low-energy sides of the main absorption peaks. This satellite peak did not change significantly with temperature, so we believe that the CEP constants do not change significantly with temperature.

The temperature dependence of the ^{57}Fe hmf must originate from the temperature dependence of $\mu_{Fe}(T)$ or $\mu_{Co}(T)$. We performed three different types of calculations for the hmf by assuming $\mu_{Fe}(T)$ to have a stronger, a weaker, or an equal dependence on temperature than $\mu_{Co}(T)$. In these calculations the magnetization of the alloy was constrained to equal the magnetization of the real alloys.[10] Calculations for the Fe–40 at. % Co alloy are presented in Fig. 3. For the most part, the ^{57}Fe hmf distribution is adequately described by allowing $\mu_{Fe}(T)$ and $\mu_{Co}(T)$ to have the same temperature dependence. Nevertheless, our data provide evidence that the temperature dependence of $\mu_{Fe}(T)$ is somewhat stronger than that of $\mu_{Co}(T)$, at least for Co concentrations below 40 at. %. The reduction with temperature of these magnetic moments could originate from a reduction in the intrinsic values of the magnetic moments, or to the reduced alignment of the moments with temperature. Changes in the intrinsic values of magnetic moments originate with changes in electronic structure, which will also affect the isomer shift. As discussed below this is not observed, so it is the alignment of the magnetic moments that depends most strongly on temperature. In measurements of the hmf, the relevant magnetic moments are time averaged in their alignment over about 2×10^{-8} sec, the ^{57}Fe Larmor precession time. The time scale for the fluctuations of the magnetic moments is evidently much shorter than 2×10^{-8} sec, so there is no significant line-shape distortion.

By measuring the areas of our spectra from 77 to 723 K, we determined how the temperature dependence of the recoil-free fraction (rff) depended on Co concentration. The dependence was not significant. For example, for each of five compositions from 0 to 60 at. % Co, the average area of the spectrum at 300 K to the area at 723 K was 0.77 ± 0.02 (consistent with a Debye temperature

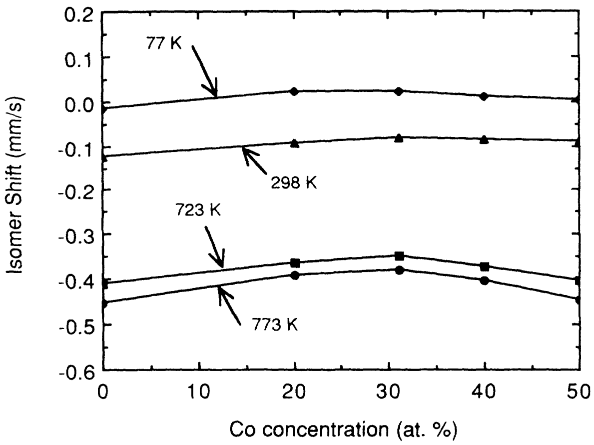

FIG. 4. The average ^{57}Fe isomer shift vs Co concentration at different temperatures.

of about 450 K). The temperature dependence of the isomer shift, presented in Fig. 4, is also insensitive to the alloy composition. The variation of isomer shift with temperature is caused entirely by the thermal shift (except for the Fe–50 at. % Co alloy, which undergoes *B*2 ordering at higher temperatures). The temperature dependences of the rff and isomer shift indicate that the mean-squared vibrational amplitudes and mean-squared velocities of ^{57}Fe atoms do not depend significantly on the number of Co atoms in their neighborhood.

These temperature dependencies of Fe-Co alloys differ markedly from the temperature dependencies of bcc Fe-Ni.[5] The ^{57}Fe hmf in Fe-Ni had a more anomalous temperature dependence; as the Ni concentration increased, the ^{57}Fe hmf decreased more rapidly with temperature. Along with this anomalous temperature dependence were found temperature dependencies of the rff and the isomer shift that indicated the lattice became softer around ^{57}Fe atoms with more Ni neighbors. These results can be understood if the hybridization of 3*d* states in Fe-Co alloys is more effective than for Fe-Ni alloys (as expected, since the atomic levels of Fe and Co lie closer in energy). The Fe—Co bond is stiffer than the Fe—Ni bond, and the mean-squared thermal displacements for Fe atoms with Co neighbors are smaller than for Fe atoms with Ni neighbors. The exchange interactions responsible for the magnetic interactions between Fe and Co atoms, presumably involving 3*d* electrons, are therefore stronger, and the temperature dependence of the ^{57}Fe hmf in Fe-Co alloys is weaker. This agrees with trends in the Curie temperature, which increases with Co concentration but decreases with Ni concentration.

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