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Crystalline and amorphous FeTi and Fe₂Ti

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Amorphous FeTi, Fe₂Ti, and their crystalline counterparts are compared by measurements of x-ray diffraction, conductivity, and ⁵⁷Fe Mössbauer spectroscopy. In FeTi one has the unique opportunity to compare a cubic crystal with its amorphous analog. X-ray diffraction and hyperfine interactions indicate no clear correlation between the crystalline and the amorphous states. The electrical conductivity exhibits distinctive behavior for the two states.

I. INTRODUCTION

Since the advent of amorphous metallic solids, there has been considerable effort devoted to elucidating the effects of structural disorder on the solid-state properties.¹ These effects can be more readily detected by studying amorphous and crystalline solids of the same or similar composition. Of particular interest are the crystalline compounds and their amorphous analogs and the alloys with compositions near the boundary separating the amorphous and the crystalline states. In the Fe-Ti system, both of these opportunities exist. There are two crystalline intermetallic compounds (FeTi and Fe₂Ti).^{2,3} The amorphous states of both can be prepared by vapor-quenching techniques. At the Fe-rich end, the composition (x) near 81 at. % Fe separates the crystalline alloys ($x \geq 82$) and the amorphous alloys ($x \leq 80$). We have recently reported the drastic differences in properties on opposite sides of $x \approx 81$, as manifested by abrupt changes in magnetic, hyperfine, conductivity, and structural properties.⁴ In this work, we will compare FeTi and Fe₂Ti in the amorphous and crystalline states.

Crystalline FeTi, well known as a hydrogen-storage material, has a simple crystal structure in which both the Fe sites and the Ti sites have *cubic* symmetry. Crystalline Fe₂Ti has a more complicated but well-characterized structure. These are the only two Fe-Ti compounds and their properties have been well studied by various measurements.³

Amorphous Fe-Ti alloys can be made by vapor-deposition techniques over a wide composition range, including those of FeTi and Fe₂Ti, thus allowing a direct comparison of the crystalline and the amorphous states. In FeTi one has the rare occasion to compare a cubic crystal with its amorphous state. Some models of amorphous solids have suggested the presence of a short-range order which is similar to, or based upon, that of the crystalline state.⁵ The validity of such models can be tested by comparing various characteristics of

the two states, particularly the structure and the hyperfine interactions.

II. EXPERIMENTAL

Amorphous films of FeTi and Fe₂Ti (hereafter referred to as *a*-FeTi and *a*-Fe₂Ti) were made by a magnetron sputtering device. Films with a thickness of 10–24 μm were deposited onto liquid-nitrogen-cooled substrates of various kinds suitable for the measurements. In some cases, substrate-free samples were obtained by physically removing the films from the substrates. The resistivity samples, deposited onto glass or sapphire substrates, were about 2 μm thick. Crystalline intermetallic compounds of FeTi and Fe₂Ti (hereafter referred to as *c*-FeTi and *c*-Fe₂Ti) were made by an arc furnace operated in a purified argon atmosphere. The samples were melted and rolled several times to insure homogeneity. Both the sputtering targets and the pellets for arc melting were made from homogeneous mixtures of pure iron (99.9%) and titanium (99.8%).

The structures of the samples were examined by the energy-dispersive x-ray diffraction method⁶ using a Si(Li) detector and tungsten bremsstrahlung x rays. The intensity of the diffraction patterns was not corrected for the efficiency of the detector or the sample thickness since that requires elaborate calibration procedures. The temperature dependence of the resistivity was measured from 4.2 to 900 K using a computer-controlled dc four-probe method. The hyperfine interactions were measured by a conventional Mössbauer spectrometer with a ⁵⁷Co in Rh source.

III. RESULTS AND DISCUSSIONS

A. X-ray diffraction

The energy dispersive x-ray diffraction patterns of amorphous and crystalline FeTi and Fe₂Ti are shown in Fig. 1.

