Design optimization through thermomechanical finite-element analysis of a hybrid piston-clamped anvil cell for nuclear magnetic resonance experiments

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ABSTRACT

The investigation of materials under extreme pressure conditions requires high-performance cells whose design invariably involves trade-offs between the maximum achievable pressure, the allowed sample volume, and the possibility of real-time pressure monitoring. With a newly conceived hybrid piston-clamped anvil cell, we offer a relatively simple and versatile system, suitable for nuclear magnetic resonance experiments up to 4.4 GPa. Finite-element models, taking into account mechanical and thermal conditions, were used to optimize and validate the design prior to the realization of the device. Cell body and gaskets were made of beryllium-copper alloy and the pistons and pusher were made of tungsten carbide, while the anvils consist of zirconium dioxide. The low-temperature pressure cell performance was tested by monitoring *in situ* the pressure-dependent ^{63}Cu nuclear-quadrupole-resonance signal of Cu_2O.

I. INTRODUCTION

Pressure is a versatile parameter to reversibly tune the structural and electronic properties of numerous types of materials, as well as to explore their phase diagrams.[1] From 1960s up to present, a large number of studies have shown that pressure can induce or significantly affect superconductivity and/or magnetic order of both simple and complex materials. For example, elemental cerium[2] or MnP[3] adopt a magnetically ordered ground state at ambient pressure but turn into superconductors at 5 and 8 GPa, respectively. More recently, theoretical calculations[4–6] suggested that, in magnetically frustrated and strongly spin-orbit coupled oxides, external pressure may induce a quantum-spin-liquid state, thus triggering a flurry of experimental studies of compounds such as α−$RuCl_3$,[7] the α- and β-phases of Li_2IrO_3,[8,9] and Na_2IrO_3.[10] Finally, pressure plays a significant role in the attempts to achieve room-temperature superconductivity. In particular, pressure-induced metallization and superconductivity were reported in hydrogen-based materials, such as H_3S[11] and LaH_{10},[12] the latter exhibiting a remarkable T_c of 215 K.[13] From the technical perspective, record pressures up to 1400 GPa were achieved to investigate the high-pressure properties of diamond.[14]

The design of efficient pressure cells is always a challenging task.[15] The most intuitive layout of a piston-clamped device, even using the most appropriate materials, such as