

## **Correlation between negative thermal expansion and polarity reduction in III-V semiconductor films**

Shaoqing WANG

*Shenyang National Laboratory for Materials Science, Institute of Metal Research, Chinese Academy of Sciences, 72 Wenhua Road, Shenyang 110016, China*

The knowledge of the thermal-expansion property is essential for the fabrications and applications of advanced semiconductor materials. The phosphides, arsenides and antimonides of boron and gallium are among the most important semiconductor materials in modern micro-electronic industry. Most of these compounds are man-made materials as thin films by epitaxial growth. The stable crystalline configurations of these phases are all in the cubic zincblende (ZB) structure. GaP and BP are excellent materials for the fabrication of light emitting devices and lasers. III-V antimonides have relative low-bandgap and are preferable for infrared and thermophotovoltaic applications. The borides III-V alloys provide the possibility to adjust the bandgap precisely for the aim of bandgap engineering.

In this study, the thermal-expansion behaviors of zincblende III-V nitrides, phosphides, arsenides, and borides are comparatively studied by the first-principles response-function calculation within the framework of the density-functional perturbation theory. Just in agreement with the experimental reports, low-temperature negative thermal expansions are observed in the III-V phosphides and arsenides phases but there are no any traces of NTE in III-V nitrides and borides. In investigating the reason for the difference, the roles of the pressure-induced redistributions of the static and dynamic charges in the lattice-dynamic process of these phases are analyzed carefully. Static charge moves closer to the bond center meanwhile dynamic effective charge decreases in these gallium compounds under pressure, but both of the static and dynamic charges behave in the inverse way for those boron phases. Thus, the polarity and ionicity will be enhanced in these borides meanwhile there is a polarity reduction in gallium phases as the crystal cell shrinks. Hence, there is an intimate correlation between NTE and polarity reduction in III-V compounds. This correlation between charge variation and thermal expansion is explained by means of the bond charge model.