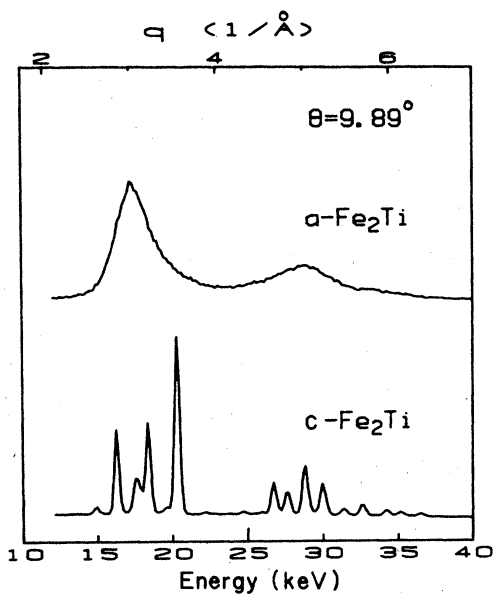
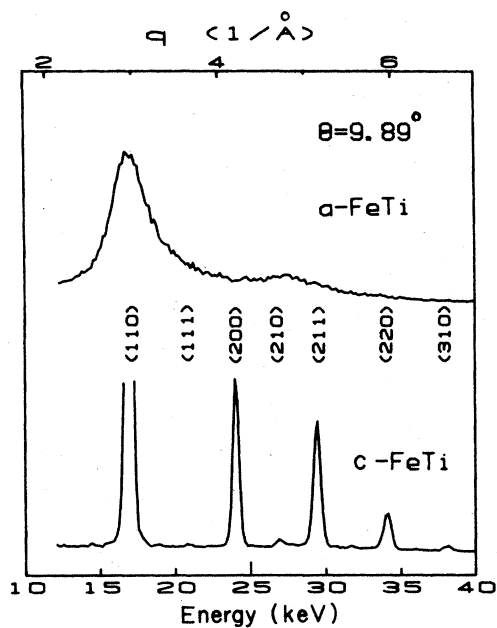


FIG. 1. Energy dispersive x-ray diffraction patterns of amorphous and crystalline samples of FeTi (top) and Fe₂Ti (bottom). The data are expressed in both keV and q (\AA^{-1}). The Bragg peaks of c -FeTi are indexed.

The amorphous samples show similar diffraction patterns with broad primary and secondary peaks up to $q = 7 \text{ \AA}^{-1}$. The second peak of a -FeTi is less pronounced due to its smaller thickness. The crystalline compounds, as expected, show a series of sharp Bragg peaks. The crystal structure of c -FeTi is of the CsCl ($B2$) type consisting of two interpenetrating Fe and Ti simple cubic sublattices. Each Fe is

surrounded by eight Ti atoms and vice versa. However, as noted by previous authors, an experimental verification of the structure of c -FeTi by x-ray diffraction turns out to be more difficult.³ This is because the scattering factors of Fe and Ti are nearly the same. Consequently, the diffraction patterns are almost indistinguishable from that of a body-centered-cubic (bcc) structure. The diffraction peaks corresponding to (111), (210), (310), etc. reflections are very weak. However, our measurements of c -FeTi, as shown in Fig. 1, observed these very weak diffraction peaks, thus confirming the CsCl structure of c -FeTi. The diffraction pattern of c -Fe₂Ti is consistent with a hexagonal Mg₂Zn ($C14$) structure.³

The diffraction patterns of a -FeTi and a -Fe₂Ti are similar, whereas rather different diffraction patterns are observed for their crystalline counterparts. Taken together, one has little evidence to suggest a strong correlation in structure between the crystalline and the amorphous states of the same composition.

B. Electrical resistivity

In the electrical resistance and its temperature dependence, one observes pronounced differences between amorphous and crystalline solids as shown in Figs. 2 and 3. The

