Unit cell angles $\alpha$, $\beta$, and $\gamma$, not fixed by symmetry, give an additional degree of freedom on the stage of crystal formation. For this reason, monoclinic crystals are the most numerous ones at ambient conditions. The oblique angles play the same role in thermal expansion; in particular they permit to demonstrate sharply anisotropic thermal expansion up to contraction along some directions. In 1982 great jump of the appearance of frequency of crystals, showing negative linear thermal expansion, was discovered between orthorhombic and monoclinic crystals [1]. It occurred that at least one third of monoclinic and triclinic crystals contracts along certain directions on heating due to so-called shear [1, 2]. This fact correlates with the existence of oblique cell angles in monoclinic and triclinic crystals only. Last quarter of a century was test and development period of the thermal contraction concept. Many types of the phenomenon were considered [2, 3 etc.]: shears, hinges, rocking polyhedra and symmetry related types etc. And now we can say that both among chemical compounds and in the earth’s crust, shears are the most fruitful case of linear thermal contraction of crystals. Taking into consideration anti-similarity of thermal and pressure deformations of crystals, the same situation should be expected in connection with linear elongation under pressure.


Keywords: negative thermal expansion, high-temperature x-ray diffraction, inorganic compounds

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**The structure of type I semiconducting clathrates under pressure**

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Semiconductor clathrates are compounds consisting of an open framework lattice of mainly, Si, Ge and Ga, containing a second large cation (alkali or alkali-earth) trapped in its cages. In this work, *in-situ* high pressure powder diffraction was performed on two Ge clathrates: $\text{AE}_{2}\text{Ga}_4\text{Ge}_{30}$, where $\text{AE} = \text{Sr, Ba}$. The pressure was applied to the samples by means of a diamond anvil cell (DAC) to 25GPa and powder diffraction data were collected with high energy (100 KeV) x-rays at the APS Sector 1 at Argonne National Lab. This technique allows data collection over a wide q range [0.2 Å⁻¹-50 Å⁻¹]. The structure of both samples was analyzed as a function of pressure, particularly with respect to the guest atom electron density and host lattice bonding. Both clathrates show amorphization of the host lattice for pressures in excess of 20 GPa, the structural characteristics of the structure factor functions S(Q) and radial distribution functions G(r) will be presented, elucidating both the local environment of the guest atoms and their short range ordering. This result suggests a promising route for obtaining periodic arrangement of guest atoms embedded in an amorphous semiconductor matrix. Oak Ridge National Laboratory is supported by the Division of Materials Sciences, U.S. D.O.E. (contract DE-AC05-00OR22725 with UT-Battelle, LLC).

Keywords: ab-initio calculations, iron compounds, molecular dynamics

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**Crystallography of intermetallic CaLi$_2$ at high pressure**

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Lithium and calcium are usually considered as simple metals because of the simple electronic structures with one and two conduction electrons, respectively. Recent studies have indicated that both lithium and calcium have anomalous properties at high pressure. Thus, the high-pressure properties of the Laves-phase CaLi$_2$, the only intermetallic compound between Li and Ca at ambient conditions, would be very interesting. Recently, Feng et al [1] have studied the electronic structure of CaLi$_2$ under pressure and found the bandwidths of the valence states decrease rapidly under compression just as in Li and Ca. Moreover, they predicted CaLi$_2$ could be a potential