Benchmark melting behavior of rhodium under megabar pressures

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Abstract

Transition metals occupy a central role in condensed-matter physics and planetary sciences due to their distinctive electronic configurations, characterized by partially filled d-electron shells. The systematic trends governing the structural stability, cohesive energy, and extreme-conditions phase diagrams of transition metals are fundamentally driven by the degree of d-band filling [1], making their study essential for constraining the internal structures of terrestrial planets and exoplanets [2]. Rhodium (Rh), a chemically inert 4d transition metal within the platinum-group metals (PGMs), lies at the intersection of fundamental physics and technological relevance. Together with Ru, Pd, Os, and Ir, PGMs play key roles in catalytic processes, electronics, and extreme-environment applications [3]. Rhodium itself is widely used in high-temperature thermocouples [4], alloy hardening, and nuclear-related technologies [5,6], owing to its high melting point, low resistivity, and exceptional chemical stability. A precise understanding of its high-pressure behavior is essential for both applied performance and fundamental materials physics. Moreover transition-metal melting at extreme pressure remains one of the least constrained problems in condensed-matter physics, with theoretical predictions often differing by several thousand kelvin. Rhodium provides an ideal benchmark for testing finite-temperature electronic structure calculations. However, its high-pressure–high-temperature phase diagram has remained largely unexplored, with experimental melting data previously limited to pressures below 10 GPa [7].

Here we determine the high-pressure–high-temperature phase diagram and melting behavior of rhodium up to 100 GPa and 5000 K using *in situ* synchrotron X-ray diffraction in laser-heated diamond anvil cell, complemented by first-principles simulations. We show that rhodium retains its face-centered cubic structure throughout the investigated range and melts at temperatures systematically lower than predicted by most theoretical approaches. Analysis of the liquid diffraction patterns reveals that molten rhodium remains only 2–5% less dense than the corresponding solid at megabar pressures, indicating a substantial reduction of the solid–liquid volume change upon compression and placing new constraints on the thermodynamics of transition-metal melting. By combining static-compression, resistive-heating, and laser-heating measurements, we additionally establish a thermal equation of state spanning 0–100 GPa and 300–4500 K.

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