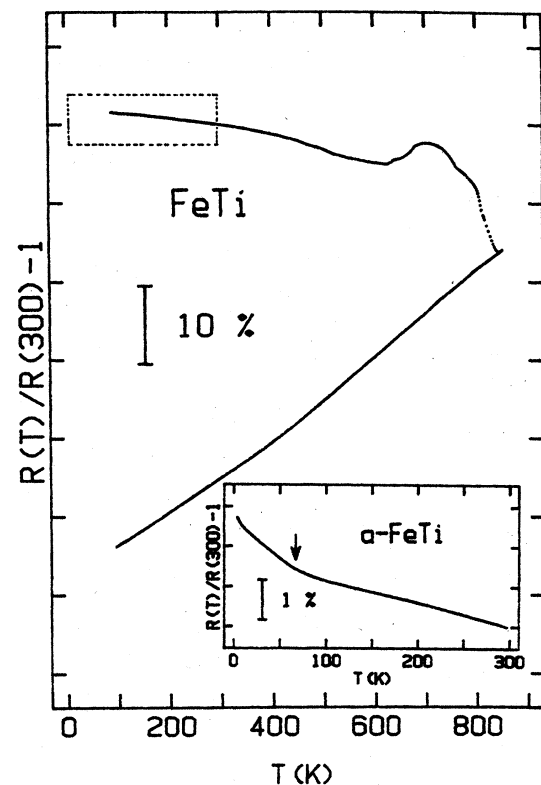


FIG. 2. The temperature dependence of the resistivity of the amorphous alloy FeTi and after crystallization. The low-temperature portion is shown in the insert plot. The arrow indicates the magnetic-ordering temperature.

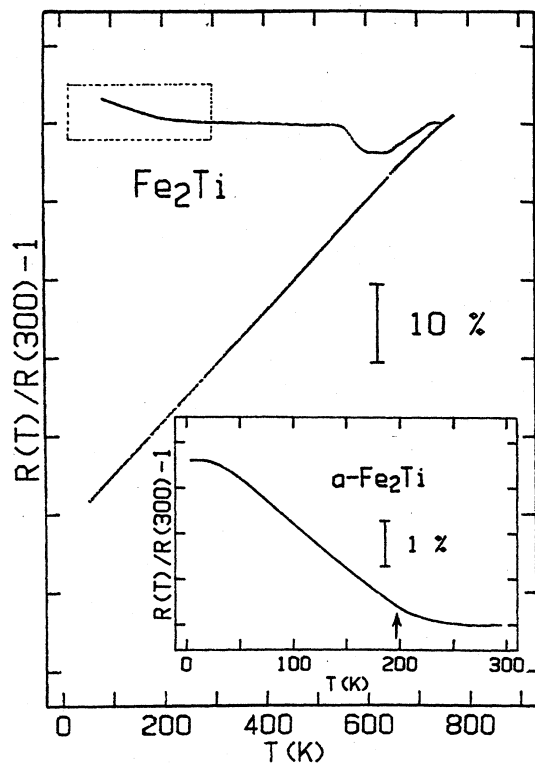


FIG. 3. The temperature dependence of resistivity of amorphous alloy Fe_2Ti and after crystallization. The low-temperature portion is shown in the insert plot. The arrow indicates the magnetic-ordering temperature.

resistivities of the amorphous solids are dominated by defect scattering. The resistivities are high ($\sim 100 \mu\Omega \text{ cm}$) but only weakly temperature dependent. The temperature coefficients of resistance (TCR) are small and, as in many other cases, negative. Over a few-hundred-degree temperature range, the resistance changes by only a few percent.¹ In crystalline solids, the electron-phonon scattering mechanism dominates. The TCR's are large, positive, and nearly linear in T . The combination of differences in resistivity and TCR gives the well-known characteristic that at low temperatures the resistivities of the amorphous alloys are much higher than those of the crystalline alloys. At high temperatures as shown in Figs. 3 and 4, the resistivities of crystalline alloys are comparable to or higher than those of amorphous alloys.

In addition to the negative TCR, the amorphous alloys show other features. Both amorphous alloys show a noticeable slope change in the resistivity at a temperature close to the magnetic-ordering temperature as indicated by the arrows. This indicates a distinct contribution to the total resistance that is related to the magnetic ordering. At low temperatures, the data of $\alpha\text{-FeTi}$ reveal a rise in resistivity which is logarithmic in T . As discussed elsewhere, this low-temperature anomaly is consistent with Kondo scattering.⁷

Despite a clear experimental distinction between the resistivity in amorphous and crystalline solids, a satisfactory theoretical account of the temperature dependence in the amorphous case remains inadequate.¹

