MEASUREMENT of the VALENCE ELECTRON FORM FACTOR of SIMPLE METALS FROM PHONON INTENSITIES(*)

A. Alatas[1,2], H. Sinn[1], E. E. Alp[1], G. Bortel[1], and E. Burkel[3]

[1] *Advanced Photon Source, Argonne National Laboratory, Argonne, Illinois 60439*

[2] *Illinois Institute of Technology, Chicago, Illinois 60616*

[3] *University of Rostock, 18055 Rostock, Germany*

Since x-rays couple to crystal lattices directly through the charge density, experimentally they are the most suitable probe to understand the nature of the metallic bonding in solids. This electron charge density response can be split into two parts; namely a rigid part which moves together with the atoms (core electrons) and the deformation part which is not strongly bound to atoms as the rigid part (conduction electrons). Details of the density response function of the valence electrons and the Fourier transform of the electron-ion interaction potential can be extracted from the second part which constitutes a correction to the usual form factor, if accurate enough intensity measurements can be made. Hartree-Fock calculation of form factors for free atoms and ions can be found in the standard literature [1]. However, form factors for the valence electrons in metals are more difficult to obtain both in theory and experiment. Access to the small momentum transfer region is required, because significant difference attributed to valence electrons occurs in that region.

Previous experimental studies for form factor measurements 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 they do not reach down to required small momentum transfer region usually smaller than the $3A^{-1}$ even for the lowest possible reflection. Therefore, one can not get any information about valence contribition

In contrast to previous experimental methods, inelastic x-ray scattering (IXS) technique can be applied to this lower region of momentum space by measuring phonon intensities. We used IXS with a very high energy resolution of 2.2 meV to measure the phonon intensities in the $[00\zeta]$ direction in beryllium. A beryllium single crystal was chosen as a sample, because half of the electrons in Be are valence electrons. From the relative intensities of the phonons, the atomic form factor have been calculated for region between $0.3A^{-1}$ and $4.5A^{-1}$. They indicate significant difference from the free atom behaviour. From this, information on a pseudo-potential can be extracted. As a second example, we have used aluminium single crystal in the $[00\zeta]$ direction to measure form factor from phonon intensities, and prelimary results have been calculated.

[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)

(*) This work is supported by US DOE BES Materials Science W-31-109-ENG-38.