High Pressure-High Temperature Synthesis and Elasticity of the Cubic Nitride Spinel $\gamma$-$\text{Si}_3\text{N}_4$

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Introduction: The compressional behavior of a new dense form of silicon nitride with the cubic spinel structure is studied by energy dispersive X-ray diffraction, following in situ synthesis from the low pressure form by laser heating in the diamond anvil cell. The unit cell dimension and the ambient temperature bulk modulus and its pressure derivative are determined to be $V_0 = 8.29(3)$ Å$^3$/atom, $K_0 = 308(5)$ GPa, for $K'_0 = 4$, in excellent agreement with theoretical calculations.

Dense nitride structures of Group III and Group IV elements (Al, Si, Ga) are well known technological materials, with high mechanical strength and hardness and useful semiconducting properties$^{1,2}$. Recently new forms of nitrides $\text{Si}_3\text{N}_4$ and $\text{Ge}_3\text{N}_4$ were found following high-pressure high-temperature synthesis.

Methods and Materials: In this study, we have obtained the cubic $\gamma$-spinel phase of $\text{Si}_3\text{N}_4$ by laser heating low pressure ($\alpha$- and $\beta$-) forms of silicon nitride in the DAC, and have studied the new phase and its decompression behavior by synchrotron (energy dispersive) X-ray diffraction. The results permit the determination of the zero-pressure bulk modulus and cell volume. Commercially obtained $\alpha$-$\text{Si}_3\text{N}_4$ (containing ~5-10% $\beta$-$\text{Si}_3\text{N}_4$) was loaded into a symmetric diamond cell for double-sided laser heating studies. Samples were loaded with ~1% amorphous boron powder to efficiently absorb the heating laser energy, and were pressurized to approximately 20 GPa. Laser heating was achieved with a Nd:YAG laser. Energy dispersive X-ray diffraction patterns were collected at the superconducting wiggler beam line station X17B1.

Results: The diffraction patterns collected at room pressure (after complete decompression) gave the value of $V_0 = 8.29(3)$ Å$^3$/atom. The calculated values of $V_0$ and $K_0$ obtained from DFT calculations compare well with the experimental values. The LDA underestimates the $V_0$ by 1.7 % but agrees with the bulk modulus within experimental error. The GGA overestimates $V_0$ by about 2.0% and underestimates $K_0$ by about 7.8 %.

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