Observation of a Strongly Nested Fermi Surface in the Shape-memory Alloy $Ni_{0.62}Al_{0.38}$

Smart alloys which exhibit shape-memory and super-elastic phenomena have been deployed in a wide variety of applications ranging from actuators in aircraft wings to surgical instruments. However, an atomic-scale understanding of the origin of the martensitic transformation, the structural transformation at the heart of these phenomena, is still lacking. It has been hypothesized that lattice vibrations are the key, an idea supported by first-principles calculations indicating that strong coupling of certain phonons to the electrons (phonon softening), due to particular features in the Fermi surface, plays a crucial role [1]. It is well-known that when parallel pieces of Fermi surface exist in a metal, there will be a strong electronic response at the wavevector which translates, or nests, one parallel piece onto the other. This role of the Fermi surface in influencing the electron-phonon coupling was extensively investigated during the last two decades where premartensitic phenomena [2] were explained in terms of Fermi surface nesting.

In order to make a direct comparison with the Fermi surface predicted by band theory, we performed *ab initio* electronic structure calculations to reproduce the earlier work of Stocks *et al.* [3] for the disordered $Ni_{0.62}Al_{0.38}$ alloy (Fig. 1). We employed the fully relativistic Koringa-Kohn-Rostoker (KKR) method within the atomic sphere approximation, and the disorder was taken into account by the coherent potential approximation.

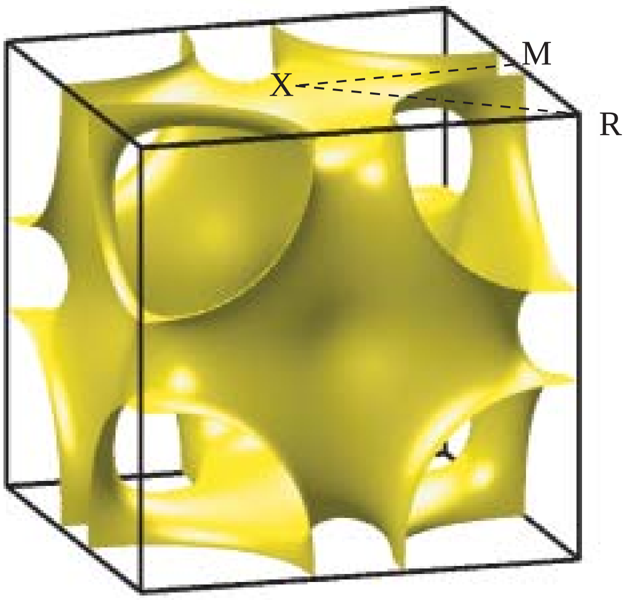

Fig. 1. Calculation of the Fermi surface using the KKR-CPA method. The Γ point is at the centre of the cubic Brillouin zone, and some other symmetry points are labelled.

Our single crystal sample was cut by spark erosion from a single grain of a large ingot of $Ni_{0.62}Al_{0.38}$ grown using the Bridgman method. A total of twenty-four Compton profiles along different crystallographic directions were measured at room temperature on the high-resolution Compton spectrometer of beamline **BL08W** [4]. This spectrometer is of the Cauchois type, consisting of a crystal analyzer and a position-sensitive detector, with a resolution FWHM at the Compton peak of ~0.16 atomic units. Compton scattering is a robust technique insensitive to defects or disorder, providing a one-dimensional projection (double integral) of the underlying bulk electron momentum distribution. For each Compton profile approximately 300,000 counts in the peak data channel were accumulated. A three-dimensional momentum density was reconstructed from this set of 24 profiles and then folded back into the first Brillouin zone to obtain the occupation density. The experimental Fermi surface (shown in Fig. 2) was extracted by contouring this density at a level fixed by an extremum in the first derivative along a direction where our calculations indicated the Fermi surface was likely to be well-defined.

