# X-ray diffraction and Raman of GaP using a laser heated diamond anvil cell

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Understanding of the crystal structure systematic among III-V and II-VI semiconductors is of fundamental to semiconductor physics and has been well established using synchrotron x-ray diffraction at high pressures.[1] A recent phonon calculation suggests that the instability of the β-Sn structure, which was absent from the ionic compounds at high pressures stems from a soft phonon.[2] EXAFS data provided a value for the bulk modulus of GaP-I and the pressure-quenched sample was claimed as amorphous.[3] However, there was no EOS information for GaP-II, which is now firmly known as an orthorhombic metallic high pressure phase of GaP. The transition pressure of GaP-II also appears in conflict.

We measured x-ray diffraction of GaP at high pressures and high temperatures to better understand physics of III-V semiconductors, to determine first isothermal EOS of GaP-I and –II, and to examine further phase transitions.

The claim that GaP did not revert to the starting low-pressure phase after compression to 35 GPa may suggest intermediate phases. However, our Raman data shows that pressure quenched GaP appears to be highly strained GaP-I. X-ray diffraction also shows very broad peaks resembling GaP-I structure. At 23 GPa, we noticed a new peak starts showing and at 24 GPa, both I and II were identified in x-ray diffraction at ambient temperature. Finally at 34 GPa, GaP-II was the only phase recognized. When we laser heated GaP at 17 GPa to ~1800 K, we noticed a new phase mixed with GaP-I and the new phase was quenched to ambient temperature. When compressed to 22 GPa, the new high temperature phase disappeared. X-ray diffraction during laser heating at 22 GPa shows the same new phase with stronger intensity suggesting that the new phase is stable at high temperature. The new phase appears to be related to β-Sn structure.

[1] Nelmes, R.J. et al., PRL, 1997, 79, 3668

[2] Ozoliņš, V. and Zunger, A., 1999, PRL, 82, 767.

[3] Itie, J.P. et al., PRB, 1989, 40, 9709.

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