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INELASTIC NEUTRON SCATTERING OF γ -IRON, AND THE DETERMINATION OF THE ELASTIC CONSTANTS BY LATTICE DYNAMICS.

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The physical properties of the various phases of iron have been the subject of numerous theoretical and experimental investigations. Of particular interest is the appearance of the fcc γ -phase between approximately 1200K and 1670K. We were able to grow in situ single crystals of fcc iron of sufficient size to perform an inelastic neutron scattering study of the lattice dynamics of this phase of iron. The phonon dispersion curves along the $[00\xi]$, $[\xi\xi0]$ and $[\xi\xi\xi]$ symmetry directions were measured at 1428K. A limited number of phonons were also measured at 1227K and 1640K to assess the temperature dependence of the phonon frequencies. The data collected at 1428K were used to evaluate the elastic constants, the phonon density of states and the lattice contribution to the specific heat. The measured dispersion curves of γ -Fe are qualitatively similar to those of Ni (measured at 296K) and $\text{Ni}_{0.3}\text{Fe}_{0.7}$ (measured at 296 and 573K).

INTRODUCTION

At ambient pressure, iron transforms from the low temperature bcc α -phase to the fcc γ -phase at approximately 1200K and then transforms back to the bcc δ -phase at approximately 1670K. The phase diagram of iron and, in particular, the appearance and stability of the closed packed γ -phase at such high temperatures is not presently very well understood and has been the subject of many theoretical investigations. For a quantitative understanding of the phase transition of iron one needs information about the vibrational [1-5] and the magnetic [6] contribution to the free energy.

The magnetic properties of γ -Fe have been the subject of many band theoretical calculations [7-13]. Although there is no general agreement about the magnetic structure of the ground state, these calculations clearly suggest that the magnetism of γ -Fe at low temperatures is very sensitive to changes in the atomic volume and support the existence of high-spin and low-spin states in γ -Fe. It is particularly encouraging that finite temperature calculations [14] based on band theory provided an explanation of the invar properties of the fcc Fe-Ni alloy.

fcc Fe with atomic volume comparable to or larger than that of Cu at low temperatures ($a=3.6\text{\AA}$) have been studied [15-19] on γ -Fe thin films on Cu or CuAu surfaces. Unfortunately, unresolved discrepancies between the results obtained in these experiments [15-19] makes it difficult to ascertain whether γ -Fe thin films order ferromagnetically, although ferromagnetic ordering corresponding to the high-spin γ -Fe state was reported [15-16]. For atomic volume less than that of Cu, experimental results have been obtained [20-24] on γ -Fe precipitates in Cu. It is interesting to note that recent experiments [24] on γ -Fe precipitates demonstrated that for small atomic volumes the ground state is a spiral-spin-density-wave (SSDW), a result which is in agreement with recent band theoretical calculations [11-13].

The experimental investigation of bulk γ -Fe, on the other hand, has been hindered by the difficulty of growing in situ single crystals of this phase of iron. To assess the spin-spin correlations in γ -Fe, we studied [25] the paramagnetic scattering from polycrystalline γ -Fe using polarized neutron scattering techniques. The results demonstrate that the correlations are of ferromagnetic nature in agreement with the results obtained [26] by Brown et al., at higher momentum transfers. More recently, we were

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able to grow in situ single crystals of γ -Fe of sufficient volume for the study of the phonon dispersion curves of this phase by inelastic neutron scattering techniques [27]. In the present paper, we discuss some of the results obtained in these neutron scattering studies of bulk γ -Fe.

EXPERIMENTAL RESULTS AND DISCUSSION

For the lattice dynamical studies, we were able to grow in situ relatively large (2-3cm³) single crystals of γ -Fe by the following procedure. High purity polycrystalline Fe was mounted in a vacuum furnace, positioned on the sample goniometer of a triple-axis neutron spectrometer. The sample temperature was raised into the δ -phase temperature range and then reduced slowly, through the $\delta \rightarrow \gamma$ transformation temperature (~ 1673 K) down to the midpoint (~ 1430 K) of the γ -phase temperature range.

The phonon dispersion curves along the $[00\xi]$, $[\xi\xi 0]$ and $[\xi\xi\xi]$ symmetry directions were measured at 1428K and are plotted in Fig. 1. The

Figure 1. Experimental dispersion curves of γ -Fe at 1428 K. The solid lines were obtained by fitting the data to a six-nearest-neighbor force-constant model.

phonon dispersion curves of γ -Fe at 1428K are quite similar to those of Ni (measured [28] at 296K) and Ni_{0.3}Fe_{0.7} (measured [29] at 296 and

573K). Furthermore, measurements of a selected number of γ -Fe phonons at 1227 and 1640K did not reveal, to within experimental precision, any anomalous behavior in the temperature dependence of the dispersion curves of γ -Fe. The only notable difference between the dispersions curves of γ -Fe and those of Ni and Ni_{0.3}Fe_{0.7} is that the T₁[110] branch of γ -Fe exhibits positive dispersion at small wave vectors (Fig. 2).

Figure 2. Transverse T₁ $[\xi\xi 0]$ branch of γ -Fe measured at 1428K. Notice the positive dispersion at small wave vectors.

To evaluate the elastic constants and the lattice specific heat the data were analyzed by conventional Born-von-Kármán models. As Fig. 1 shows a six-nearest-neighbor force-constant model provides an adequate fit to the experimental results. The elastic constants obtained from this model are listed in Table I.

Table I. Elastic constants (10¹² dyn/cm²) obtained by fitting the 1428K data to a six-nearest-neighbor model.

C ₁₁	1.54 ± 0.14
C ₄₄	0.77 ± 0.08
C ₁₂	1.22 ± 0.13

Information about the temperature dependence of the lattice specific heat can be obtained by assuming that the phonon density of states is independent of temperature. With this assumption, we performed the calculations using the phonon density of states obtained at 1428K. The results expressed in terms of an effective Debye temperature, $\Theta_D(T)$, are plotted in Fig. 3. The initial rise (Fig. 3) in $\Theta_D(T)$ is due to the positive dispersion of the $T_1[110]$ branch at small wave vectors and it is similar to that observed [30] in gold.

Figure 3. Temperature dependence of the effective Debye temperature of γ -Fe.

No detailed theoretical calculations are presently available to compare with the experimental results on the lattice dynamics of γ -Fe. The lack of any unusual features in the measured dispersion curves indicates, however, that the vibrational contributions to the free energy cannot by itself account for the occurrence and stability of the γ -phase of iron at high temperatures. Thus, the difference in the magnetic properties between the α and γ -phase of iron appears to be of importance. Our study [25] of the paramagnetic scattering in γ -Fe and that [26] by Brown et al., clearly demonstrate that the spin-spin correlations are of ferromagnetic nature over a quite wide range of wave vectors. Unfortunately, no detailed theoretical calculations are available for a comparison with these experimental results.

In conclusion, although considerable progress has been made towards an understanding of the low temperature properties of γ -Fe thin

films and precipitates in Cu, the properties of the actual γ -phase of Fe are still not very well understood.

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