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Femtosecond X-ray Diffraction

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Keywords: time-resolved X-ray diffraction, time-resolved structural studies, X-ray free-electron lasers

In this paper we provide a review of the revolution that has taken place over the past few years in our ability to produce and exploit ultra-bright, ultra-short pulses of X-radiation. For some time, nanosecond and picosecond optical lasers have been used to generate K-shell line radiation to interrogate rapid structural changes in matter. A good example of such work is the recent observation of the shock-induced alpha-epsilon transition in iron. [1] However, relatively small femtosecond lasers are now routinely used to produce bursts of X-rays with pulse-lengths of a few hundred femtoseconds. Such systems can be used to study rapid changes in materials -for example the atomic motion in both coherent acoustic and optical phonons have been directly followed.[2] Sub-bunch-length temporal resolution can also be achieved on third generation sources, either by use of streak-cameras to get to picosecond timescales, [3] or by laser-slicing to achieve 100-fsec resolution. [4] Within the next few years hard X-ray free-electron lasers (FELs) will come on line. These systems, with X-ray pulse-lengths of order 100-fsec, will have spectral brightnesses ten orders of magnitude greater than any extant synchrotron. [5] They will be fully spatially coherent, and temporal coherence can easily be achieved by spectral filtering. Such systems will have many unique applications, and considerable effort is already being devoted to designing experiments to enable diffraction from single bio-molecules.[6] An ability to obtain in a direct manner structural information from molecules that do not crystallize clearly has wide-ranging applications. The non-lasing precursor to such sources - the short pulse photon source at Stanford - has already produced remarkable results, with the shortest X-ray bursts yet produced being used to follow non-thermal melting in laser-irradiated semiconductors.[7] We also note that once the pulse lengths of the X-rays, and/or the time-scales of the phenomena of interest, start to become comparable with an extinction-depth traversal time, the diffraction process itself becomes time-dependent.[8]

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Incommensurate high-pressure and high-temperature structures in group VI elements

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Keywords: high-pressure crystallography, incommensurate modulated structures, chalcogens

The high-pressure behaviour of the group VI elements S, Se and Te have long been of considerable interest, because of their pressure-induced semi-conductor to metal transition, their dramatic changes in superconductivity temperature with pressure increase, or their unusual melting curves to name only a few exceptional properties. Recent high-pressure studies using diamond anvil cells and synchrotron radiation of these elements not only changed the generally accepted transition sequence with increasing pressure, but also discovered an incommensurately (IC) modulated structure for S-III, Se-IV, and Te-III [1]. Together with an IC modulated structure in group VII elements and incommensurate host/guest structures in group I, group II, groups V and even transition elements of the periodic table this shows the great occurrence of aperiodic structure elements at high pressure. [2-7]
The IC modulated structure of S, Se and Te has symmetry $I'2/m(0q0)s0$ and is stable from 75-153GPa in S-III, from 41-80GPa in Se-IV and from 4.5-29.2GPa in Te-III at room temperature. The wavevector q is dependent on both temperature and pressure (Fig. 1). On pressure decrease q increases from ca. 0.275 (depending on element and pressure) to ca. 0.31, where the IC structure transforms to a triclinic structure. In this triclinic structure one lattice parameter is three times as big as in the IC modulated structure, as if the wave vector q has locked in at 1/3.
In order to understand the driving force for the development of the incommensurability and structural modulation recent first-principles calculations indicate the IC modulated structures are due to a charge-density wave [8].

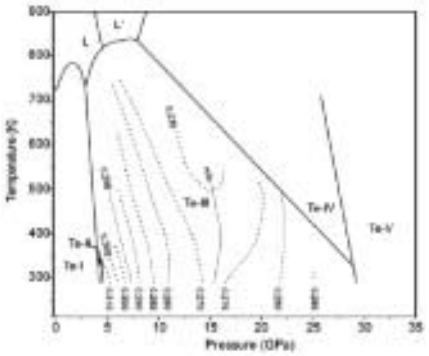

Fig. 1: Phase diagram of Te showing the P-T dependence of the wave vector q.

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