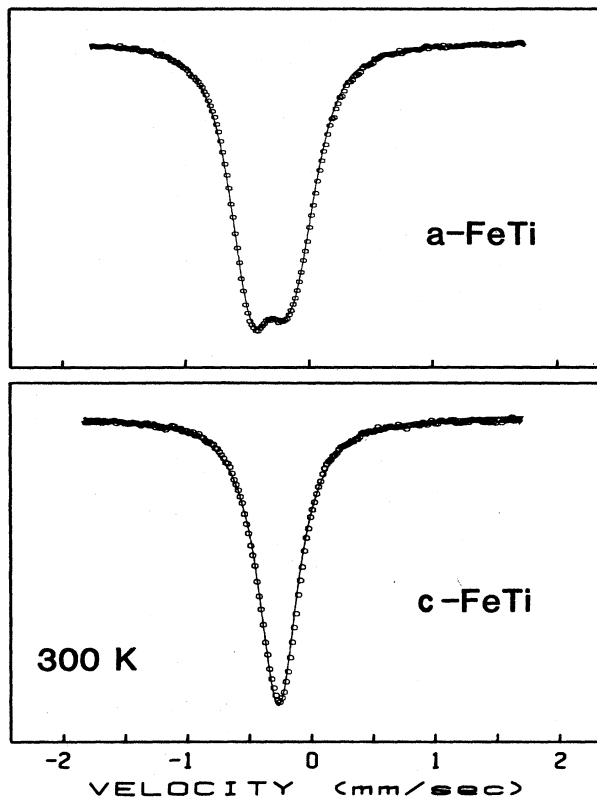


FIG. 4. Mössbauer spectra of amorphous and crystalline FeTi at 300 K.

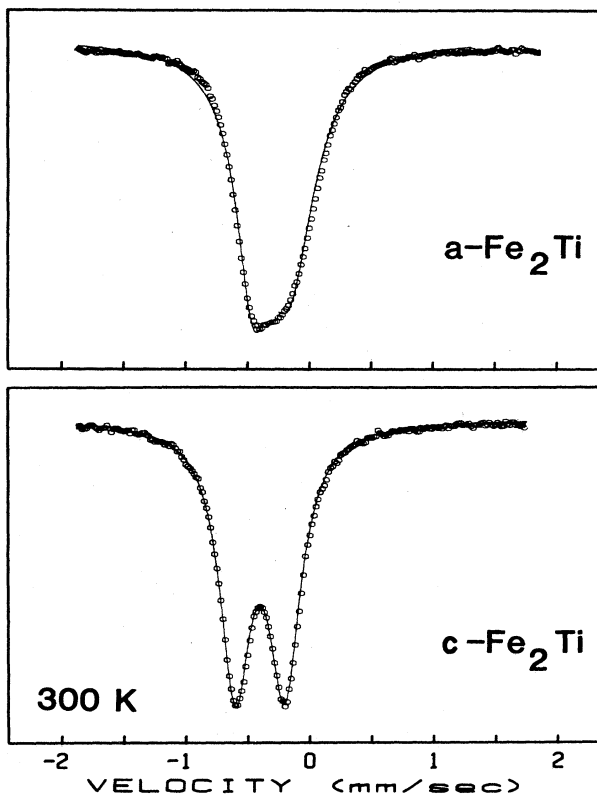


FIG. 5. Mössbauer spectra of amorphous and crystalline Fe_2Ti at 300 K.

