Using High-pressure Diffraction to Design and Understand Functionality

The Preferential Orientation of Silicon Phases Formed During Non-Hydrostatic Compression

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Keywords: High Pressure, Non-Hydrostatic, Silicon

Semiconducting materials are vital for the electronics industry with one of the most important materials being Si. Typically Si has a diamond cubic (dc) structure, however Si possesses other phases that are accessible via the application of high pressure. It has been reported that when compressed to 10-11 GPa dc-Si transforms into the metallic β-Sn-Si phase [1] and then upon decompression one of several metastable phases forms: bc8-Si, r8-Si, and hd-Si depending on the temperature, decompression rate and whether shear is present [2, 3]. As most investigations utilise hydrostatic compression the effects of shear are poorly understood [1, 3, 4]. In this work, we investigated compressing randomly orientated dc-Si powder in a diamond anvil cell (DAC) up to 20 GPa (see figure 1(a)). A high shear environment was induced by loading the cell without a pressure medium, instead filling the DAC entirely with dc-Si powder. In-situ x-ray diffraction (XRD) was performed parallel and perpendicular to the compression axis in order to explore the crystallography of the phases formed. The microstructure of the recovered samples were also analysed using transmission electron microscopy (TEM) using site specific specimen preparation via focused ion beam milling. TEM of the sample recovered from 20 GPa compression (see figure 1(b)) reveals that the bc8-Si was preferentially orientated with its <110> direction perpendicular to the compression axes. This preferred orientation may be caused by the non-hydrostatic compression conditions which drive crystals to align in such way that minimizes strain energy [5]. Our finding that non-hydrostatic compression can be used to produce oriented bc8-Si may allow the synthesis of larger and higher quality bc8-Si crystals that have properties suitable for a range of applications including multiple exciton generation solar cells [6].

Figure 1. (a) Schematic of the method used in which dc-Si in a compressed in a DAC. (b) Cross sectional TEM image of a sample retrieved following compression to 20 GPa. Selected area diffraction pattern (top right) from the crystal indicated by red circle indexed to bc8-Si with its <110> direction perpendicular to the compression axes (as shown bottom right).