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1995 J. Phys.: Condens. Matter 7 919

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Compton profile difference between HCP and BCC Ti measured *in situ*

N G Alexandropoulos†‡

† Department of Physics, University of Ioannina, PO Box 1186, Ioannina, GR 45110, Greece

‡ Department of Physics, Polytechnic University of New York, New York, USA

Received 3 May 1994, in final form 19 October 1994

Abstract. Compton profiles (CPs) of the allotropic forms of Ti, HCP and BCC, have been measured and their difference has been compared with the existing literature. To avoid ambiguities in obtaining the CP differences introduced by the many corrections needed to derive these differences through the absolute CP deduced from the raw data, the spectra of scattered γ -ray radiation by the two Ti allotropic forms were measured *in situ*. To achieve this, the γ -ray spectrometer was modified in such a way that the Ti sample could be heated to 1280 K in order to transform it to its BCC structure while the scattering geometry remained exactly the same as in the case of the HCP structure (Ti at room temperature). The comparison between existing theories and this experiment demonstrated that the long-range periodicity influences the electron momentum distribution somewhat less than the band-structure theory suggests.

1. Introduction

The motivation for this investigation rests on the old question of the influence of the long-range periodicity on the electron momentum distribution; interest has been lost in γ -ray Compton spectroscopy [1, 2], which for more than two decades has been a routine method in the condensed-matter study of electron momentum distribution. Although the method is experimentally simple and inexpensive in data collection, data processing requires many time-consuming corrections before theory and experiment can be compared. The corrections for detection efficiency, absorption coefficient, Compton cross-section dependence on energy, multiple scattering, internal bremsstrahlung and spectrum truncation limits include parameters not always of a single value, leading to ambiguities. The above-mentioned difficulties can be eliminated in the cases where Compton profile (CP) differences are of *physical importance instead of the absolute CP itself* [3]. This should be true also in the case of x-ray Compton spectroscopy with synchrotron radiation, although the high flux and high collimation of the incident beam in conjunction with the spectrometer's high energy resolution reduces significantly the ambiguities.

The present investigation, part of a broader project that focuses on the long-range crystal lattice periodicity variation with the electron momentum distribution, demonstrates the method in the case of the two allotropic forms of Ti, the HCP and the BCC structures.

Ti at room temperature has the HCP structure with two atoms in the unit cell with $c = 4.6833 \text{ \AA}$ and $a = 2.9504 \text{ \AA}$, leading to a density ρ of 4.508 g cm^3 , very close to an equivalent FCC close-packed structure with $a = 4.095 \text{ \AA}$ and four atoms per unit cell. The above observation meant that the CP [4, 5] of FCC Ti and its density of states [6] were considered to be a good approximation for HCP Ti. Ti also has a BCC structure at a

temperature of 1153 K with two atoms in the unit cell with $a = 3.3065 \text{ \AA}$ corresponding to a density ρ of 4.400 g cm^3 .

The CP difference $\Delta J(q) = J_{\text{BCC}}(q) - J_{\text{HCP}}(q)$ has been derived by subtracting the raw data of the two γ -ray scattered spectra, one by Ti at room temperature and the other by Ti and 1280 K, without disturbing the scattering geometry.

2. Experiment and data reduction

The ^{241}Am γ -ray Compton spectrometer, which has been described elsewhere [7], has been employed to measure the spectra of scattered γ -ray radiation of incident energy 59.54 keV, in the spectral range from 35.9 to 61.9 keV by Ti at room temperature (HCP form) and by Ti at 1280 K (BCC form). The two sets of raw data, after changing variables from channel number to momentum atomic units and from counts per second to intensity in reciprocal atomic units, have been subtracted and their difference has been normalized to zero. The elastically scattered component which is independent of the sample's crystal structure has been used as an internal standard to estimate the actual uncertainty in determining $\Delta J(q)$. For that purpose, the two sets of elastically scattered radiation have been treated in the same manner as the inelastically scattered components, leading to an uncertainty of 0.02 (au)^{-1} .

