# High-pressure behavior of the double perovskite $Sr_2CrReO_6$

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Double perovskites have the general formula $A_2BB'O_6$, where A is an alkali metal or a lanthanide, and B and B' are transition metals. A high magnetoresistance at room temperature has been discovered in these compounds. $Sr_2CrReO_6$ has a Curie temperature of 635 K [1]. First band-structure calculations, including predictions of the magnetic moments for $Sr_2CrReO_6$, were published by Vaitheeswaran *et al*. [2] and later experimentally confirmed by Majewski *et al*. [3].

The parent structure of $Sr_2CrReO_6$ is tetragonal with space group *I4/mmm*. The lattice parameters are $a_{0,\,tet}$=5.52 Å, and $c_0$=7.82 Å [1]. It is seen that the *c/a* ratio is close to √2, indicating that a larger face-centered cubic (fcc) unit cell can describe the lattice at ambient conditions. The fcc cell has the lattice parameter $a_0$=7.82 Å and twice the volume of the tetragonal cell.

Room temperature, high-pressure powder x-ray diffraction (XRD) spectra were recorded at Station F3 to determine the parameters of the equation of state of the material. Calculations were performed using density-functional theory (DFT) and the all-electron full potential linear muffin-tin orbital (FP-LMTO) method.

Cubic indexing has been assumed at low pressure, but a tetragonal distortion becomes evident above 9 GPa (Fig. 1). The inset graph in figure 1 shows that the width of the Bragg peaks increases steadily with increasing pressure.

Figure 2 shows the volume compression. There is no observable volume change at the transition from pseudo-cubic to tetragonal structure, although the scatter of the data points becomes larger at high pressure. The experimental bulk modulus is $B_0$=170±4 GPa, and the pressure derivative is $B_0'$=4.7±1.0.

DFT calculations of total energies are indicating that the cubic phase is stable at zero pressure, whereas the tetragonal phase is favored under pressure. The calculated lattice parameter of the fcc unit cell at ambient conditions is $a_0$=7.872 Å, which agrees within less than 1% with the experimental value. If instead a tetragonal unit cell is assumed, the calculated lattice parameters at ambient conditions are $a_{0,\,tet}$=5.5478 Å and $c_0$=7.8477 Å. Thus, the *c/a* ratio is practically equal to √2 at zero pressure.

The calculated equation of state is shown by the dashed curve in figure 2. The bulk modulus is 172.6 GPa and the pressure derivative 5.7. Thus, the calculated and experimental bulk moduli agree

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within 1.5%. This close agreement must be considered very satisfactory. To our best knowledge, there are no published data with which to compare the present results.

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## References

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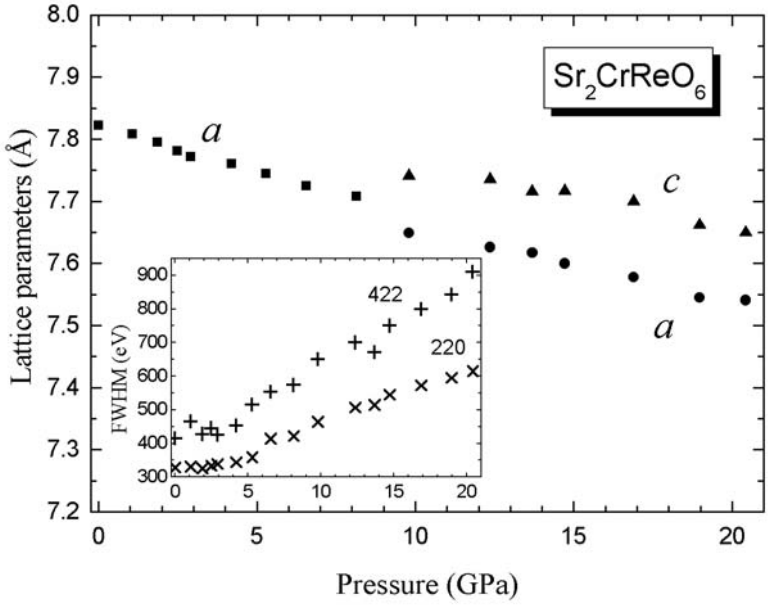


Figure 1.

The lattice parameter, *a*, of the pseudo-cubic unit cell, and the parameters *a* and *c* of the tetragonally distorted cell of $Sr_2CrReO_6$ as functions of pressure.

The inset shows the full width at half maximum (FWHM) of the 220 and 422 peaks as functions of pressure.

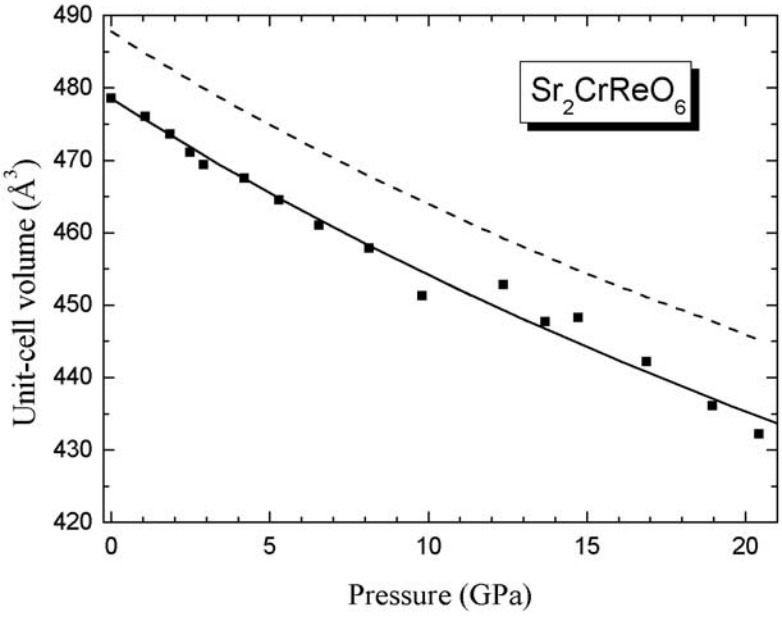


Figure 2.

Unit-cell volume of $Sr_2CrReO_6$ as a function of pressure. The full curve through the experimental data points has been calculated from the Birch-Murnaghan equation of state.

The dashed curve is the result of the DFT calculation.