Segregation of Si and Sn to the Fe(100) Surface in the Fe-6.2% Si-0.03% Sn Alloy

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SUMMARY ABSTRACT

Surface segregation of Si and Sn and the site competition between them in a polycrystalline sample of an Fe-6.2% Si-0.03% Sn alloy were reported in a previous work by the authors. In the experiments reported here a single crystal having the same composition as the polycrystalline sample was used. The following temperature dependence of segregation on the (100) surface was observed.

At lower temperature (25-400°C) C segregated to the surface. After heating at 500°C for 20 hours, Si was the only solute segregated to the (100) surface. At 600°C Sn segregated to the surface and replaced all the segregated Si on the surface. Fig. 1 shows this replacement of Si by Sn. This was similar to that observed and described previously for a polycrystalline sample.

Si segregates to the surface at a lower temperature than Sn because it has a higher bulk diffusivity and the bulk concentration of Si is higher than Sn. The replacement of Si by Sn at the higher temperatures (600°C) indicates a larger driving force for the segregation of Sn compared to Si.

There are several LEED patterns observed for the various surface phases. The C impurities when segregated to the surface at low temperature form a c(2x2) structure. Likewise the Si also creates a c(2x2) structure shown schematically on Fig. 1.
contrast a saturated layer of Sn forms a (1x1) structure.

An approximate depth profile of the Si and Sn in the surface region can be measured using the relative changes in the XPS core level intensities as the angle of collection is varied. As the angle (measured from the normal) is increased the depth probed by the XPS measurement decreases. Fig. 2 shows the relative intensity of the Sn 3d peaks with respect to the Fe 2p and the Si 2p with respect to the Fe 3s. Several qualitative observations are obvious from the data shown in Fig. 2. (1) Both the Si and Sn concentrations in the surface region are higher than in the bulk. (2) The Sn to Fe signal increases with increasing angle of collection indicating that the Sn is on the surface above the Fe. (3) The Si to Fe signal decreases with increasing collection angle, indicating that there is a high concentration of Si some where below the Fe surfaces. A comparison of the intensity variation of the Sn 3d's to the Si 2p's shows that Sn is above the Si. Fig. 3 shows a model for the composition of the surface region that is consistent with Fig. 3. It must be stressed that this concentration gradient is not unique, but it shows the basic facts. Sn is on the surface and Si is positioned some where below the outer most Fe layer. 1

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Fig. 1 The process of replacement of Si by Sn on the (100) surface of an Fe-Si-Sn alloy.
600°C 10,000 min
$\hbar \omega = 1254$ eV

Binding Energies:
Sn 3d: 484.65 eV normalized by Fe 2p: 706.15 eV
Si 2p: 99.15 eV normalized by Fe 3s: 91.3 eV.

Fig. 2 Relative intensities of Si 2p and Sn 3d photoemissions as functions of the emission angle.
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