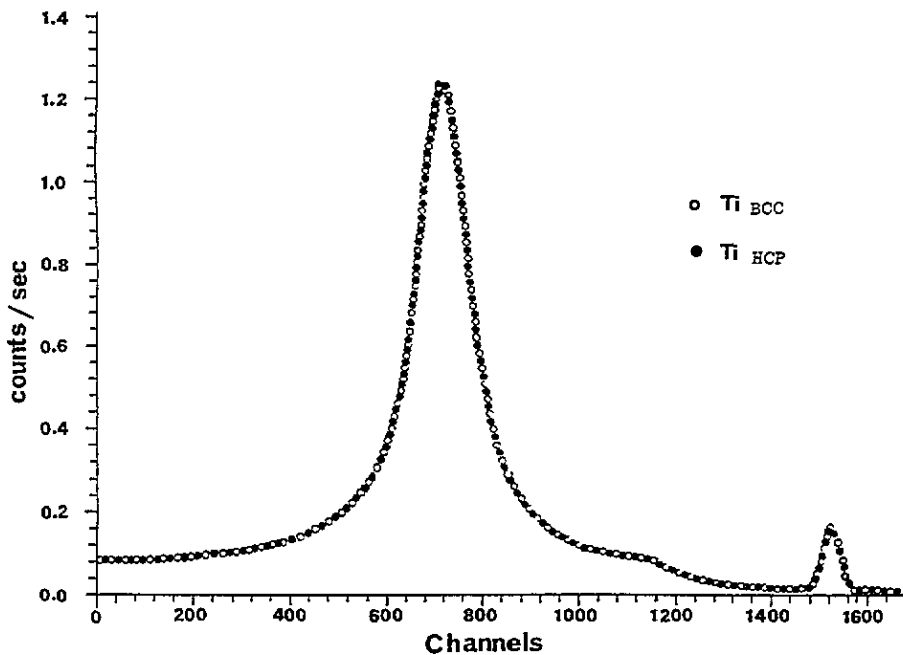


Figure 1. The γ -ray 59.54 keV scattered spectra by HCP Ti (room temperature) and by BCC Ti (1280 K). Because the two spectra overlap, they are not drawn for the same value of energy but for alternate values. The size of the dots indicates the largest value of the statistical error.

