ESRF

Experiment title: Effect of thermal disorder on Compton profiles of Lithium	**Experiment number:** HE-394

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Report:

The results of this experiment have been published as:

C. Sternemann, G. Döring, C. Wittkop, W. Schülke, A. Shukla, T. Buslaps, P. Suortti, *Influence of lattice dynamics on electron momentum density of lithium*, J. Phys. Chem. Solids **61**, 379 (2000)

Abstract:

High resolution Compton profile measurements of single crystalline Li were performed for momentum transfer $\vec{q} \parallel [110]$ with 0.12 a.u. momentum space resolution at room temperature and at 95 K using the Compton spectrometer of ID 15 B at ESRF. The valence electron Compton profile at room temperature is higher around $p_z = 0$ a.u. and lower for $|p_z| > 0.4$ a.u. when compared with the one at 95 K. The experimental results are in good agreement with calculations using an empirical pseudopotential scheme, where the variation of lattice constant with temperature is taken into account when calculating the Fermi energy and Fourier coefficients of the empirical pseudopotential are multiplied by the corresponding Debye-Waller factor to simulate the thermal disorder. Thus the measured temperature effect can be traced back not only to the variation of the lattice constant with temperature but also to the decreasing contributions of higher momentum components to the total momentum density with increasing temperature.

C. Sternemann, T. Buslaps, A. Shukla, P. Suortti, G. Döring, and W. Schülke, *Temperature influence on the valence Compton profiles of aluminium and lithium*, Phys. Rev. B **63**, 094301 (2001)

Abstract:

We present temperature-dependent valence Compton profiles of single-crystalline Al and Li measured with 30 keV incident energy and 173° scattering angle with momentum space resolution of 0.1 a.u. The valence profiles for both samples measured at low temperature are above the high-temperature ones at momentum $p_z \approx p_F$, the Fermi momentum, and below at $p_z = 0$ a.u., which corresponds to a narrowing of the valence Compton profiles with increasing temperature. This fundamental temperature dependence can be attributed to the variation of the lattice constant and thus the variation of the Fermi momentum with temperature when the experimental results are compared with jellium calculations of the valence Compton profiles utilizing a correlation corrected occupation number density. In addition the Li experiment shows a significant temperature dependence even fur $p_z > p_F$, which is assigned to the diminished contribution of higher momentum components to the valence Compton profile with increasing temperature. The Li results are in good agreement with calculations using an empirical temperature-dependent local pseudopotential.