

AN INVESTIGATION OF THE STRUCTURE OF AMORPHOUS $\text{Si}_{1-x}\text{Ni}_x$
THROUGH THE METAL-INSULATOR TRANSITION

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The metal-insulator transition (MIT) in a-Si:metal alloys is generally accepted to be of Anderson type, where localised states at the Fermi level become delocalised. Of particular interest as dopants are transition metals which, when alloyed in the form $\text{a-Si}_{1-x}\text{M}_x$ introduce impurity states deep within the band-gap, with the MIT expected at around $x = 0.15$. Whilst much work has been reported on the MIT in amorphous silicon thin films doped with transition metals, it is far from obvious how the metal impurity atoms are incorporated into the system. Without a more direct knowledge of the structure it is difficult to understand the precise nature of the process responsible for MITs in such systems.

Samples of hydrogenated amorphous silicon:nickel ($\text{a-Si}_{1-x}\text{Ni}_x\text{:H}$) have been prepared using rf reactive co-sputtering^[1]. There was no evidence for c-Si in Raman spectra from any of the samples and IR absorption results indicated the presence of Si-H covalent bonds at all compositions. D.C. conductivity measurements^[2] showed qualitative agreement with those of Rogachev et al.^[3]. EXAFS measurements on both Si and Ni edges were taken at the SRS, Daresbury Laboratory (UK). Si edge data were collected by the total electron drain current method, whilst Ni edge experiments were performed in transmission. The data were analysed using the EXCURV88^[4] program available at the SRS, and the use of multi-shell fitting was made subject to the criteria of Joyner et al.^[5]. The Ni edge data were fitted to 2 shells whereas only 1 shell was used for the Si edge analysis.

The Ni K-edge results indicate that there is no significant change (within errors) in the local environment of the nickel atoms over the composition range studied, $0 < x < 0.3$. The total co-ordination of the nickel is surprisingly high (10.5) with each nickel atom having, on average, six Si and four Ni near-neighbours. This leads us to suggest that the nickel is not entering substitutionally

or interstitially, but that some form of clustering must be occurring. However, this clustering cannot consist simply of metal atoms but must also contain some Si atoms in the form of a close-packed silicon:nickel alloy.

Raman spectroscopy confirms that an a-Si matrix is present at all compositions; thus the system appears to have two distinct regions each containing some silicon. At low nickel content the Si K-edge EXAFS is dominated by the a-Si, giving the expected interatomic distances and co-ordination numbers. As the nickel content increases, Si:Ni regions increase the absorption, resulting in a decrease in statistical accuracy of the spectra and results obtained from them. However, the overall trend appears to be a slight increase in the average Si-Si distance with a decrease in the corresponding co-ordination number as more nickel is incorporated into the sample. The distances measured correspond to interatomic distances found in several phases of crystalline Ni_xSi_y [6]. However a neutron scattering experiment on a single sample of a-Si:Ni:D showed no evidence of crystallinity; we conclude that the clusters are a disordered form of nickel silicide.

We speculate that the system contains two amorphous phases: one being semiconducting and the other being semi-metallic. These results indicate that the assumption that the MIT observed in such systems is of Anderson type may not be as well founded as previously thought. Indeed, the evidence for a two-phase system suggests that the application of classical percolation theory may be more appropriate.

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