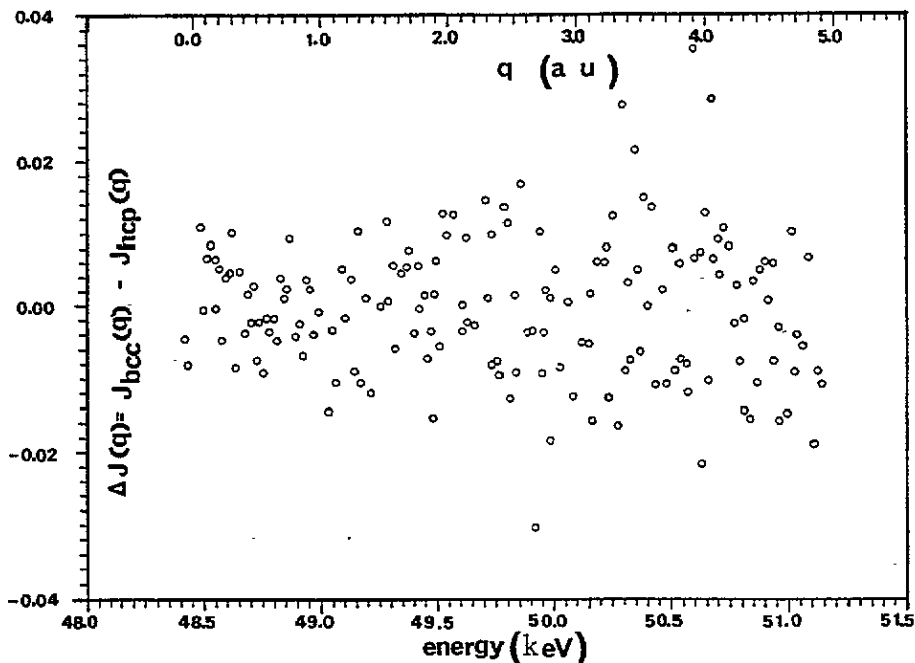


Figure 2. Raw data differences for the inelastically scattered components after renormalization of the spectrum axes. The horizontal axis is the scattered photon energy and the vertical axis is the scattering cross-section in reciprocal atomic units. The scale at the top is the momentum in atomic units used for normalization of the vertical axis. The large spread in difference values on the right is a result of the poor statistics owing to the small number of counts accumulated in the tails of the Compton spectrum. The scale at the top of the graph is a gross scale of the scattered electron's momentum in atomic units.

3. Results and discussion

In figure 1, the two spectra of 59.54 keV γ -ray radiation scattered by the two allotropic forms of Ti are shown; the two spectra overlap. The small line on the right is the elastically scattered component which is independent of the sample's structure and has been used as an internal standard to provide the actual uncertainty in the magnitude of the CP differences. For that reason it has been treated as the inelastically scattered component; that is, after changing the spectra's variables from channel number to momentum transferred, the total line area has been normalized to 0.85 electrons. This number is the product of the 22 Ti electrons with the ratio of the areas of the two spectra from 43.5 to 53 keV inelastic component to the area from 58.5 to 60.5 keV elastic component. After the above procedure, these simulated CPs were subtracted, providing a zero average value with a spread of 0.01 (au)^{-1} which is the actual uncertainty of the CP differences. This difference is drawn in figure 2 which presents the raw data differences after recalibrating the axes; the horizontal axis is the photon energy and the vertical axis is the scattered intensity in reciprocal atomic units. The scale at the top represents the electron momentum in atomic units used for normalization of the vertical axis. Figure 3 is the theoretical CP difference between FCC Ti and BCC Ti as has been reported in [4, 5], after convolution of the instrumental resolution of 0.59 au (broken curve) for the experimental set-up employed. The solid curve in the same figure is the CP difference between HCP Ti calculated within the RFA [8] and BCC Ti calculated within the APW approximation after convolution.

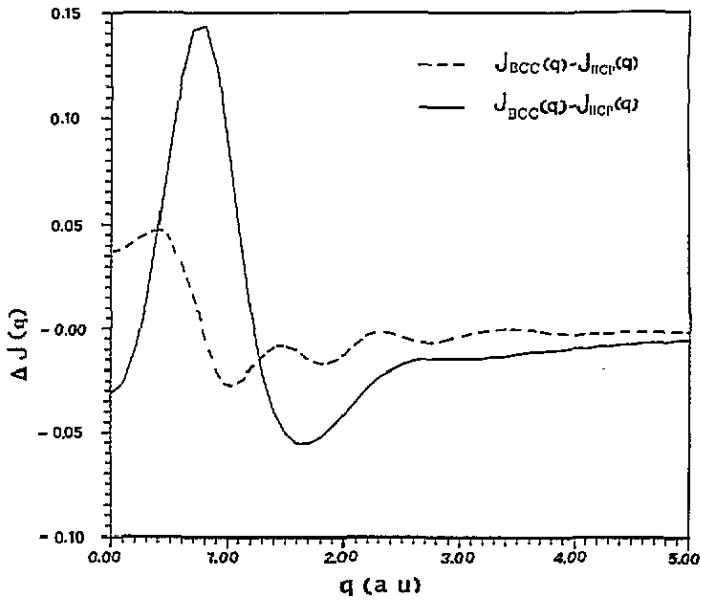


Figure 3. The difference between FCC and BCC theoretical average CPS owing to the band electrons of Ti [5] after convolution with a Gaussian of FWHM 0.59 au. The calculations have been made using the self-consistent augmented-plane-wave method (APW) (---). The CP between BCC Ti calculated within the APW and the HCP Ti within the RFA is also shown (—).

