been suggested to solve this problem, including doping with other elements such as nitrogen.[7,8] In this study, we have shown that the optical conductivity decreases with increasing nitrogen content, in agreement with experiment. At the time of writing, no theoretical study had confirmed this effect.

A main driving force in the search for new materials is to reduce the wavelength of the laser used for reading, writing and erasing bits. By decreasing the wavelength, the size of the written bits decreases and thereby the storage density increases. Pure GST exhibits a high reflectivity contrast in the red and infrared spectral range. One way to decrease the wavelength of the writing laser is by altering the stoichiometry of GST.[8] In this study, we show that nitrogen-doped GST has a higher reflectivity contrast between hexagonal and cubic GST in the visible and ultraviolet spectral range (shorter wavelengths) as compared with pure GST. Moreover, the reflectivity contrast is found to increase with increasing nitrogen content within the range 0–25 at.%. At the time of writing, no theoretical study had investigated this aspect.

As already stated, the amorphous-to-cubic tran-

DFT, has been considered in this study. The cubic phase has a rocksalt-like structure, in which *Te* atoms occupy the anion (4a) sites whereas *Ge* atoms, *Sb* atoms and intrinsic vacancies randomly occupy the cation sites.[14,15] In this work, the cubic phase has been replaced by an equivalent hexagonal lattice for purposes of implementation. This has been achieved by taking the atomic arrangement along the [1 1 1] direction in the fcc lattice. The result is a unit cell having 27 atoms and 3 vacancies (v) in the sequence *Te*-*Ge*-*Te*-*Sb*-*Te*-v-*Te*-*Sb*-*Te*-*Ge* repeated three times along the *c*-axis. Figure 1 shows one-third of the resulting unit.

The atomic radius of *Ge*, *Sb* and *Te* atoms is approximately twice that of *N*.[16] Hence, *N* is quite small and cannot substitute *Ge*, *Sb* or *Te* under normal circumstances. As such, *N* can only occupy interstitial sites (Fig. 2). The relative concentration of nitrogen was set to 10 at.% and 25 at.%, in which relative concentration has been defined as the ratio of the number of dopant atoms to the total number of atoms in the unit cell.

As Ge, Sb and Te are heavy atoms, 10 at.% and 25 at.% *N*-doping levels were chosen to avoid larger supercells in an effort to reduce computational time.