MS41-O5 Strain mapping in Ge microstructures using X-ray white beam Laue microdiffraction

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Strain-engineering of the band structure in germanium in currently intensively investigated to achieve a direct bandgap material suitable for a CMOS-compatible laser source. Theory predicts that the required tensile strain is relatively large (> 2% biaxial or > 4% uniaxial), yet such strain values have already been achieved using strain concentration in patterned suspended membranes.[1-2] A local probe of the full strain tensor would therefore be much needed to measure the actual strain distribution across the pattern.We have used X-ray Laue micro-diffraction (µLaue) at beamline BM32 at the European Synchrotron Radiation Facility to measure the strain tensor in different suspended Ge structures. We combined this technique with energy resolved measurements, such as rainbow-filtering[3-4] or direct energy determination using a silicon drift detector on a Bragg peak. The combination of the measurement of the deviatoric strain tensor with at least one measurement of a Bragg energy allowed us to measure the full strain tensor, *i.e.* including the hydrostatic part. Several conclusions were drawn from such measurements. First, the experimental results were confronted to numerical calculations of the full strain tensor obtained from the generalized Hooke's equation using the measured deviatoric strain tensor and the assumption of no normal stress on the free surfaces of the membranes. The excellent agreement evidenced the absence of changes in the values of the Ge elastic parameters up to 5% uniaxial strain. Experimental maps of all strain components were also consistent with Finite Element Method simulations. Furthermore, a comparison of the strain values measured by X-ray scattering with the spectral shift of the phonon modes measured using Raman spectroscopy showed a non-linear strain-shift relation for uniaxial strain larger than 3%. The non-linear dependence of the Raman shift on the strain was also observed in ab initio calculations. Finally, we show that experimental results in stretched Ge nanowires have allowed plotting the position of their direct bandgap as a function of strain and a remarkable agreement with the theoretical calculations was obtained.[5][1]M. Suess et al., Nature Photonics **7**, 466-472 (2013)[2]A . Gassenq et al., Appl. Phys. Letters **107**, 191904 (2015)[3]O. Robach et al., Acta Cryst. A **69**, 164-170 (2013)[4]S. Tardif et al., arXiv:1603.06370 (2016)[5]K. Guilloy et al., Nano Letters **15**, 4 (2015)

Keywords: X-ray Laue micro-diffraction, strain mapping, strained Ge

MS42 Advances in neutron scattering under non-ambient conditions

Chairs: Jiri Kulda, Stefan Klotz

MS42-O1 The role of oxygen packing in the structural transformations of oxide glasses

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Liquid and glassy oxide materials play a vital role in multiple scientific and technological disciplines. Here we investigate the structural transformations in silica, a building block of geophysically relevant silicates, as well as germania and B_2O_3. We show that an interplay between experiment and simulation leads to a new understanding of the pressure induced changes within these materials. A new structural map is devised for predicting the likely regimes of topological change. It is shown that this can be applied to a range of oxide materials. The information obtained can be used to forecast when changes may occur to the transport properties and compressibility of, e.g., fluids in planetary interiors, and is a prerequisite for the preparation of new materials following the principles of rational design.

Keywords: high pressure, glass, oxygen packing