

*Effect of pressure on anisotropic momentum density of BeH<sub>2</sub> polymorphs*K B Joshi<sup>1</sup>, D K Trivedi<sup>2</sup>, K L Galav<sup>1</sup>, B K Sharma<sup>3</sup><sup>1</sup>Department Of Physics, ML Sukhadia University, Udaipur, India, <sup>2</sup>Department of Physics, Government Polytechnic College, Dungarpur, India, <sup>3</sup>Faculty of Science, Manipal University Jaipur, Jaipur, India  
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Electron momentum density (EMD) is an important ground state property of materials. The quantity is directly related to the ground state wave functions of solids in the momentum space. Experimentally it can be accessed by measuring 2 Dimensional Angular Correlation of Annihilation Radiation (2D-ACAR) spectra. The technique offers good resolution. However, electron-positron interaction, role of positrons in sensing defects in solids and Coulomb interaction of positron with nuclei pose limitations [1,2]. Alternatively, the inelastic scattering of X-rays at large momentum transfer i.e. Compton scattering does not suffer from these drawbacks. Within the validity of impulse approximation, the technique is applied to measure projection of EMD along direction of the scattering vector. The  $\gamma$ -ray Compton scattering experiments offer limited resolution. At synchrotron radiation sources, it is possible to achieve high resolution and very good statistics. The technique has been applied to unfold Fermi surface topology, nature of bonding and directional bonding behavior in a variety of solids [1]. Magnetic Compton scattering is applied to study field and temperature-dependent magnetic properties, distribution of magnetic moment, separation of orbital and spin part of the magnetic moment in novel rare earth materials [1]. Despite such a success, attempts to study pressure-dependent EMD or the Compton profiles are rare. In these experiments, pressure exerting assemblies such as diamond anvil cell are necessary. The pressure assembly poses serious problems in background measurements. Nevertheless, a few experiments are performed to see the effect of pressure on Compton profiles [2]. Thereafter, attempts to study effects of pressure on EMD, Compton profile, or the autocorrelation functions experimentally are very rare. However, first-principles study of effect of pressure on the isotropic Compton profiles, its first and second derivatives are investigated for several polymorphs of MgO [2]. It is observed that the valence electrons Compton profiles are sensitive to the applied pressure. The first and second derivatives before and after the transition pressure suggest reorganization of momentum density in the B1→B2 structural phase transition. To our knowledge, effect of pressure on the anisotropies has not been attempted either experimentally or theoretically to ascertain significant effect.

BeH<sub>2</sub> is an important metal hydride which exists in orthorhombic ( $\alpha$ ), tetragonal-anatase( $\beta$ ), tetragonal-rutile ( $\delta$ ) and cubic( $\epsilon$ ) structures. Under ambient conditions BeH<sub>2</sub> is found in the orthorhombic ( $\alpha$ ) phase. Pressure induced  $\alpha$ → $\beta$ ,  $\alpha$ → $\delta$ ,  $\alpha$ → $\epsilon$ ,  $\beta$ → $\delta$ ,  $\beta$ → $\epsilon$  and  $\delta$ → $\epsilon$  structural phase transitions are observed to take place at 8.75, 12.75, 18.34, 39.53, 55.57 and 76.60 GPa respectively [3]. Interestingly values of transition pressures are experimentally achievable. So it is worthwhile to study effect of pressure on anisotropies in the directional Compton profiles and the total Compton profiles of BeH<sub>2</sub> polymorphs. Results obtained by performing calculations of the Compton profiles at various values of pressure shall be presented. Changes in the anisotropies shall be examined. The current study invites experiments to perform anisotropy measurements varying pressure. We could then definitely see if Compton profiles carry signatures of the structural phase transitions.

[1]. Cooper M.J. et al. (2004) X-ray Compton Scattering. Oxford University Press, Oxford (UK).

[2]. Joshi K.B. et al. (2012) J Mater Sci, 47,7549-7557 and references therein

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