A plane-by-plane inspection of the Fermi surface throughout the Brillouin zone revealed that a vector ~ 0.18 [1,1,0] ($2\pi/a$) connects a large area in the manner predicted in [1]. The plane through the BZ at k_z = 0.48 (π/a) is shown in Fig. 3, with the nesting vector indicated.

Clearly, the general shape of the experimental Fermi surface (Fig. 2) agrees well with the calculation (Fig. 1). As discussed above, the regions of Fermi surface responsible for the nesting are observed experimentally to be relatively flat. This, in conjunction with the large density of states (predicted by the calculations) spanning these wavevectors, provides a large propensity for nesting. There is, however, some noteworthy discrepancy between the calculated and experimental Fermi surfaces.

Experimentally, a neck is observed to open around the X-point of the Brillouin zone whereas according to the calculations this sheet remains closed. The calculated bandstructure reveals flat (almost dispersionless) bands along X-M and M-R, lying just below the Fermi level, leading to a van Hove singularity in the density of states at that energy. The opening up of a Fermi surface neck along Γ-X implies that the Fermi level has crossed below this van Hove singularity and may be indicative of the impending lattice instability at the martensitic transformation (where the Fermi surface would undergo more substantial rearrangement).

In conclusion, we have presented the experimental Fermi surface of the disordered alloy $Ni_{0.62}Al_{0.38}$ from the results of Compton scattering experiments, providing evidence in support of the intimate link between the electronic structure and the observed phonon softening.

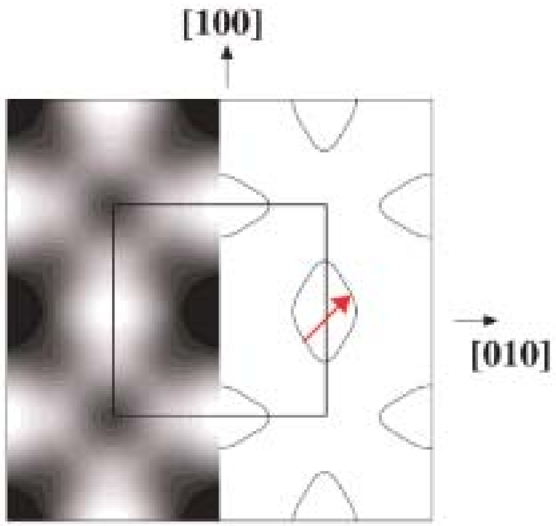

Fig. 3. A slice through the $k_z = 0.48(\pi/a)$ plane of the experimental data, for comparison with Fig 1. Shown on the left is the occupation density through this slice, where brighter shades represent a larger occupation. On the right is the experimentally determined Fermi surface, with the nesting vector shown in red.

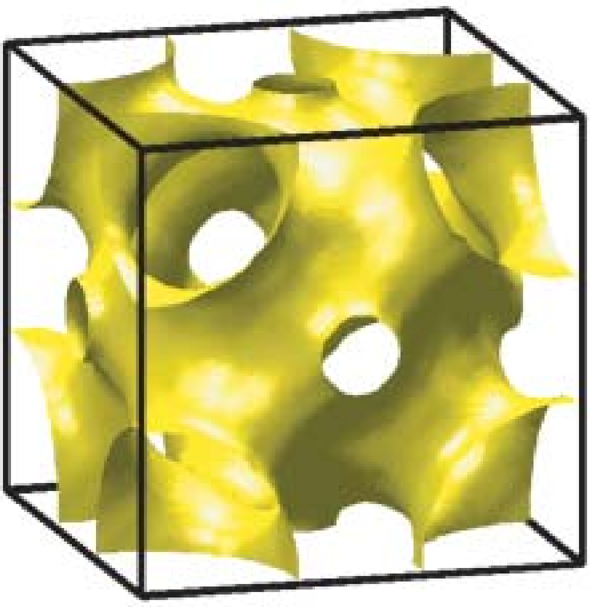

Fig. 2. Reconstruction of Fermi surface from 24 measured directional Compton profiles.

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References

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