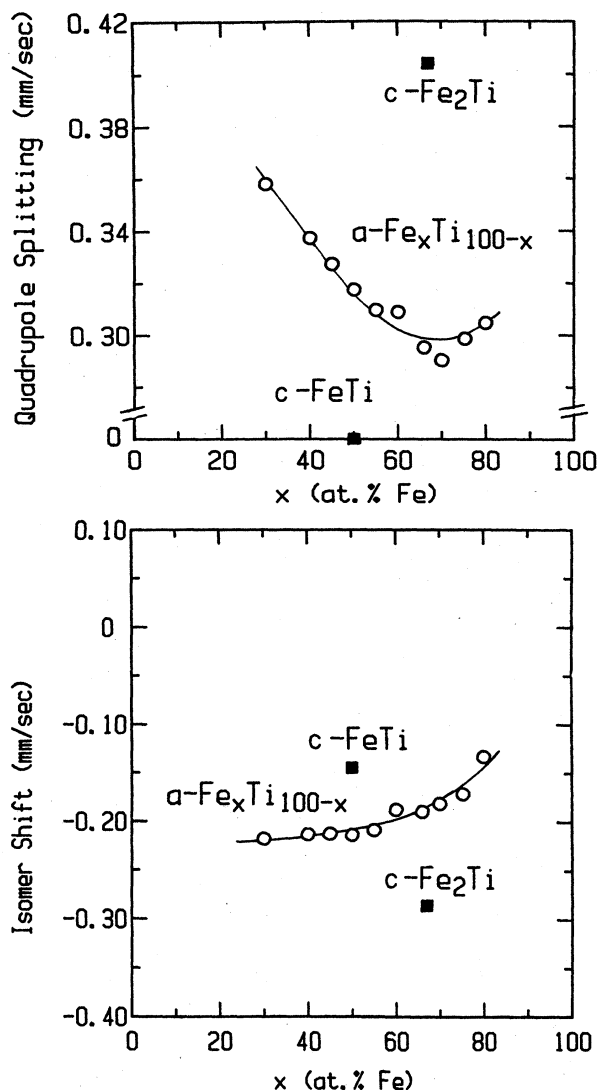


FIG. 6. Quadrupole splittings and isomer shifts of amorphous $\text{Fe}_x\text{Ti}_{100-x}$ and crystalline FeTi and Fe_2Ti at room temperatures as a function of Fe content. The isomer shifts are relative to that of $\alpha\text{-Fe}$.

C. Hyperfine interactions

Cubic symmetry and random atomic arrangement are the two extremes of ordering in solids. The composition of FeTi is unique in that both of these states can be realized. In this respect, a comparison of the hyperfine interactions of $c\text{-FeTi}$ and $\alpha\text{-FeTi}$ is particularly interesting. Mössbauer spectra of $\alpha\text{-FeTi}$ and $c\text{-FeTi}$ at 300 K are shown in Fig. 4. The CsCl ($B2$) structure of $c\text{-FeTi}$ assures a cubic symmetry at the Fe sites. Consequently, the Mössbauer spectrum shows a single line with zero quadrupole splitting. On the other hand, a sizable quadrupole splitting of 0.32 mm/sec is observed in $\alpha\text{-FeTi}$, indicating that the local symmetries at the Fe sites are generally lower than cubic. This is in agreement with some models of amorphous solids.^{8,9} For example, Lines has shown in solids amorphized from cubic crystals that there is a minimal and nearly zero probability of finding sites with cubic symmetry.⁹

Mössbauer spectra of $\alpha\text{-Fe}_2\text{Ti}$ and $c\text{-Fe}_2\text{Ti}$ at 300 K are also shown in Fig. 5. The Fe sites in $c\text{-Fe}_2\text{Ti}$ have low symmetry resulting in a large quadrupole splitting of 0.40 mm/sec which is in good agreement with the value of 0.404 mm/sec reported by Wertheim, Wernick, and Sherwood.³ A considerably smaller quadrupole splitting is observed in $\alpha\text{-Fe}_2\text{Ti}$.

It is informative to examine the quadrupole splittings and the isomer shifts of all the amorphous $\text{Fe}_x\text{Ti}_{100-x}$ alloys ($30 \leq x \leq 80$). These values, varying continuously with Fe content, are rather different from those of $c\text{-FeTi}$ and $c\text{-Fe}_2\text{Ti}$ as shown in Fig. 6. Similarly, the isomer shifts of the amorphous alloys vary systematically among themselves without obvious correlation with those of $c\text{-FeTi}$ and $c\text{-Fe}_2\text{Ti}$. These results indicate that the random atomic arrangement of the amorphous state is unique to the disordered state. The inherent short-range order, as far as hyperfine interactions are concerned, bears no resemblance to that of the crystalline state.

ACKNOWLEDGMENT

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