Lattice Distortions near Impurity Atoms in \(\alpha-Fe_{1-x}Si_x\) Alloys

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Abstract—Lattice distortions near impurity atoms in \(\alpha-Fe_{1-x}Si_x\) alloys \((x = 0.05–0.06)\) are studied both experimentally using x-ray diffraction and theoretically by means of ab initio calculations. It is found that the distortions are more complex than experimental data suggest. The displacements of atoms near impurities are not determined by the concentration dependence of the average lattice constant nor by a difference in the ion radii.

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1. INTRODUCTION

It is convenient to study the structure of materials and its effect on the magnetic properties of these materials using single crystals and then apply the results of the study to explain the rules governing the properties of objects with a broken crystal symmetry, such as thinmetals and metal glasses. \(\text{Fe–Si}\) alloys are excellent subjects for this approach.

Investigations of \(\text{Fe-based}\) alloys with a small content of silicon (below 20 at %) have a long history because of the numerous practical applications of these alloys. The benefits of adding silicon to iron to enhance its magnetic properties were first reported in 1900 [1]. Now, crystalline, nanocrystalline, and amorphous materials based on the \(\text{Fe}_{1-x}\text{Si}_x\) alloy can be produced using modern technologies.

The phase diagram of the \(\text{Fe–Si}\) alloy in the crystal state and a number of its features are well known [2–6]. At low and moderate concentrations, silicon atoms substitute for Fe atoms in bcc lattice sites and, as a result, the following three phases can form depending on the temperature and silicon content: the \(\alpha\) phase (a disordered phase or a phase with \(\text{A2}\)-type short-range ordering), \(\alpha_1\) phase (with \(\text{DO}\) type long-range ordering), or \(\alpha_2\) phase (with \(\text{B2}\)-type ordering). For example, at room temperature, the \(\alpha\) phase forms for silicon concentrations up to 6–7 at % and the \(\alpha_1\) phase exists for higher concentrations [4]. It has been demonstrated using neutron diffraction [6] that a \(\text{Fe}_{1-x}\text{Si}_x\) single crystal with \(x = 0.061\) is a substitution alloy with short-range order at temperatures up to 873 K. As far as we aware, there is no published data on the details of the short-range ordering, including on the bcc-lattice distortions, for Si concentrations below 6 at %.

Previously [7–9], we made preliminary investigations of the local atomic structure of single-crystal \(\text{Fe–Si}\) alloys with 5–6 at % of silicon using x-ray diffraction. It was demonstrated that the local ordering was of the \(\text{B2}\) type and that there was no half-integer superstructure peaks (which are characteristic of \(\text{DO}\) ordering). Simultaneously, bcc-lattice distortions near silicon atoms were found. The distortions manifested themselves in diffraction patterns as shifts (to smaller angles) in the positions of the maxima of diffuse superstructure reflections for which the sum of the \((hkl)\) indices is an odd number from the positions calculated for the bcc lattice.

The present work is devoted to detailed experimental and theoretical study of bcc-lattice distortions near silicon atoms in \(\text{Fe}_{1-x}\text{Si}_x\) alloys with small \(x\).

2. EXPERIMENT

Single-crystal \(\text{Fe}_{1-x}\text{Si}_x\) alloy samples were prepared in the form of thin disks in two varieties: \(\text{C}\)-type samples had a cubic texture, with the sample surface coinciding with the \((010)\) crystallographic plane, and \(\text{G}\)-type samples had a Goss texture, with the sample surface being parallel to \((110)\). Cubic-textured samples \((x = 0.049)\) were cut from a single crystal grown under laboratory conditions, and Goss samples \((x = 0.06)\) were cut from large grains of rolled electric steel sheets.

All samples were initially 8–10 mm in diameter and 0.30–0.35 mm in thickness and were subjected to the following types of processing:

(1) refining by annealing at 1150°C during 2–5 h, which reduces the number of interstitial impurities (for example, the carbon content was below 0.005 wt %);

2. EXPERIMENT

(2) annealing at 873 K for 1–5 h

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(2) disordering by annealing at 850°C followed by quenching into water, with the cooling rate estimated to be 400 K/s (samples \( C_0 \) and \( G_0 \)); and

(3) ordering by annealing at 450°C for several minutes (samples \( C_1 \) and \( G_1 \)).

Also, we produced a single-crystal iron sample in the form of a thin plate with the surface close to the (113) crystallographic plane containing less than 0.06 wt. % of carbon. The diffuse scattering data obtained on the Fe single crystal were compared with the data obtained on alloy samples in order to extract the contribution due to the chemical ordering of Si atoms in samples \( C_0, C_1, G_0 \), and \( G_1 \).

For x-ray diffraction measurements, each sample was ground to a thickness of 100 μm and then chemically polished down to 40–50 μm, which is optimal for Mo \( K_α \) radiation (\( λ = 0.071 \) nm). Measurements were performed using a four-circle x-ray diffractometer at room temperature. The characteristic radiation of an x-ray tube was monochromated using a pyrolytic graphite single crystal. Scattered radiation was registered by a semiconducting Si(Li) detector. The high voltage applied to the x-ray tube was below the excitation threshold for the \( 1/2 \) radiation in the continuous spectrum; therefore, this radiation did not contribute to the measured intensity. Since the diffuse scattering is three to five orders of magnitude weaker than the main bcc reflections, its intensity was measured using a beam 2 mm in diameter with a less than 0.5° divergence in the transmission geometry. This technique slightly reduces the intensity but makes it possible to perform measurements in a wide region of reciprocal space, in particular, for the case where the scattering vector is parallel to the sample plane.

We measured the profiles of the \((h00)\) and \((00l)\) reflections for \( h, l = 2, 4, 6 \) for samples \( C_0 \) and \( C_1 \) and the profiles of the \((hh0)\) reflections for \( h = 1, 2, 3, 4 \) and the \((00l)\) reflections for \( l = 2, 4, 6 \) for samples \( G_0 \) and \( G_1 \). Using the angular positions of these reflections, we determined the lattice constant \( a_α \), which was found to be 0.2863(1) nm for samples \( C_0 \) and \( C_1 \) (with 4.9 at % Si) and 0.2862(1) nm for samples \( G_0 \) and \( G_1 \) (with 6.0 at % Si).

As was reported earlier [7, 8], wide diffuse peaks were found for all samples near the angular positions for which the sum of the indices \( h + k + l \) is an odd number. For a bcc lattice, the reflections at these sites are the difference between the reflections from the two simple cubic lattices that form the bcc lattice. For an alloy with the \( B2 \) type of ordering, narrow superstructure reflections form at these sites because all silicon atoms are situated on one sublattice. The fact that only diffuse peaks occur indicates that there is no long-range order in the arrangement of silicon atoms. The profiles of the superstructure \((100)\) and \((001)\) peaks are shown in Fig. 1 for samples \( C_0, C_1, G_0, G_1 \). Solid lines in Fig. 2 show Gaussian least square fits, which were used to determine the peak heights, the full widths at half-maximum (FWHM), and