A NEED FOR HIGH RESOLUTION COMPTON SCATTERING STUDY OF hcp METALS WITH THE USE OF SYNCHROTRON RADIATION

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Abstract: One-directional electron momentum density distributions (Compton profiles) of hexagonal structure metals (Mg, Zn and Cd) were measured using high energy (662 keV – ^{137}Cs isotope gamma source) and medium resolution (0.4 a.u.) Compton spectrometer in the Institute of Experimental Physics, University of Bialystok. The experimental data were compared with corresponding first principles Korringa-Kohn-Rostoker coherent potential approximation calculations (KKR-CPA). Small anisotropy of Compton profiles measured in all three metals makes observation of fermiological features exceedingly difficult. We show that to achieve this goal, high-resolution experimental data are essential. Judging from recently obtained results for much easier case of cubic $Ni_{75}Cu_{25}$ and $Ni_{75}Co_{25}$ alloys one needs the resolution below ~0.15 a.u. Such experiment can be carried out at the synchrotron radiation source only with the energy above ~40 keV.

Streszczenie: Kierunkowe rozkłady gęstości pędów elektronów (profile komptonowskie) metali o strukturze heksagonalnej (Mg, Zn i Cd) zostały zmierzone przy użyciu spektrometru komptonowskiego z izotopowym źródłem promieniowania gamma ^{137}Cs (o energii 662 keV) i stosunkowo niskiej rozdzielczości (0.4 a.u.) w Instytucie Fizyki Doświadczalnej Uniwersytetu w Białymstoku. Dane eksperymentalne zostały porównane z obliczeniami teoretycznymi z pierwszych zasad metodą KKR-CPA (Korringa-Kohn-Rostoker - Coherent Potential Approximation). Mała anizotropia profili komptonowskich, występująca we wszystkich trzech badanych metalach, bardzo utrudnia obserwację efektów związanych z topologią powierzchni Fermiego („fermiologicznych"). Pokazujemy, iż w celu obserwacji takich subtelnych szczegółów niezbędne jest wykonanie pomiarów z wysoką rozdzielczością. Sądząc po ostatnich wynikach uzyskanych dla dużo prostszego przypadku stopów $Ni_{75}Cu_{25}$ i $Ni_{75}Co_{25}$, krystalizujących w strukturze regularnej, potrzebna jest zdolność rozdzielcza poniżej ~0.15 a.u. Eksperyment taki może zostać przeprowadzony przy użyciu promieniowania synchrotronowego o energii powyżej ~40 keV.

1. Introduction

Directional electron momentum density distribution $J(p_z)$, which can be measured via Compton scattering experiments is called Compton profile (CP):

$$J(p_z) = \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty} n(\boldsymbol{p})dp_x dp_y .$$

CP is one dimensional projection of the electron momentum density distribution $n(\boldsymbol{p})$:

$$n(\boldsymbol{p}) = \frac{1}{(2\pi)^3}\sum_j \left|\psi_j(\boldsymbol{r})e^{i\boldsymbol{p}\cdot\boldsymbol{r}}d^3\boldsymbol{r}\right|^2 ,$$

where $\psi_j(\boldsymbol{r})$ are the ground-state electron wavefunctions and the summation extends over all occupied states. The knowledge of wavefunctions is essential for theoretical calculations of physical parameters and properties of the studied material. Thus the experimental results can be used for a direct test of solid state theory.

2. Theory

The electronic band-structure computation of hexagonal metals are based on the KKR Green function method, utilizing the muffin-tin approximation to the crystal potential [1]. All electrons were included and the von Barth-Hedin [2] local density approximation (LDA) to the exchange-correlation potential was used. The two-dimensional integrations involved in the evaluation of CPs were carried out by using the tetrahedral method of Lehmann and Taut [3]. The Lam-Platzman isotropic correction for electron correlation effects was incorporated in the final stage of calculations.

3. Experimental Results

Medium-resolution (0.4 a.u.) directional Compton profiles have been measured along [001], [110] and [100] directions for single crystals of hexagonal metals (Mg, Zn, Cd) [4], as well as along [100], [110], [111] directions for single crystals of cubic $Ni_{75}Co_{25}$ and $Ni_{75}Cu_{25}$ disordered alloys. In order to compare the data of medium and high resolution for cubic alloys, the first ones were collected in Bialystok and the latter in the ESRF, Grenoble [5].

The total CPs were extracted from the experimental spectra after a number of energy-dependent corrections included in the standard data handling procedures [6-7]. The effect of multiple scattering of photons in the sample was simulated by the Monte Carlo Method [8] and subtracted from the final CPs.

The directional anisotropies of CPs (differences of directional CPs) were calculated for all hcp metals (Fig. 1) and cubic alloys (Fig. 2).