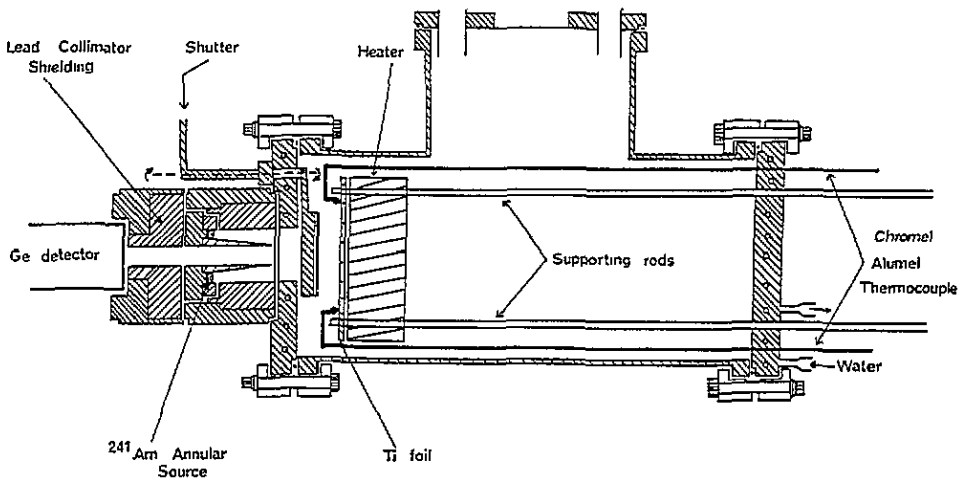


Figure 4. A schematic representation of the heating equipment used in the experiment.

4. Conclusions

This work demonstrates another method in the CP difference studies that reduces the number of steps required to obtain the experimental $\Delta J(q)$ from the raw data and it is compared with that derived from theoretical considerations. The reduction in the number of steps required and the use of the coherently scattered component as an internal standard reduced the magnitude of the actual uncertainty in $\Delta J(q)$. The method has been applied to the case

of HCP Ti and BCC Ti while the theoretical CP for HCP Ti has not been calculated within the APW approximation and instead the CP of FCC Ti has been used, assuming that the close-packed similarity of the FCC and HCP material should provide the same CP. The CP of HCP Ti has been calculated within the RFA [8]. The present experimental evidence indicates that within the limits of experimental accuracy it does not verify the above assumption. However, on comparison of figures 2 and 3 it is clear that the band-structure predictions of [4, 5] are closer to reality.

Acknowledgments

Part of the experimental work and calculations has been performed by the late T Chatzigeorgiou-Alexandropoulou. The author expresses his thanks to Professor N Papanicolaou for providing figure 3 and for constructive discussions. Thanks are also extended to Mr G Tsoumanis for the spectrometer modification and his assistance in the data collection. Dr I Theodoridou, Professor K Kotsis and Mr S Danakas deserve the author's thanks for their assistance with the present work.

References

- [1] Williams B G (ed) 1977 *Compton Scattering* (New York: McGraw-Hill)
- [2] Cooper M J 1985 *Rep. Prog. Phys.* **48** 415
- [3] Alexandropoulos N G, Chatzigeorgiou T and Theodoridou I 1988 *Phil. Mag.* **B 57** 191
- [4] Bacalis N C, Papanicolaou N I and Papaconstantopoulos D A 1986 *J. Phys. F: Met. Phys.* **16** 1471
- [5] Papanicolaou N I, Bacalis N C and Papaconstantopoulos D A 1991 *Handbook of Calculated Electron Momentum Distributions, Compton Profiles and X-ray Form Factors of Elemental Solids* (Boca Raton, FL: CRC)
- [6] Moruzzi V L, Jának J F and Williams A R 1978 *Calculated Electronic Properties of Metals* (Oxford: Pergamon)
- [7] Alexandropoulos N.G, Theodoridou I and Cooper M J 1987 *J. Phys. C: Solid State Phys.* **20** 1201
- [8] Manninen S and Paakkari T 1976 *J. Phys. C: Solid State Phys.* **9** 95