Compositions, structures, and properties of chlorides system under high pressure

Jun KONG (Center for High Pressure Science and Technology Advanced Research, China),
Lei SU (Center for High Pressure Science and Technology Advanced Research, China)
Xiao DONG (Nankai University, China)

Abstract

With the rapid development of high‑pressure techniques and computational methods, research on chloride systems has expanded to unconventional stoichiometries, leading to new materials with novel electronic properties. This work employs high‑pressure techniques to investigate the composition, structure, and properties of several representative chloride systems. (I) The Grüneisen parameter (γ), a key thermodynamic quantity describing anharmonic effects, connects different equations of state (isotherms, isentropes, Hugoniots). In view of slow progress in high‑pressure γ measurements, we developed a technique using a dynamic diamond anvil cell (dDAC) combined with a fast signal acquisition system. Using this method, we determined γ of NaCl at room temperature over a broad pressure range (3.80–21.33 GPa) for the first time and successfully derived its Hugoniot curve. (II) Calcium–chlorine system under high pressure (0–100 GPa) was investigated by theoretical simulations and experiments. Calculations show that CaCl, Ca_5Cl_6 and Ca_3Cl_4 are stable under high pressure and contain monovalent calcium ions. Using a laser‑heated diamond anvil cell, we synthesized CaCl and obtained its high‑pressure isothermal compression curve. (III) We identified a stable chlorine‑rich compound, $CaCl_3$, which exhibits a Rubik's cube‑like Fermi surface and quasi‑flat bands in its band structure. Using a tight‑binding model, we show that the unique electronic properties originate from intrachain (nearest‑neighbor) interactions within one‑dimensional chlorine chains.

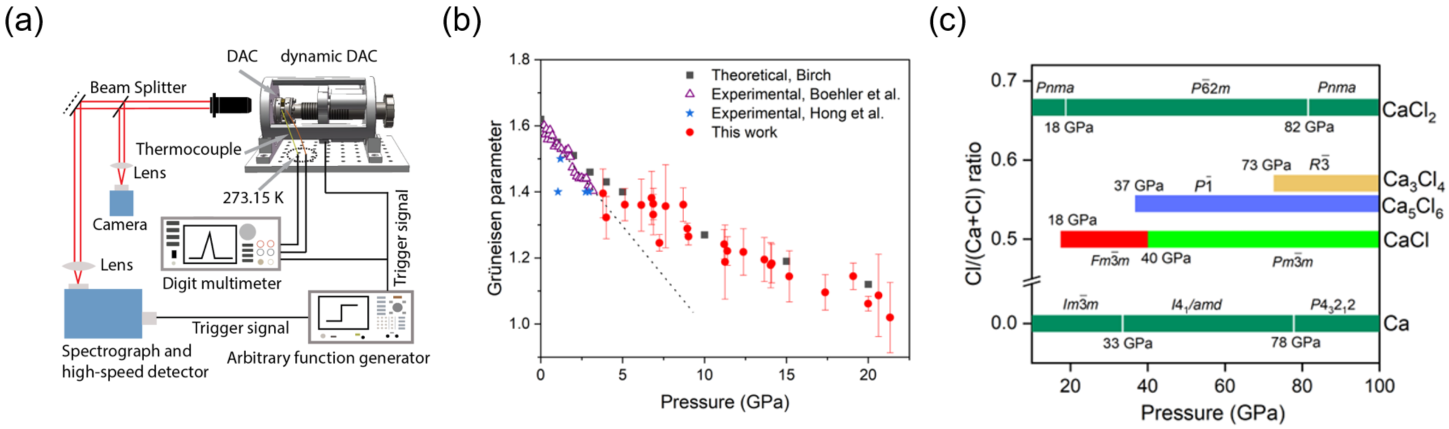

Figure1 (a) Schematic illustration of the programmable automatic high pressure jump and temperature detection apparatus. (b) Grüneisen parameter vs. pressure for sodium chloride from our data and previously published data. We measured the Grüneisen parameters in a wide pressure range. The dashed line is the extrapolation from the previous experimental data. (c) Phase diagram of calcium-chlorine system.

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