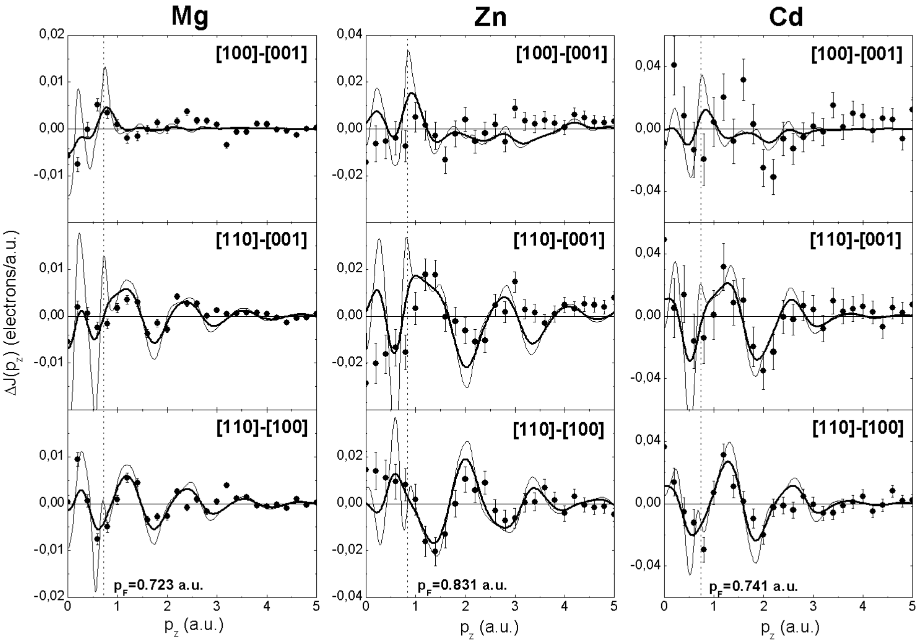

Fig. 1. Directional anisotropies of the CPs in single crystals of three hexagonal metals. Medium resolution experimental data (0.4 a.u. – measured in Bialystok University laboratories) are represented by solid circles, KKR calculations convoluted to medium (0.4 a.u.) and high (0.15 a.u.) resolution are shown by thick and thin solid lines respectively, dashed vertical lines show location of the Fermi momentum.

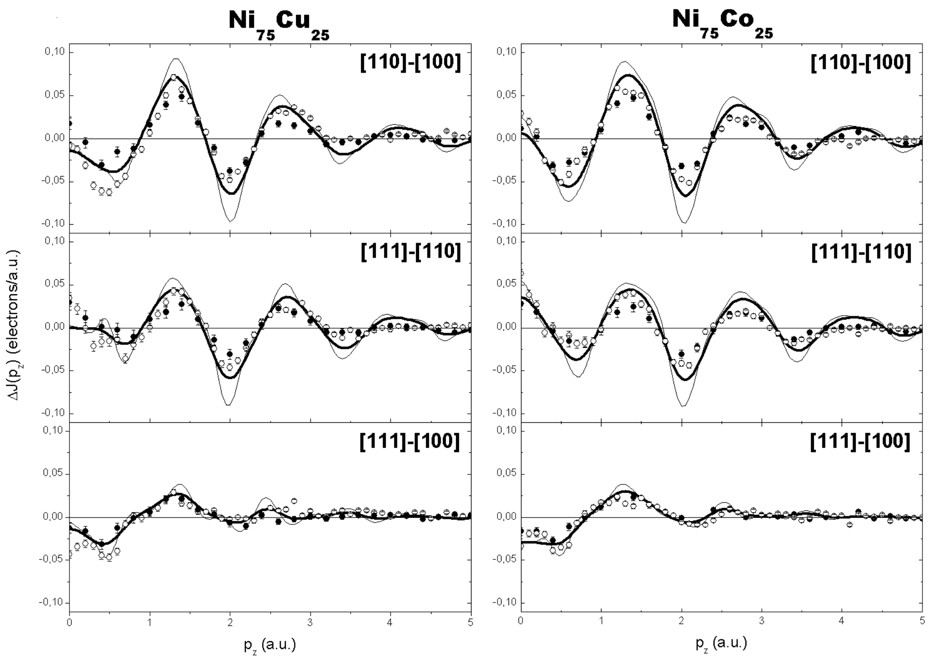

Fig. 2. Directional anisotropies of the CPs of $Ni_{75}Cu_{25}$ and $Ni_{75}Co_{25}$ disordered cubic alloys. Experimental data measured in Bialystok (medium resolution – 0.4 a.u.) and ESRF (high resolution – 0.15 a.u.) are represented by solid and empty circles respectively, KKR calculations convoluted to experimental resolutions are shown by thick (0.4 a.u.) and thin (0.15 a.u.) solid lines.

Taking into account very small anisotropy of directional CPs and therefore assuming isotropic momentum distribution, this momentum density were calculated using the formula:

$$n(p) = -\frac{1}{2\pi p_z} \left. \frac{dJ(p_z)}{dp_z} \right|_{p_z = p} .$$

The results for hcp metals are shown in Fig. 3 and for $Ni_{75}Co_{25}$, $Ni_{75}Cu_{25}$ alloys in Fig. 4.

