MEASUREMENT of the VALENCE ELECTRON FORM FACTOR of BERYLLIUM USING INELASTIC X-RAY SCATTERING(*)

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In order to understand the nature of the metallic bonding in solids, it is crucial to obtain the valence electron charge density. The Fourier-transform of the charge density, the atomic form factor, can in principle be derived from an x-ray scattering experiment. Hartree-Fock calculation of form factors for free atoms and ions can be found in the standard literature [1]. However, atomic form factors for the valence electrons in metals are more difficult to obtain both in theory and experiment.

We used inelastic x-ray scattering (IXS) with a very high energy resolution of 2.3 meV to measure the phonon intensities in the $[00\zeta]$ direction in beryllium. A beryllium single crystal was chosen as sample, because half of the electrons in Be are valence electrons. Figure 1 shows the form factors of the Be free atom and the ion as a function of momentum transfer. As seen in the figure, the significant difference which can be attributed to valence electrons occurs at momentum transfers k smaller than $3A^{-1}$. Therefore, in order to understand the valence electron contribution, one must have access to this small k region.

Previous experimental studies for form factor measurement of beryllium have been performed by using x-ray and electron diffraction [2],[3]. In these measurements, the form factor was obtained from intensity measurement of bragg reflections. But for the lowest possible reflection, the form factor determined in these experiments lies around $k = 2.8A^{-1}$ in momentum space.

In contrast to previous experimental methods, IXS technique can be applied to this lower region of momentum space by measuring phonon intensities. Prelimary measurements of the form factor of Be from IXS are included in figure 1. The measured form factor is in good agreement with the Hartree-Fock calculation except for the region around $k = 1.3A^{-1}$, where the experimental data indicate a slightly reduced charge density.

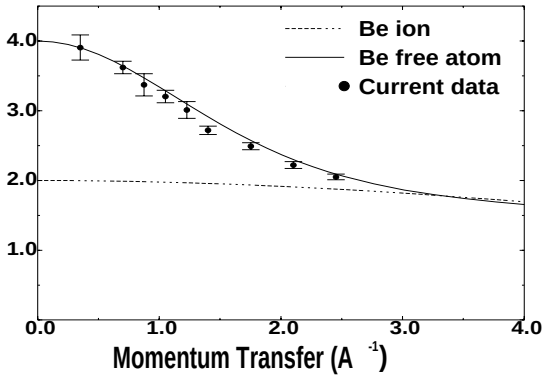

Figure 1:Atomic form factor of the Be free atom (solid line) and ion (broken line) taken from International tables for crystallography. Data from IXS measurements are shown as dots.

References

[1] A.J.C. Wilson, International Tables for Crystallography **C**, (1995)

[2] P.J. Brown, Phil. Mag. **26** 1377 (1972)

[3] A.G. Fox *et al*, Phil. Mag. B **57 No 2** 197 (1988)

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