Structural changes in elemental germanium at high pressure and high temperatures

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Materials under extreme conditions often exhibit interesting properties and can adopt novel structural configurations that differ greatly from those occurring at ambient. Often these transformations result in a great change in material properties leading to such effects as metals becoming insulators and vice versa.

Being semiconductor with a band-gap of 0.66 eV germanium has been the subject of numerous theoretical calculations [1] and high-pressure experimental studies, which have uncovered several high-pressure phases up to 170 GPa at 300 K [2-5]. These studies also have demonstrated that at room temperature phase transitions of germanium follow the same sequence with increasing pressure as those of silicon, another member of the group 14 [1]. Whilst the melting curve of Ge has been measured up to pressures of 40 GPa [6] and the phase I-II boundary is well understood above room temperature [7], currently there are no published experimental studies on the high temperature behaviour of germanium above 40 GPa.

In this study we explore the high temperature structural behaviour of germanium at pressures above 40 GPa though simultaneous x-ray powder diffraction, laser-heating experiments and theoretical calculations. We will discuss our evidence of a number of structural transitions in elemental germanium at high temperature, including a structural transition to a potential new high temperature phase of germanium which is not recoverable to room temperature.

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