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Electron momentum density in a shape-memory alloy TiNi

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Introduction

The intermetallic compound TiNi is one of a number of β-phase alloys which undergo a reversible martensitic transformation upon cooling. Inelastic neutron scattering experiments have found that the TA_2[110] phonon branch in the β-phase is temperature dependent and becomes soft near $\mathbf{Q_0}$=1/3(110)2π/a at about room temperature[1]. The origin of the phonon softening has long been speculated to be due to Fermi surface nesting. However, there has been no experimental information about the geometry of the Fermi surface simply because traditional spectroscopy for Fermiology could not be applied. Recent progress in reconstructing three-dimensional electron momentum density from Compton scattering data has made it possible to map out three-dimensionally the Fermi surface. In this report we present the three-dimensional momentum density which would eventually lead to the Fermi surface of TiNi.

Experiment

The Compton profiles are measured at the PF-AR NE1A1 beamline of the KEK, where for the incident beam of 60 keV x-rays are available with a rate of $1.5x10^{13}$ photons/s. The Compton spectrometer is unique in design and consists of four independent analyzing systems arranged on the surface of a cone that provides a scattering angle of 160° to all the analyzing system. The reader is referred to Sakurai et al.[2]. Two of the analyzing systems are used for the present measurements, one in the horizontal and the other in the vertical position viewed from the base of the cone, to obtain 28 directional profiles. The directions along which the Compton profiles were measured are show in Fig. 1. The overall instrumental resolution was 0.13 atomic units (a.u.) in full width at half maximum. The total accumulated counts under each profile were about $2x10^8$. The measured profiles were corrected for the necessary energy dependent corrections such as absorption, detector and analyzer efficiency, and scattering cross-section. The contribution of double scattering was estimated by a Monte Carlo simulation. The valence electron profile is obtained by subtracting from the corrected profile the core electron contributions which are assumed to be given by the weighted sum of theoretical profiles of electrons from $(1s)^2$ to $(3p)^6$ of Cu atom and from $(1s)^2$ to $(2p)^6$ of Al atom calculated by Biggs et al.[3].

Reconstruction and Results

The method we employed to reconstruct the three-dimensional electron momentum density from the obtained 28 profiles is called the direct Fourier transform method [4-6]. The reconstructed three-dimensional momentum density on the (100) plane is show in Fig. 2.

References

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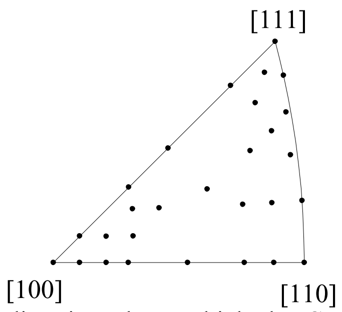

Fig.1 The direction along which the Compton profiles are measured are represented by the full circles in the irreducible orientation triangle.

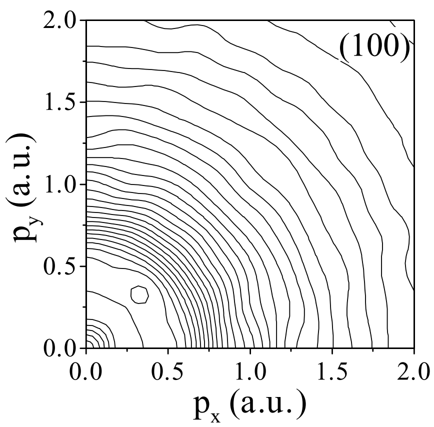

Fig.2 The reconstructed three-dimensional momentum density on the (100) plane.