

Anomalous Electronic Correlations in Momentum Density of $\text{Al}_{97}\text{Li}_3$

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Introduction

For technological and fundamental reasons the electronic structure of Al-Li alloys has been the subject of considerable attention over the years. We directly probe changes in the electronic ground state of Al due to presence of Li impurities via Compton scattering measurements. We find that the modifications in the momentum density of Al induced by just a few percent Li atoms are surprisingly large and cannot be accounted for within the standard Fermi-liquid-type model of correlated homogeneous electron gas.

Theoretical and Experimental Results

A single crystal of $\text{Al}_{97}\text{Li}_3$ was grown by the Bridgeman method. Disc-shaped samples, 10 mm in diameter and 1.5 mm thick, were cut parallel to the (100), (110), and (111) crystallographic planes. The Compton profiles were measured with the high resolution Compton spectrometer at the NE1A1 beam line. The incident energy of photons was 60 keV, the scattering angle 160 degrees, and the momentum resolution was estimated to be 0.12 a.u. The valence electron profiles of Al for comparison were measured by Ohata et al.[1] under the experimental conditions of the present measurements. Concerning the theoretical profiles, the self-consistent electronic structures of pure Al and the alloy were first obtained using the KKR-LDA-CPA scheme. Then, from that, the momentum density and Compton profiles were computed.

We consider the measured and computed changes in the profiles due to addition of Li atoms,

$$\Delta J_{\text{sph}}(p) = J_{\text{sph}}(p)_{\text{Al}} - J_{\text{sph}}(p)_{\text{Al}_{97}\text{Li}_3}$$

Although the profiles of both Al and $\text{Al}_{97}\text{Li}_3$ have small anisotropies, here we take spherical average of the profiles because the anisotropies are smaller than the changes we are considering and do not affect the essential features. In Fig. 1 the experimental $\Delta J_{\text{sph}}(p)$ is shown by the full circles, the KKR-CPA theoretical $\Delta J_{\text{sph}}(p)$ is represented by the full squares. It is obvious that the KKR-CPA theory differs substantially from the experiment near $p=0$ and 1 a.u. Deviations in the Compton profile of pure Al compared to the KKR-CPA predictions can be explained reasonably well within the standard electron gas picture. Such standard correlation effects are also present in $\text{Al}_{97}\text{Li}_3$ with a magnitude very similar to that of Al because the electron density in Al and $\text{Al}_{97}\text{Li}_3$ is nearly the same with the Fermi momentum

differing by only about 1%. Therefore, when the difference $\Delta J_{\text{sph}}(p)$ is formed, we would expect such standard electron-gas type correlation effects to be canceled. The key to understanding this discrepancy is to recognize that correlation effects can be viewed as exciting some electrons into higher energy unoccupied levels as a way of modifying the character of the ground-state wave function. The lowest unoccupied orbitals in Al and Li are the $2p$ and the $3p$ orbitals, respectively. It is natural therefore to consider the effect of promoting an electron from an s to a p orbital. The full line in Fig. 1 represents the KKR-CPA theory corrected in a way that 3% valence electrons in $\text{Al}_{97}\text{Li}_3$ are promoted from s - to p -states. We may look upon the good agreement between the corrected theory and the experiment as indicating that correlations and the associated changes in the effective potentials produce an enhanced p character of the ground-state wave function in $\text{Al}_{97}\text{Li}_3$. Given the increasing current interest in understanding correlation effects in the inhomogeneous electron gas, our results indicate that Al-Li alloys present an example of a simple binary system which exhibits unusual correlation effects even though each of its two constituents is commonly thought as being a free-electron-like metal.

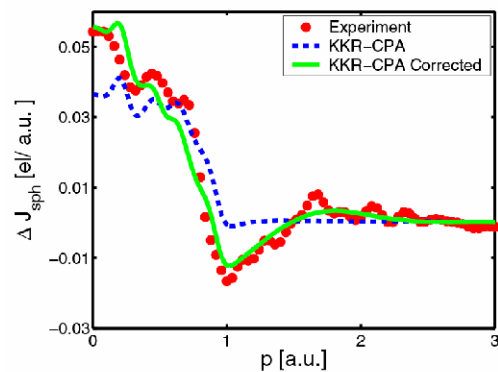


Fig. 1 Experimental $\Delta J_{\text{sph}}(p)$ is compared with corresponding KKR-CPA result with and without corrections.

References

- [1] T. Ohata et al., Phys. Rev. B 62, 16528 (2000).