4. Discussion

Medium resolution (0.4 a.u.) experimental results show good agreement with theoretical KKR calculations convoluted to experimental resolution (Fig. 1, 2).

The measured and calculated profiles of hcp metals show very small anisotropy of the electron momentum density (Fig. 1), significantly lower than observed in cubic metals (Fig. 2). Although the amplitudes and zero crossing positions of experimental anisotropies agree well with calculated ones, relatively low resolution of the experiments and moderate statistical accuracies are insufficient to reveal fine structure in the directional anisotropies, resulting from Fermi surface topology predicted by KKR theory.

There are many sharp details observed in theoretical directional anisotropy of CP's and directional momentum densities of hcp metals, especially in the region of Fermi momentum and below, when theory is convoluted to resolution 0.15 a.u. which are accessible at high resolution experiments on synchrotron sources (Figs. 1 and 2).

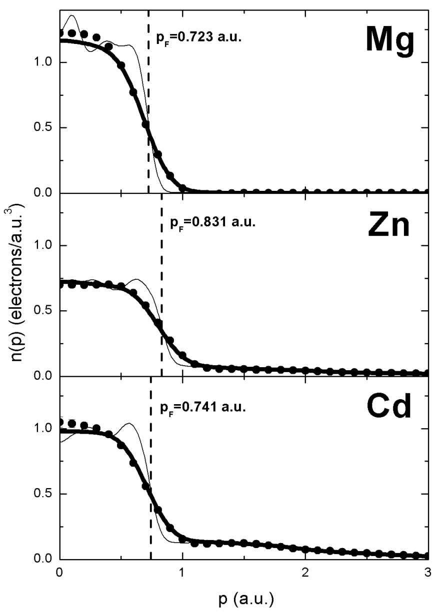

Fig. 3. Momentum densities of valence electrons, *n(p),* in three hexagonal metals. Densities calculated on basis of the medium resolution experimental data (0.4 a.u.) are represented by solid circles, densities calculated on basis of the KKR theoretical CP's convoluted to medium (0.4 a.u.) and high (0.15 a.u.) resolution are shown by thick and thin solid lines respectively, dashed vertical line shows location of the Fermi momentum.

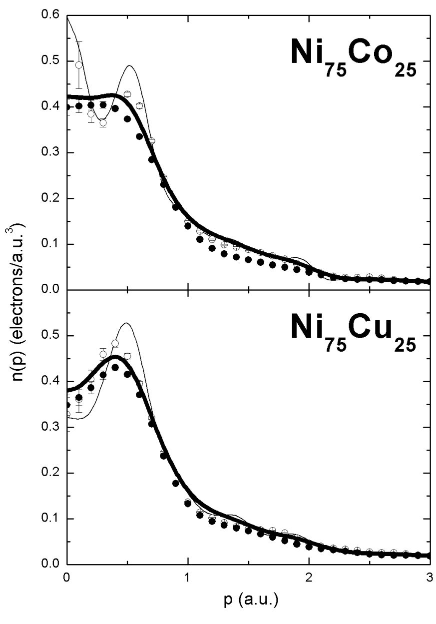

Fig. 4. Momentum densities of valence electrons, *n(p),* in $Ni_{75}Cu_{25}$ and $Ni_{75}Co_{25}$ disordered cubic alloys. Densities calculated on basis of the medium (0.4 a.u. – Bialystok) and high (0.15 a.u. – ESRF) resolution experimental data are shown by solid and empty circles respectively, densities calculated on basis of the KKR theoretical CP's convoluted to experimental resolutions are shown by thick (0.4 a.u) and thin (0.15 a.u.) solid lines.

High resolution experiments performed on single crystals of disordered cubic alloys of $Ni_{75}Co_{25}$ and $Ni_{75}Cu_{25}$ show that the sharp features present in theoretical calculations may be observed also in the experimental results (Fig. 4). In addition the Compton experiment performed on synchrotron source, due to high intensity of the beam, lasts about 50-100 times shorter time.

Differences between theoretical calculations convoluted to medium (0.4 a.u.) and high (0.15 a.u.) resolution for hexagonal metals (even up to 500% - Fig. 1) are much bigger than in mentioned cubic alloys (below 50% - Fig. 2), thus this effects should be easily observed in high resolution experiment.

As shown in the paper, high resolution experiment is the only one which could confirm or disprove theoretical predictions of the KKR.

Comments: *All figures presented in this work are taken from article: M. Brancewicz, A. Andrejczuk, L. Dobrzyński, H. Reniewicz and E. Żukowski "A need for high resolution Compton scattering study of hcp metals with the use of synchrotron radiation", Nuclear Insruments and Methods in Physics Research B (in press).*

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