

s11.m33.o4 **Novel Chain Structures in Group VI Elements.**
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Sulfur is a well studied element, having one of the most complicated phase diagram among elements, with 12 solid and 5 liquid phases up to pressures of 4 GPa [1]. A wealth of interesting phenomena has been observed *in situ* under pressure, such as metallization at 95 GPa [2] and observation of superconductivity up to 230 GPa with high temperature of superconducting transition [3]. However, the diffraction studies on sulfur reported in literature so far are of poor quality; hence there is little reliable information on the crystal structures of its high pressure phases [4,5]. The most recent *in situ* study on the low-pressure phase diagram of sulfur [6], provided the first high-quality diffraction data on high-pressure sulfur and reported breaking down of the ambient-pressure molecule rings and formation of a chain structure. However this study [6] was restricted up to 5 GPa, and the high-pressure behavior of the chain structure remains unknown.

Present study shows that the existing knowledge about the high-pressure structures of sulfur is in fact archaic: we present first high-quality diffraction data for high-pressure forms of sulfur stable between ambient pressure and approximately 80 GPa. Using new *in situ* diffraction techniques we show that the phase diagram of sulfur is very different from that previously proposed, with three stable phases between ambient pressure and 75 GPa and temperatures from 300 K and 1100 K. The structures of two high-pressure phases, S-II, previously observed in Ref. [6], and S-III, reported here for the first time, are solved in the present work.

Most significantly, we find that both phases have novel chain structures that have not been previously described for any element. The newly determined non-metallic chain structures of sulfur provide information that is critical for understanding its higher pressure behavior. Further, we show that the next member of chalcogen family, selenium, has a high-pressure phase that is identical to S-III. Thus, selenium is shown to have a chain structure in its non-metallic state, showing that this chain structure is not just a peculiarity of sulfur.

- [1] D.A. Young, *Phase Diagrams of the Elements*, Univ. of California Press, (Oxford, England 1991).
- [2] H. Luo, S. Desgreniers, Y. Vohra and A. Ruoff, *Phys. Rev. Lett.* **67**, 2998 (1991).
- [3] V.V. Struzhkin, R.J. Hemley, H.K. Mao and Yu.A. Timofeev, *Nature*, **390**, 382 (1997)
 E. Gregoryanz, V.V. Struzhkin, R.J. Hemley, M.I. Erements, H-K. Mao, and Y.A. Timofeev, *Phys. Rev. B* **65**, 64504 (2002).
- [4] Y. Akahama, M. Kobayashi, and H. Kawamura, *Phys. Rev. B* **48**, 6862 (1993).
- [5] H. Luo and A.L. Ruoff, *Phys. Rev. B* **48**, 569 (1993).
 H. Luo, R.G. Greene and A.L. Ruoff, *Phys. Rev. Lett.* **71**, 2943 (1993).
- [6] M. Mezouar, *Program of the School on Crystallography at High Pressure*, Erice, 2003.

s11.m33.o5 **Crystallography at extreme conditions: state of the art.** Natalia Dubrovinskaia and Leonid Dubrovinsky,
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High-pressure studies of geophysically important materials have historically been a vital part of the geosciences. In last few years as a result of extraordinary developments in high-pressure techniques, the field emerged as a distinct discipline. New methodologies, which include diffraction, spectroscopic, and imaging techniques, allow investigate relations between structures and phase transformation, chemical reactions, and thermophysical properties at conditions covering pressure and temperature ranges from ambient to Earth's inner core. "On-line" experimental facilities provide opportunity to investigate behavior of materials under extreme conditions and link scale of electrons and nuclei with global processes of crystals grows and performance in technological devices. We will discuss new prospects and challenges in the field.