

**High pressure EDXD and Raman studies on nanoscale 3C-SiC**

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Beamlines: X17C, X17B1

**Introduction:** The stability of nanocrystalline materials has drawn increasing attention in recent years since the high density of interfaces in nanostructured materials may provide a significant driving force for grain growth or phase transitions. Silicon carbide is one of the important model compound [1,2], thus the high pressure behavior of 3C-SiC powder with 30nm mean grain size is studied, especially compared the (quasi-)hydrostatic and nonhydrostatic compression to highlight the influence of the interfaces of nanoscale powder on the compressibility, and the dynamical charge change estimated from the pressure dependence of splitting between longitudinal optical (LO) and transverse optical (TO) phonon modes in its Raman spectra.

**Results:** Fig. 1 shows the relation between volume and pressure of (quasi-)hydrostatic and nonhydrostatic compressions for nanoscale SiC. The fit of Birch EoS for (quasi-)hydrostatic case (red line) demonstrates almost same as bulk SiC case (dash line,  $K_0=260\text{GPa}$ ), the corresponding bulk modulus  $K_0$  estimated as  $266\text{GPa}$  when  $K'=2.9$ . Hard to compress behavior is observed in non pressure medium case that is similar to the results of lattice strains research on gold and rhenium [3]. However, it is noted that nonhydrostatic compression could be treated as 2 stages process based on a simple model, in which the compressibility is mainly controlled by surface of grain (below  $10\text{GPa}$ ) and by the core of the grain (above  $10\text{GPa}$ ), respectively

Fig. 2 shows the pressure dependence of  $w_{\text{LO}}$  and  $w_{\text{TO}}$ , in which the experimental results [2] of bulk 3C-SiC (dot line) are illustrated as reference. In the zincblende structure SiC, the Born's transverse effective charge  $Z^*$  has a relation with the LO-TO splitting which results from the macroscopic electric field associated with the LO phonon displacement. Phonon frequencies of nanoscale crystal 3C-SiC and their pressure coefficients and corresponding mode Gruneisen parameters, as well as the dynamical charge  $Z^*$  and their pressure dependence were achieved, and negative pressure dependence of  $Z^*$  was observed, in contrast with positive value for its bulk counterpart. Thus the nanostructured 3C-SiC becomes more covalent upon compression in contrast to the behavior of bulk SiC which shows an increase of ionicity upon compression. However, Raman data for LO mode is available only within  $5\text{GPa}$  which is still in surface control zone, further investigation is necessary for reveal the strange dynamical charge transfer behavior for nanoscale 3C-SiC under pressure.

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Fig. 1

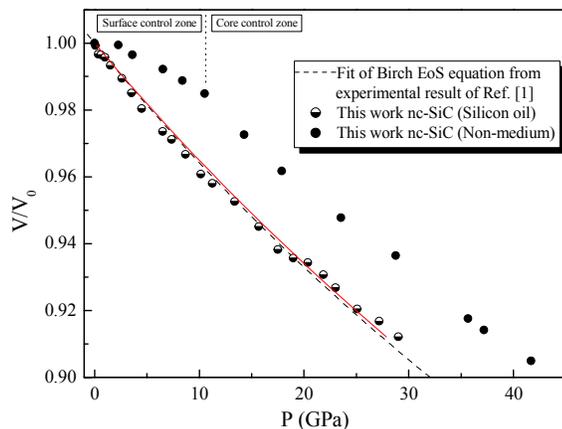


Fig. 2

