Study of the Debye-Waller factor near the temperature of a phase transition of the first kind in cobalt

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Values of the Debye-Waller factor f' in cobalt containing 7 wt. % Fe are calculated on the basis of nuclear gamma-resonance spectra for temperatures between 20 and 250 K. A considerable decrease in f' is observed near the temperature of the beginning of a first-order phase transition, $M_S = 140 \pm 5°$ C. It is suggested that this effect may be due to a decrease in the lattice force constants near M_S.

A first order phase transition (PT-I) takes place in Co at a temperature of ~420° C; upon cooling, the face-centered cubic (FCC) lattice transforms into a hexagonal close packed (HCP) lattice. The transition is accompanied by a thermal effect of 100 cal/mole, which definitely indicates attribution to PT-I. A distinguishing feature of PT-I in Co is the nondiffusive character of the transformation (martensitic transformation): the FCC lattice transforms into an HCP one by way of a certain deformation of the initial structure.

Inasmuch as the PT-I in Co is martensitic, a fundamental role in it is usually ascribed to structure defects, by means of which lattice deformation occurs. However, in the study of the mechanical properties, phase composition and dislocation structure of Co whiskers, which possess a high degree of perfection of structure, a series of features have been discovered.[1] On the one hand, plastic deformation in the whiskers under the action of external stresses σ was extraordinarily difficult and began at σ close to the theoretical shear stress (for favorable orientation ot the slip system relative to the external stresses $\sigma = 0.01\ \mu$, where μ is the shear modulus). On the other hand, a nondiffusive PT-I went to completion in most Co whiskers in which dislocations were not observed in x-ray analysis, while structural defects prevented phase transitions. On the basis of these facts, the assumption was made that structural defects do not play a leading role in the nondiffusive PT-I in Co, and the possibility of PT-I is connected with a change in the dynamic characteristics of the lattice near the initial temperature of the PT-I.[1]

To test this assumption, we measured the Debye-Waller factor f' in an alloy of Co—7 wt. % Fe by the method of nuclear gamma ray resonance spectra in a temperature range including the temperature of the initial PT-I in cooling (M_S). Fe was introduced into the Co as a Mössbauer isotope. Measurement of the temperature dependence of the electrical resistance showed that $M_S = 140 \pm 5°$ C in the alloy Co—7 wt. % Fe. As in pure Co, the PT-I was nondiffusive, as was indicated by the macrorelief on the surface of the samples after the transition.

The samples investigated consisted of foil of 30-μ thickness, annealed at 900° C. The Mössbauer absorption spectra were recorded on a multichannel spectrometer operating in the constant-acceleration mode. The isotope Co^{57} in Cr served as the source and was held at room temperature at all times. Immediately before the measurement cycle, the samples were heated to 600° C for the purpose of obtaining a single-phase FCC structure. After the corresponding cooling in an inert
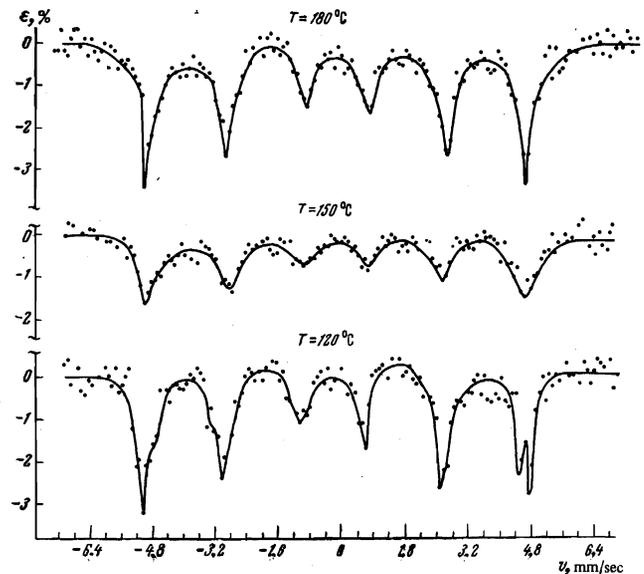

FIG. 1. Absorption spectra of samples of the alloy Co—7wt.% Fe for various temperatures.

atmosphere, spectral exposures were made at nine temperatures in the range 250–20° C (±1°). Up to M_S, six-peaked absorption spectra were observed that were somewhat broadened (in comparison with pure iron) in the direction of lower velocities (Fig. 1, T = 180° and 150° C). At T = 150° C, the intensity of the absorption lines decreased clearly in comparison with T = 180° C. In cooling below M_S, two weakly-resolved sixfold lines were distinguished in the spectrum, connected evidently with the existence under these conditions of FCC and HCP phases simultaneously (Fig. 1, T = 120°).

The value of the Debye-Waller factor f' was determined from the total area of the experimental absorption spectrum. In the case of total splitting,[2]

$$S_{бэ} = \frac{\Gamma}{2} \pi a f \sum_{i=1}^{6} K(C_{iA}). \tag{1}$$

In the investigated samples, $C_A \approx 0.6$ and $K(C_A) \approx C_A$; therefore

$$S_{бэ} \approx \frac{\Gamma}{2} \pi a f \sum_{i=1}^{6} C_{iA}, \tag{2}$$

where $\Gamma = 0.097$ mm/sec is the width of the emission line; α the fraction and f the probability of emission of γ quanta without recoil; $C_{iA} = \beta_i C_A = \beta_i \sigma_0 n_A f'$; C_A is the effective thickness of the absorber; β_i is the relative intensity of the ith component of the spectrum; σ_0 is the maximum absorption cross section for γ
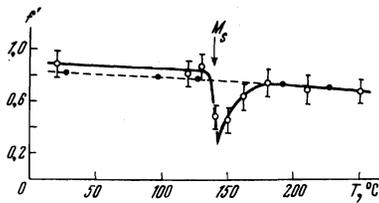
FIG. 2. Temperature dependence of the Debye-Waller factor: O—experimental points; ●—calculated in the Debye approximation, $\Theta = 450°$K.

quanta; n_A' is the number of atoms of Fe^{57} in 1 cm^3 of absorber; f' is the probability of absorption of γ quanta without recoil (the Debye-Waller factor of the absorber).

The computed values of f' are given in Fig. 2. During cooling of the samples, a monotonic increase of f' is first observed, which is well-described by the Debye approximation with $\Theta = 450$ K. The resultant value of Θ is in agreement with the value of the Debye temperature of Co ($\Theta = 445$ K).[3] However, a significant decrease in the denominator of f' occurs near M_S; this indicates an increase in the root-mean-square displacements of the atoms. Upon cooling below M_S, the quantity f' increased rapidly, and the temperature change of f' again corresponded to the Debye approximation from 130° C on. Evidently, the value of Θ of the low-temperature phase with HCP lattice is somewhat higher than the Θ of the FCC lattice (dashed line in Fig. 2); however the change of Θ lies within the limits of error.

Thus, near the temperature of onset of the PT-I, a significant decrease takes place in the Debye-Waller factor in Co, which indicates an important change in the dynamic characteristics of the lattice near M_S. Inasmuch as the Fe atoms differ little (in mass or size) from the Co atoms, it is natural to assume that the observed increase in the root-mean-square displacements is a consequence of the change in the force constants of the matrix. Similar results were obtained near the ferroelectric transition point in $BaTiO_3$[4] and $Pb(Fe_{1/2}Nb_{1/2})O_3$,[5] and also near M_S in an Fe-Ni alloy.[6] In the last case, however, the nearness of the Curie point to PT-I does not allow a unique interpretation of the experimental results.

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