

### **Complex Structures in Barium at High Pressure**

Richard Nelmes, Malcolm McMahon, Clivia Hejny, Sara Falconi, Lars Lundegaard, Scott Belmonte, *School of Physics and Centre for Science at Extreme Conditions, University of Edinburgh, Mayfield Road, Edinburgh EH9 3JZ, UK.* E-mail: r.j.nelmes@ed.ac.uk

Barium has a bcc structure at ambient pressure, transforms to an hcp phase II at 5.5 GPa, and then to phase IV at 12 GPa which transforms to another hcp phase at 45 GPa. Phase IV is characterised by complex structures and a number of different forms. IVa, which exists from 12 to 12.5 GPa, was the first example discovered of a composite incommensurate host-guest structure in an element [1]. The structure comprises a ‘host’ framework, with 8 atoms in a tetragonal unit cell, and chains of ‘guest’ atoms that lie in channels formed by the host framework. These chains form tetragonal and monoclinic guest structures that are incommensurate with the host along the *c*-axis of the host. Similar composite structures have now been found in Sr, K, Rb, As, Sb and Bi. In barium above 12.5 GPa, there is a IVb form with the same host structure as IVa but with the guest chains forming an orthorhombic structure. There is evidence of further structural changes to a IVc form at ~16 GPa and a IVd form at ~18 GPa [1]. New structural studies have revealed these to have remarkably complex structures.

[1] Nelmes R.J., Allan D.R., McMahon M.I., Belmonte S.A., *Phys. Rev. Letters*, 1999, **83**, 4081.

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