The Layered Structures of Bi-Te Compounds Under Pressure

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Keywords: bismuth tellurides, crystal structure, x-ray diffraction

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Binary bismuth-telluride compounds are part of an *infinitely adaptive series* of the form $(Bi_2)_m(Bi_2Te_3)_n$ with end members Bi_2Te_3 and elemental bismuth. These materials adopt layered crystal structures at ambient conditions, with different compositions formed by stacking of regular Bi_2 and Bi_2Te_3 blocks along the c-axis to achieve the desired stoichiometry. Several Bi-Te compounds exhibit interesting properties such as thermoelectricity, topological insulation and pressure-induced superconductivity. Despite this, comprehensive high-pressure structural studies have not yet been completed across a wide range of compositions.

The thermoelectric power factor of Bi_2Te_3 has been reported to be significantly enhanced by the application of several GPa of pressure, while exhibiting the same layered crystal structure as at ambient conditions. However, subsequent theoretical and experimental studies have reported conflicting results, such that the effect of pressure is not yet clear.

Within the stability range of the crystal structure observed at ambient and under pressures up to a few GPa, a structural anomaly has been reported to occur in Bi₂Te₃ and attributed to an 'electronic topological transition (ETT)'. Detailed studies of the crystal structures as a function of pressure would provide a valuable starting point for understanding the changes in physical properties and for electronic structure calculations.

Here we report the results of high-pressure synchrotron x-ray powder diffraction studies of several $(Bi_2)_m(Bi_2Te_3)_n$ compounds in diamond anvil cells. The pressure dependences of the structural parameters were obtained with Rietveld refinement analysis. They allows us to identify pressure-induced anomalies and yield information about the interplay between inter- and intralayer compression in these layered crystal structures.

Acknowledgments: KF acknowledges studentship funding from EPSRC under grant no. EP/L015110/1.